INTRODUCTION TO QUANTUM CHAOS

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Contents

Summary

The authors provide a pedagogical review of the subject of Quantum Chaos. The subject's origins date to the debut of the twentieth century when it was realized by Einstein that Bohr's Old Quantum Theory could not apply to chaotic systems. A century later, the issues arising in trying to understand the quantum mechanics of chaotic systems are actively under research. The main theoretical tools for exploring how chaos enters into quantum mechanics and other wave mechanics such as optics and acoustics, are semiclassical methods and random matrix theory. Both are briefly reviewed in their own chapters. The kicked rotor, an important simple paradigm of chaos, is used to illustrate some of the main issues in the field. The chapter proceeds with applications of quantum chaos research to understanding the results of three very different experimental systems.

1. Introduction

It is not trivial to compose a concise statement that defines the meaning of quantum chaos precisely. In fact, it may be more helpful to begin with a description. One branch of quantum chaos encompasses a statistical mechanics based on the nature of a system's dynamics, be it chaotic, diffusive, integrable, or some mixture. This means that one is not relying on the thermodynamic limit in which the number of particles tends to infinity. Another branch is an analysis of what the behaviors of linear wave equation solutions may be in a short wavelength or asymptotic limit. It applies equally well in the contexts of quantum mechanics, acoustics, optics, or other linear wave systems, and quantum chaos is sometimes referred to as wave chaos, which is really the more general moniker. As the subject has developed, these two branches have become intimately intertwined with each other and with parts of the theory of disordered systems. From investigations of quantum chaos, many unexpected and deep connections have emerged between quantum and classical mechanics, and wave and ray mechanics as well as newly identified asymptotic and statistical behaviors of wave systems. Hopefully, the meaning of these somewhat abstract statements will develop into a clearer mental image as you proceed through the general subject introduction provided here.

The study of quantum chaos has multiple, important motivations. First, it is absolutely essential if one wishes to understand deeply the interface between the quantum and classical mechanical worlds. Together they form the foundation for all of physics and there is still much left to uncover about their connections and the Correspondence Principle. In addition, quantum chaos has pushed the development of new theoretical techniques and methods of analysis that apply to a wide variety of systems from simple single particle systems to strongly interacting many-body systems to branches of mathematics. These developments are still underway and are still being applied to new domains.

A fascinating feature of quantum chaos is that it reveals a significant amount of *universality* in the behavior of extraordinarily different physical systems. For example, acoustic wave intensities found in problems with strong multiple scattering that lead to a probability density known as the Rayleigh distribution, Ericson fluctuations in the cross-sections of neutrons scattering from medium to heavy nuclei, and conductance fluctuations found in chaotic or disordered quantum dots can be seen to possess a common underlying statistical structure. One is thus able to see essential parallels between systems that would normally otherwise be left uncovered. Universality implies a lack of sensitivity to many aspects of a system in its statistical properties, i.e. an absence of certain kinds of information. Furthermore, quantum chaos brings together many disparate, seemingly unrelated concepts, i.e. classical chaos, semiclassical physics and asymptotic methods, random matrix ensembles, path integrals, quantum field theories, Anderson localization, and ties them together in unexpected ways. We cannot cover all of these topics here, and so make a selection of important foundations to cover instead. However, we will list a few references at the end to some of what has been left out for the interested reader.

It is not surprising then to see that quantum chaos has found application in many domains. A partial list includes: i) low energy proton and neutron resonances in medium and heavy nuclei; ii) ballistic quantum dots; iii) mesoscopic disordered electronic conductors; iv) the Dirac spectrum in non-Abelian gauge field backgrounds; v) atomic and molecular spectra; vi) Rydberg atoms and molecules; vii) microwave-driven atoms; viii) ultra-cold atoms and optical lattices; ix) optical resonators; x) acoustics in crystals and over long ranges of propagation in the ocean; xi) quantum computation and information studies; xii) the Riemann zeta function and generalized L-functions; and xiii) decoherence and fidelity studies. There are many other examples.

