An Introduction to Quantum Chaos

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Abstract

Nonlinear dynamics ("chaos theory") and quantum mechanics are two of the scientific triumphs of the 20th century. The former lies at the heart of the modern interdisciplinary approach to science, whereas the latter has revolutionized physics. Both chaos theory and quantum mechanics have achieved a fairly large level of glamour in the eyes of the general public. The study of quantum chaos encompasses the application of dynamical systems theory in the quantum regime. In the present article, we give a brief review of the origin and fundamentals of both quantum mechanics and nonlinear dynamics. We recount the birth of dynamical systems theory and contrast chaotic motion with integrable motion. We similarly recall the transition from classical to quantum mechanics and discuss the origin of the latter. We then consider the interplay between nonlinear dynamics and quantum mechanics via a classification and explanation of the three types of quantum chaos. We include several recent results in this discussion.

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1 Introduction

"In the beginning, there was Chaos." These words, though somewhat pretentious, serve as a microcosm for the excitement that has been engendered by nonlinear dynamics, which is often called *chaos theory* among general audiences. Nonlinear dynamics is at the heart of the modern interdisciplinary approach to science. Many people, however, appreciate this subject only in a very limited sense. Chaos theory was annointed a glamorous field of study when James Gleick's introduction to it appeared in print in 1987. 16 References to chaos are prevalent in popular culture. It has been mentioned, for example, in Jurassic Park, the movie Pi, and an episode of The Simpsons. In such references, it is often grossly misapplied, demonstrating that although chaos is glamorized in popular culture, it is not really understood by the general public. People outside the scientific community are far more aware of fractals and the pretty pictures that can be created with them than with the analysis behind them and the fact that such behavior serves as a good model for systems in several scientific fields, including physics, chemistry, biology, economics, and geology.⁴⁷

Quantum mechanics has achieved a similar lofty status in the public eye. There have been references to it in countless movies, magazines, and television shows. It has even encroached upon the English language. Like dynamical systems theory, however, it is grossly misunderstood by public audiences. The term quantum leap, for example, refers to a very large change, even though the quantum regime encompasses quantities that are so tiny that one cannot properly analyze the behavior they describe as part of a continuum. Indeed, the quantal regime is one of small jumps rather than large ones.

One of the goals of studying quantum chaos is to combine the paradigms encompassed by nonlinear dynamics and quantum mechanics into one coherent theory describing regimes in which both theories are relevant. Unlike the two separate concepts, this notion is not well-developed. Additionally, quantum chaos is virtually unknown to the general public, despite the fact that this subject seeks to reconcile two objects of the world's fascination. In scientific circles, the notion of quantum chaos is well-known, but its facets are not understood as well as its two underlying theories. The purpose of the present paper is to remedy this situation by providing an introduction to quantum chaos as well as a brief survey of some of the prevalent ideas in this area of research. Toward this end, we introduce some of the fundamental concepts of quantum mechanics and nonlinear dynamics before attempting to marry these two fields. We contrast chaotic behavior with integrable motion and discuss how dynamical systems theory arose from the study of celestial mechanics. Similarly, we contrast classical and quantum mechanics and then recount the origin of the latter. Finally, we present an introduction to quantum chaos that includes a classification of its types, a survey of recent

results, and an attempt to explain what quantum chaotic behavior actually represents.

2 Order and Chaos

One of the hallmarks of nonlinear dynamics is the concept of equilibria, which helps characterize a system's behavior–especially its long-term motion. There are numerous types of equilibrium behavior that can occur in continuous dynamical systems, but such long-time behavior is restricted by the number of degrees-of-freedom (that is, by the dimensionality) of the system. In other words, one ignores the transient behavior of a dynamical system and only considers the limiting behavior as $t \longrightarrow \pm \infty$. In dissipative systems, one considers the basins of attraction and repulsion of a given dynamical system. The extent of the possible complexity of a dynamical system's attracting and repelling sets is determined by the dimension of the system. Hamiltonian systems (which are conservative) do not possess global attractors or repellors, but their dynamics also becomes more complex as their dimensionality increases.

A one-dimensional system may be described by a single (unforced) ordinary differential equation (ODE) of first order. Its phase space is a line. All solutions must either approach a steady state or blow up, because the topology of the phase line implies that all equilibrium points separate it into two distinct regions. Moreover, any observed blow-up must be monotonic; there cannot be any spiraling or other complex behavior.