The structure of this contribution is the following. The next section covers critical background and historical developments. This is followed by the introduction of a historically important, simple dynamical system, the kicked rotor, which illustrates the notion of the quantum-classical correspondence, and provides in this way some intuition of why, and in what way, one should expect classically chaotic dynamics to influence the quantum mechanical properties of a system. Section 4 goes into the more formal aspects of the quantum-classical correspondence, and in particular gives a more concrete sense to different approximation schemes going under the name of *semiclassical approximations*. It covers a brief review of the Bohr (or more generally Einstein-Brillouin-Keller) quantization scheme, and discusses why this approach can be applied only to integrable systems. This is followed by a description of *semiclassical trace formulae*, applicable for a much wider range of dynamics, and in particular of the *Gutzwiller trace formula* valid in the chaotic regime. Section 5 introduces random matrix theory, which has proven extremely fruitful in the context of the quantum dynamics of classically chaotic systems, namely the statistical description of the spectrum and eigenfunctions. Finally, in Section 6 we select a few systems, or problems, for which the concepts of quantum chaos have proven useful. We will in particular show how the tools described in Sections 4 and 5 can be applied in different physical contexts by considering the examples of the Hydrogen atom in a strong magnetic field, the Coulomb Blockade in ballistic quantum dots, as well as some aspects of orbital magnetism.

2. Background Context and History

2.1. Chaos

At the end of the nineteenth century, the paradigm most physicists (as well as most everyone actually) were relying on to understand the physical world was derived from the motion of planets. Within this paradigm, physical objects could be described by their position and velocity, quantities which could be known arbitrarily well or at least as precisely as one was able to measure them. Their time evolution was governed by Newton's laws, which form a completely deterministic set of equations, and the subject is known as classical mechanics. However, exact solutions of these equations were derived only in certain simple cases, and it was usually assumed that sophisticated approximation schemes could provide arbitrarily accurate solutions – as long as one was willing to put enough effort into the calculations.

A limitation to this notion that, at least in principle, it is possible to have complete predictive power with respect to the dynamics of physical objects, arose with the realization that the solutions to Newton's equations could be exponentially unstable. Already, Poincaré, in his study of the "three-body problem" of celestial dynamics knew that under many circumstances, a qualitatively different and significantly more complex kind of dynamics was taking place now known as chaos. It is worth understanding how it differs from the dynamics of more readily solvable systems.

Let us begin by considering a stable, effectively one body, dynamical system, the Earth revolving around the Sun at position $\mathbf{r}$ and with a momentum $\mathbf{p}$ relative to the Sun. Assuming the Sun's mass is immensely greater than the Earth's, the Earth's motion is governed by the classical Hamiltonian (the total energy of the system - kinetic plus potential)

$$H_{\mathrm{cl}} = \frac{\mathbf{p}^2}{2M_\oplus} + V(\mathbf{r}), \tag{1}$$

associated with the gravitational potential energy

$$V(\mathbf{r}) = \frac{GM_\odot M_\oplus}{|\mathbf{r}|}, \tag{2}$$

where $\{M_\oplus, M_\odot\}$ are the Earth's and Sun's masses, respectively, and G is the gravitational constant. The derivative changes in position and momentum $\dot{\mathbf{r}}$ and $\dot{\mathbf{p}}$ are given by Hamilton's equations

$$\begin{aligned} \dot{\mathbf{r}} &= +\frac{\partial H_{\mathrm{cl}}}{\partial \mathbf{p}} = \frac{\mathbf{p}}{M_\odot} \\ \dot{\mathbf{p}} &= -\frac{\partial H_{\mathrm{cl}}}{\partial \mathbf{r}} = -\frac{\partial V}{\partial \mathbf{r}} \end{aligned} \tag{3}$$

which can be shown to be equivalent to the Newton equations of motion $M_\oplus \ddot{\mathbf{r}} = -\partial V / \partial \mathbf{r}$. Depending on the initial conditions, $(\mathbf{r}(0), \mathbf{p}(0))$, Eq. (3) is solved with Eqs. (1, 2) to give the known (Keplerian) elliptical orbits that are excellent approximations to Earth's true motion.