Systems consisting of either an autonomous pair of first order ODEs or a single (unforced) second order ODE have two dimensions. (A forcing term corresponds to a non-autonomity, which increases the dimensionality of the system when it is suspended into autonomous form.⁵¹) Such systems are aptly described by a phase plane. Closed trajectories separate the plane into two parts, and if the qualitative behavior is different in those two regions of phase space, then the trajectories in question are known as *separatrices* (see Figure 1). Such separatrices are common in Hamiltonian systems, coming in the guise of *homclinic* and *heteroclinic* orbits. Limiting behavior may include steady states, limit cycles, and blow up (which need not be monotonic). Systems that are not Hamiltonian may thus exhibit various flavors of attractors and repellors.

The phase space of systems with $n \in [3, \infty)$ dimensions is embedded in \mathbb{R}^n . In addition to the behavior that can show up in systems described in spaces of one or two dimensions, those with at least a third dimension may exhibit quasiperiodicity, chaotic ("strange") attractors and repellers in addition to other manifestations of chaos such as ergodicity. (Once again, attractors and repellors cannot occur in Hamiltonian systems, so one must distinguish chaotic behavior in those systems from that in dissipative and absorptive ones. Such structures may prove to be relevant to the study of dissipative quantum chaos.^{9,21}) In many contexts, the concept of dimension is related to the number of degrees-of-freedom (dof) of a system. The number of dof of a system is defined as the number of variables required to uniquely specify its orientation and position in physical space.²⁵ This corresponds to the number of directions the system may move in configuration space. For example, an unconstrained particle in open space may move in three different directions. A (holonomic) system with k degrees-of-freedom has a

2k-dimensional phase space. We will not treat non-holonomic systems^{17,32} in the present work. Such systems have velocity spaces of lower dimensionality than their configuration spaces so that a k dof nonholonomic system has a phase space of dimension n < 2k. Hamiltonian systems are holonomic and conservative. They may behave chaotically as well (as long as they possess at least two degrees-of-freedom), although their brand of chaos is somewhat different from that in other types of systems.

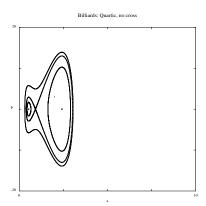


Figure 1: A separatrix that occurs in an integrable configuration of a vibrating quantum billiard in a double-well potential. Trajectories inside the separatrix behave qualitatively differently from those outside the separatrix.

Let us now compare periodic, quasiperiodic, and chaotic behavior. To contrast the former two, consider the arcade game *Asteroids*. When the ship that the player controls flies off the screen on one side, it appears at the corresponding point on the other side, and the same is true of the top of the screen with respect to the bottom. In other words, the game's playing field is

a 2-torus, which is properly embedded in 3-dimensional space (which is why quasi-periodic behavior is possible). More precisely, consider the following vector field on the torus:

$$\dot{x} = 1,$$
 $\dot{y} = \omega.$ (1)

If ω is rational, the line in phase space eventually reaches its initial point so that it is periodic, whereas if ω is irrational, the line is quasiperiodic, approaching every point on the torus arbitrarily closely. Another contrast between periodic and quasiperiodic motion occurs with planetary motion. According to Kepler's First Law, each planet's orbit is an ellipse with the Sun at one of its foci. A better model, however, is one in which planetary motion is described by precessional ellipses. The latter motion is a quasiperiodic analog of the elliptical motion that describes the celestial body at any given instant. The quasiperiodicity comes from the fact that the properties (eccentricity, angle of inclination, etc.) of the ellipse that describe the instantaneous motion change gradually over time. Interaction with the other planets, in fact, leads to this evolution of the orbital parameters. (Directly considering such time evolution is a way to incorporate perturbations due to the other planets in the solar system as a small perturbation of the two-body problem.)