It turns out that both the kinetic energy term $\mathbf{p}^2 / 2M_\oplus$ and the gravitational potential $V(\mathbf{r})$ are invariant under a rotation of the physical space. This implies that one can construct two independent constants of the motion associated with angular momentum. Adding another to this list, Earth's total energy, which is conserved because the Hamiltonian, Eqs. (1, 2), has no explicit time dependence, there are three constants of the motion. Any system, such as this, which has as many constants of motion as degrees of freedom is said to be integrable. Integrability implies that the motion of the system is stable in the sense that a small change in the initial position or velocity implies a small change, with a linear time-dependence of the final position and velocity. In the same way, a small perturbation of an integrable Hamiltonian, as could be realized by accounting for Jupiter's gravitational pull on the Earth, would not drastically alter the trajectories or stabilities.

Before modern computers made it possible to perform extensive numerical simulations, the class of problems physicists or mathematicians could effectively solve were either integrable or sufficiently near integrability that a perturbative scheme could be applied. This class included both the "two-body problem", i.e. two bodies interacting via a central force such as the Earth example, and small perturbations around stable equilibrium points. The theory was very successful for this broad range of physical situations, and at times it was erroneously assumed that to broaden the range of treatable problems, one had merely to work harder doing longer calculations or calculate more terms in a perturbations series.

However, integrability and/or near-integrability is a rather exceptional property for a dynamical system to possess. Systems with three or more bodies interacting often behave radically different from integrable systems. The motion of Earth's Moon and Pluto are both chaotic as each are effectively part of a three body system (Sun, Earth, Moon or Sun, Neptune, Pluto). Even deceptively simple looking systems may display chaos. Consider Bunimovich's stadium billiard, mathematically proven completely chaotic, shown in Figure 1, and consider a point-like particle of mass m moving freely (that is in a straight line) inside the billiard and subject to specular reflection on the boundaries. Contrary to the Earth's orbit around the Sun, a particle's motion within this billiard is highly unstable. As illustrated in Figure 1, two trajectories initiated with slightly different initial conditions diverge exponentially quickly from each other, and after just a few bounces are not correlated anymore. In the same way, even the slightest perturbation would completely change a trajectory after a relatively small number of bounces. The motion within the stadium billiard is associated with the strongest form of chaotic dynamics. It is perfectly deterministic, so that exact knowledge of position and velocity at some initial time fixes the evolution to all times, and yet the evolution is so unstable that any uncertainty in the initial conditions quickly makes both position and velocity unpredictable.

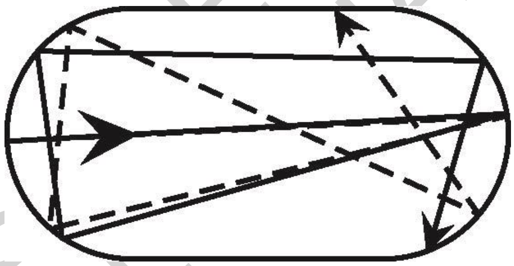

Figure 1. An example of a strongly chaotic system: the Bunimovich stadium billiard. The two trajectories indicated by the solid and dashed lines begin with a slightly different starting point. Their divergence is an illustration of exponential sensitivity to initial conditions.

After the pioneering work of Poincaré, little progress was made in the study of chaotic systems and, more generally, of systems far from integrability until the 1960's or 1970's. Then computer simulations made it possible to develop one's intuition about their behaviors and to motivate more formal work concerning their qualitative and statistical properties. Note that integrable and chaotic systems correspond to the two limiting cases of the most stable and most unstable dynamics. Typical low dimensional systems usually fall in the intermediate category of *mixed dynamics* in which integrable-like and chaotic-like motions coexist in different regions of phase space.

2.2. Quantum Mechanics

A second, quite fundamental limitation to the notion that one could have complete predictive power over physical objects, arose with the realization that microscopic systems, such as atoms and molecules require a description in terms of quantum mechanics. Classically and non-relativistically, the Hydrogen atom, other than the values of its constants and microscopic size, leads to equations identical to that of the Sun and Earth system; i.e.

$$H_{\mathrm{cl}} = \frac{\mathbf{p}^2}{2m_{\mathrm{e}}} + V(\mathbf{r}) \tag{4}$$

with

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0 |\mathbf{r}|} \tag{5}$$

where m_{e} is the mass of the electron, e the electric charge, and ϵ_0 the permittivity constant. The electron then in a classical world would follow elliptical orbits around the proton in a Hydrogen atom just like the Earth moves around the Sun.

Quantum mechanics implies however drastic conceptual changes. Rather than being entirely characterized by it's position and velocity, the electron is now described by a wave-function $\psi(\mathbf{r},t)$, whose modulus square $|\psi(\mathbf{r},t)|^2$ specifies the probability that the particle can be found at position $\mathbf{r}$ at time t. As a consequence position, as well as velocity, can be known only in a probabilistic way, not with an arbitrary precision, and not simultaneously. The time evolution of the wavefunction is then given by the [time-dependent] Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}_{\mathrm{qu}} \psi \, , \tag{6}$$

where the quantum version of the Hamiltonian

$$\hat{H}_{\mathrm{qu}} \stackrel{\mathrm{def}}{=} -\frac{\hbar^2}{2m_e} \Delta + V(\mathbf{r}) \tag{7}$$

is obtained from the classical counterpart H_{cl} Eq. (4) through the substitution $\mathbf{p} \to -i\hbar\nabla_{\mathbf{r}}$.

From the Schrödinger equation, Eq. (6), we see that in quantum mechanics a particular role will be played by the static solutions, called eigenenergies and eigenfunctions, of the quantum Hamiltonian $\hat{H}_{\mathrm{qu}}$, i.e. the set of real numbers ϵ_n and functions $\varphi_n(\mathbf{r})(n = 0,1,2,\ldots)$ fulfilling the eigenvalue equation (or stationary Schrödinger equation)

$$\hat{H}_{\mathrm{qu}}\varphi_n = \epsilon_n \varphi_n \,. \tag{8}$$

Indeed, from Eq. (6) the time evolution of the n'th eigenfunction is $\varphi_n(t) = \varphi_n(0)\exp[-i\epsilon_n t/\hbar]$. Therefore to within the phase $\exp[-i\epsilon_n t/\hbar]$, which is not a measurable quantity, φ_n is a stationary function. In a more rigorous theory of the Hydrogen atom, in which the interaction with the electromagnetic environment is included, the energies $\hbar\omega$ of the photons emitted or absorbed by the atom are generally given by the difference $(\epsilon_n - \epsilon_{n'})$ between two eigenenergies. This indicates that the Hydrogen atom has switched from the state φ_n to the state $\varphi_{n'}$. As the most natural way to probe the properties of an atom or a molecule is to look at the color of the light they emit or absorb, i.e. at the energy of the corresponding photons, the spectrum of an atom or molecule (that is the set of all energies of the corresponding quantum Hamiltonian) is the most immediate quantity to access. In addition, many important properties of quantum systems, and in particular thermodynamic quantities, are entirely determined by their energy spectra. More focus ahead is on the description of the quantum energy spectra, keeping in mind however that this does not exhaust the richness of the quantum world.

2.3. Correspondence Principle & Quantum Chaos

In the early twentieth century quantum mechanics began with a primitive form known as the "Old Quantum Theory." It was the statement that among all possible trajectories, only one with the classical action $J \stackrel{\mathrm{def}}{=} \oint \mathbf{p}d\mathbf{r}$ being a multiple of Planck's constant $2\pi\hbar$ could actually correspond to a stationary state of the quantum particle. The action, and thus the energy of the electron had to be "quantized".