In addition to the theoretical distinction between periodicity and quasiperiodicity, there is an issue as to whether one can actually observe this difference. (Equivalently, can nature tell if a number is rational or irrational in this context?) Every irrational number can be approximated arbitrarily closely as a rational one,³¹ a fact that is very important for numerical simulations. If

one considers a single time series in Fourier space, one cannot in principle tell the difference between periodic and quasiperiodic motion, because computers approximate every irrational number as a rational one. (Thus, the computer indicates that the result is periodic—though the period might be very long.) However, one can distinguish periodicity from quasiperiodicity based on the variation of a parameter if one computes multiple time-series plots. For periodic motion, one observes that the ratio of given frequencies and higher harmonics remains constant, whereas this ratio varies across different time series in the quasiperiodic case. On a computer, there is really no such thing as quasiperiodicity simply because every number is rational. From a practical standpoint, however, one can tell the difference between perioic and quasiperiodic behavior as long as the reduced form of the rational number contains reasonably small integers (that is, as long as the period is not too long). One must nevertheless be careful when doing dynamical computer simulations, as it may not always be easy to distinguish a quasiperiodic orbit and a periodic orbit with a very long period.

We are now ready to contrast quasiperiodic and chaotic motion. For motion to be chaotic, it must satisfy three properties: boundedness, infinite recurrence, and sensitive dependence on initial conditions. The first property simply means that one can find a ball of sufficiently large radius that contains the chaotic attractor. The second one implies that if one considers an arbitrarily small neighborhood about the initial point of a trajectory, it will return to the neighborhood infinitely many times. The last property means that two trajectories that emanate arbitrarily closely diverge from each other at an exponential rate. (That is, the trajectories are character-

ized by a positive Lyapunov exponent.) Quasiperiodic motion satisfies the first two properties but does not satisfy the third. Two nearby quasiperiodic trajectories remain "close" to each other in the sense that they only diverge linearly.

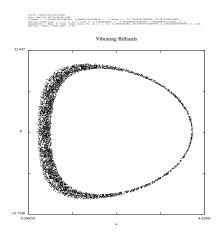


Figure 2: An example of hard Hamiltonian chaos.

One can also distinguish several different types of chaos. There is Hamiltonian chaos as well as chaotic behavior in dissipative and absorptive systems. Both classes of systems exhibit numerous flavors of chaos. In the former, one can observe stochasticity (Figure 2), in which a Poincaré map displays a bounded set within which there is complete disorder. One can also observe so-called "soft chaos" or "local chaos" (Figure 3), in which there is some fuzziness near otherwise well-defined curves. If the curves are completely well-defined in a Poincaré map—that is, they lack fuzziness—they describe quasiperiodic behavior, and if one has a collection of dots rather than a curve, then the depicted motion is periodic. One can also observe chaotic

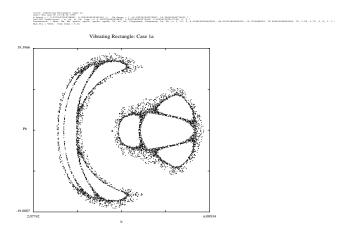


Figure 3: An example of soft Hamiltonian chaos.

behavior that falls between these two cases. This quasiperiodic route to chaos is described by KAM theory. ^{18,51}

Finally, one can extend dynamical systems theory to partial differential equations (PDEs). A PDE, which may be treated as an infinite set of coupled ODEs, has infinitely many degrees-of-freedom.⁴⁹ Such systems may exhibit chaotic behavior in both spatial and temporal variables. (The chaotic behavior discussed above is temporal chaos.) Possible manifestations of such spatio-temporal chaos include a spiral wave route to chaos anologous to the period doubling route to temporal chaos described by the Feigenbaum sequence.¹⁰ Research concerning such spatio-temporal complexity is quite active.

3 The Origin of Dynamical Systems Theory

The historical evolution of dynamical systems began with the advent of

celestial mechanics.^{11,37} The orbits of the planets were described as the "Music of the Spheres," and the solar system was treated as something both magical and mystical. Considered strong evidence of Divine creation, many scientists set out to explain this extraordinary natural symmetry. Nicholas Copernicus (1574–1642), an early celestial mechanician, waited until he was on his deathbed to publish his heliocentric theory because he knew that it would be considered blasphemy. Other pioneers in celestial mechanics, such as Galileo Galilei (1564–1642) and Johannes Kepler (1571–1630), also had to be careful with that they published on the subject. (Kepler studied celestial bodies in part to explain their divine symmetries, whereas Galileo's work was treated quite harshly by the Church.) Sir Isaac Newton (1642–1727) used Kepler's three laws of planetary motion and three laws of his own to derive the inverse square law of gravitational attraction. Essentially, Newton solved the (unperturbed) 2-body problem.

A natural progression of these results was the attempt to derive a solution to the *n*-body problem. According to the intellectual climate prior to the 20th century, the universe was a giant orrery that could be completely solved. Nobody had yet succeeded in solving the *n*-body problem, but surely somebody would if given the proper motivation. Scientists such as Pierre Simon de Laplace (1749–1827), Joseph Louis Lagrange (1736–1813), Siméon Denis Poisson (1781–1840), and Spiru Haretu (1851–1912) attempted to analyze the stability of the solar system by examining the *n*-body problem, but their results were inconclusive. Moreover, Haretu showed that the methods they were using were doomed to indeterminacy. The problem was of such a magnitude that the development of new methods was essential to its

resolution.

In Volume 7 (1885–86) of Acta Mathematica was an announcement that King Oscar II of Sweden and Norway would award a substantial prize and medal to the first person to obtain a global general solution to the n-body problem. Jules Henri Poincaré (1854–1912) had developed new techniques for studying differential equations, and he felt that these would provide a good intuitive basis for his attempt at this solution. After more than two years of study, the nature of the situation began to take shape. One of the problem's secrets was revealed by the special case n = 3. Poincaré proved that there did not exist uniform first integrals other than the one that had already been found. This showed that the 3-body problem could not be solved quantitatively by Hamiltonian dynamics (by using first integrals to reduce the problem to a solvable one of lower dimension), as even the restricted three body problem needed two degrees-of-freedom to describe it fully. The n-body problem was thus considerably more difficult than anyone had realized. Mathematicians would have to change the way they treated systems of this sort. They could no longer rely on quantitative methods to study the universe, a fact that countered the prevailing philosophy. The presence of chaotic behavior showed that determinism did not imply accurate prediction, because even a small perturbation of the initial data of a problem could cause an arbitrarily large alteration in the behavior of its solution.

From Poincaré's discovery arose dynamical systems theory. In addition to showing that the *n*-body problem could not be solved analytically, Poincaré discovered the first manifestation of chaotic behavior in the form of homoclinic tangles. Poincaré's work served as the foundation for that of several

mathematicians and scientists—including such luminaries as George Birkhoff, Stephen Smale, Andrei Kolmogorov, Vladimir Arnold, and Jürgen Moser and the theory and methods he originated now hold prominent places in mathematics, science, and popular culture.

4 Classical and Quantum Physics

When introducing quantum mechanics to his students, Richard Feynman called it "the description of the behavior of matter in all its details and, in particular, of the happenings on an atomic scale." Dijects on this scale behave like neither particles nor waves. The quantum behavior of all atomic objects is the same; there are respects in which they behave like particles and other respects in which they behave like waves. The reconciliation of this particle-wave duality of matter is at the heart of the transition from classical to quantum mechanics.

In quantum mechanics, quantities such as position, momentum, and energy play roles as operators as well as variables (depending on the representation in use). In classical mechanics, only the latter role is played. Concomitant with this additional interpretation is the issue of compatibility of observable quantities. Incompatible observables do not commute, and so there is an 'uncertainty relation' between them.⁴² In such relations, the more precisely one knows one quantity, the less precisely one can determine the other. The canonical Heisenberg Uncertainty Principle expresses this phenomenon between position and momentum, a pair of complementary quantities. From a mathematical point of view, this example of quantum-mechanical uncertainty is a consequence of the Fourier Integral Theorem.⁷ (One must be

careful in more general situations, as this result depends on the fact that position and momentum are Fourier transforms of each other.)

Another contrast between classical and quantum physics is that the former has a continuous energy spectrum, whereas that of the latter is discrete. This is perhaps best illustrated by comparing a classical oscillator with a quantum-mechanical one. In both cases, one can find 'normal modes' ('eigenfunctions', 'wavefunctions') $\psi_n(r,t)$ and their associated eigenvalues ('eigenenergies'). One then considers an arbitrary superposition of these normal modes:

$$\psi(r,t) = \sum_{n=0}^{\infty} c_n \psi_n(r,t). \tag{2}$$

Equation (2) is traditionally interpreted differently in classical and quantum mechanics. In the former, $\psi(r,t)$ is a linear combination of all the normal modes of an oscillator. One can observe this superposition, for example, when conducting experiments with a string or a Slinky. One such experiment is to demonstrate that 'travelling waves' are a solution of the canonical wave equation by showing that they are one example of a superposition of normal modes. In quantum mechanics, one can only observe a single wavefunction at one time. Instead of being an expression for the degree of expression of a given normal mode, the coefficients c_n in the eigenfunction expansion for $\psi(r,t)$ are instead interpreted as a measure of the likelihood that the *n*th wavefunction $\psi_n(r,t)$ manifests in a given experiment. The superposition $\psi(r,t)$, then, represents an expectation of possible wavefunctionns rather than a linear combinations of observed ones as in classical mechanics.