In the modern form of quantum mechanics the link between the quantum and the classical world is less immediate, but still exists through what is referred to as the Correspondence Principle. For instance, the quantum Hamiltonian Eq. (7) describing the Hydrogen atom could be associated with a classical counterpart, here given by Eqs. (1)-(5). This remains true on a very general basis. Quantum Hamiltonians can be associated with a classical analog, which, in some sense corresponds to its classical limit as $\hbar \to 0$ (or more correctly when all action variables are large compared with $\hbar$).

Even before the emergence of the full quantum theory, it was recognized that the primitive form can only apply to integrable systems. With the modern form of quantum mechanics, the Correspondence Principle is effective irrespectively of the nature of the dynamics. A question that naturally arises then is whether this concept of chaos, which has been developed in the context of classical physics, is relevant when studying a quantum system.

This interrogation could actually be approached in two rather different ways. The first one would be to decide whether, for instance, by making a choice different than Eq. (5) of the potential $V(\mathbf{r})$, there exists a class of quantum Hamiltonians such that the Schrödinger equation (6) is chaotic. One possible sense of the term "chaos" here could be that two slightly different initial wave functions $\varphi_1(\mathbf{r}, t=0)$ and $\varphi_2(\mathbf{r}, t=0)$ diverge "exponentially" rapidly from one another with time. It turns out however that one can answer this question under relatively general conditions, and the answer is negative. Indeed, the simple fact that the Schrödinger equation is linear (i.e. that a linear combination of two solutions of Eq. (6) is also a solution of this equation) makes it impossible that chaos, in any sense similar to classical mechanics, develops in quantum mechanics.

Another more interesting and productive approach to the role of chaos in quantum mechanics is associated with exploring the interrelations mentioned above between a quantum system and its classical analog through the Correspondence Principle. Indeed, within this framework it becomes meaningful to ask whether the quantum mechanics of some system is qualitatively different if its classical analog displays a completely chaotic and irregular behavior. The answer to this question is positive, and one purpose of *quantum chaos* is to determine in what ways. We shall illustrate this statement in the next section using the particular example of the kicked rotor, and come back after that to a discussion of the role of chaos in quantum mechanics with a broader perspective.

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Biographical Sketches

Denis Ullmo earned a Ph.D. in theoretical physics from the university of Paris-Sud in 1992 under the direction of Oriol Bohigas. He then worked within the Theoretical Division of the Nuclear Physics Institute of Orsay until he was appointed resident visitor at the Bell Laboratories (Murray Hill, NJ) from December 1994 to May 1997. After this, he joined the LPTMS (Laboratoire de Physique Théorique et Modèles Statistiques, Paris-Sud university) where he now holds a Directeur de Recherche position at the French CNRS (Centre National de Recherche Scientifique). During that period, he spent three years (from 2002 to 2005) as a visiting professor at Duke University (North Carolina) in the group of Harold Baranger.
Denis Ullmo's scientific interests include quantum chaos and its applications to mesoscopic physics. He has worked in particular on quantum tunneling in the presence of chaos, as well as on the thermodynamic and transport properties of quantum dots.

Steve Tomsovic earned a Ph.D. in theoretical and statistical nuclear physics from the University of Rochester in 1987 with J. B. French. Afterward he received a Joliot-Curie Fellowship and IN2P3 stipend to work with Oriol Bohigas in Orsay, France for two years. He then spent six years working with Eric Heller at the University of Washington, one year of which was spent visiting the Harvard-Smitsonian Center for Astrophysics as a Fellow. Now a professor at Washington State University, he was department chair of Physics and Astronomy for eight years. He has been an invited visiting professor at the *Laboratory for Theoretical Physics and Statistical Models* in Orsay, France, and at the *Indian Institute for Technology Madras* in Chennai, India, and was also recently awarded a *Senior Research Fulbright Fellowship* for work in Germany, and held the *Martin Gutzwiller Fellowship* of the *Max Planck Institute for the Physics of Complex Systems* in Dresden, Germany. He has organized a number of international programs and conferences.
Steven Tomsovic research specialties include the wave mechanics of chaos and disorder, semiclassical methods, random matrix theory, statistical nuclear physics, mesoscopic systems, and long range ocean acoustics.