In the above discussion, we were careful to indicate that we were referring to the discreteness of energy rather than of the eigenvalues some other quantum-mechanical operator, for which one may yet have a continuum. The momentum operator, for example, may admit such a continuum. Additionally, the distinction in the preceeding paragraph is in many ways cosmetic, as classical Sturm-Liouville operators have discrete energy spectra. Nevertheless, this distinction is a convenient one to use from a historical and expository perspective—it is extremely useful for elementary discussions of quantum mechanics. In truth, however, the situation is subtler and more complicated, as there are important dynamical differences depending on whether a quantum system's spectrum is discrete, continuous, or contains regions with each property. In fact, such differences lie at the heart of the search for genuine quantum chaos, because any candidate system that might exhibit such behavior must be (spatially) bounded and unforced with a spectrum that is not discrete. It must also be fully quantum and describe a finite number of particles. 14

The probabilistic interpretation of quantum mechanics highlights an important difference between classical and quantum physics. In quantum-mechanical experiments, it is impossible to predict exactly what can happen in a given circumstance in the same sense as in classical experiments, as one can only observe a single mode at a time. Instead, one predicts the probabilities of different events, which can then be measured by repeated experimentation. However, this distinction between classical and quantum mechanics is, in some sense, cosmetic. One can, for example, compute probabilities in classical mechanics—the key difference is that all observable quantities may be measured simultaneously so that the expressions that correspond to the off-diagonal elements in a quantum-mechanical matrix calculation must

necessarily vanish. This, moreover, is intimately related to what is perhaps the fundamental difference between the classical and quantum theories. In classical physics, particles can be labeled by their position and velocity at a given time and their trajectories are thereby distinguished. In the quantum regime, however, particles do not have definite trajectories, so this distinction cannot be made. Indeed, in any experiment, one can switch the labeling of two identicle particles without altering its outcome.

Like dynamical systems theory, quantum mechanics has important philosophical implications.¹² The Heisenberg Uncertainty Principle implies that making (highly non-perturbative) observations of a phenomenon affects the phenomenon itself. This effect, moreover, cannot be minimized arbitrarily by altering experiments. There is a minimum disturbance that one simply cannot avoid. In classical physics, an observer is important only in a passive sense, whereas in quantum mechanics, the effects of an observation can be highly nontrivial.

5 The Origin of Quantum Mechanics

Now that we have highlighted several distinctions between quantum and classical mechanics, let us review its history. The physics community was in turmoil as the 19th century faded into oblivion and the 20th century began.²⁴ Amidst this maelstrom lay the origin of quantum mechanics. There were many experimental observations that were inexplicable according to the firmly grounded classical theory. As with nonlinear dynamics, the theoretical answer to these questions required a new way of thinking. At its very core lay subjective probability rather than objective determinism.

One of the aforementioned experimental observations was that light exhibits interference fringes and is therefore a wave phenomenon. However, erroneous results are obtained if one attempts to explain the photoelectric effect using the postulate that light is a wave. One finds that the energy of an emitted electron depends only on the frequency of the incident radiation rather than on its intensity as one might expect from the classical optics.

In 1901, Max Planck (1858–1947) observed blackbody radiation, showed that energy due to radiation could only exist in the form of discrete packets, and introduced his constant \hbar . In formulating his explanation of radiation packets, Planck had to abandon the notion that the second law of thermodynamics was an absolute law of nature. It was instead a statistical law. In 1905, Albert Einstein (1879–1955) discovered the photoelectric effect. Six years later, Ernest Rutherford (1871–1937) found that an atom has a positive central core surrounded by satellite electrons. Such circulating (and hence accelerating) particles radiate energy and so—based on classical theory—one would expect the electron to collapse into the nucleus. Why, then, does one not observe a burst of ultraviolet radiation emitted as an electron spirals into the nucleus? Why, moreover, is the frequency spectrum of light emitted from an atom discrete rather than continuous? Niels Bohr's (1885–1962) response, published in 1913, was his quantum theory of spectra.

In 1922, Arthur Compton (1892–1962) discovered that photons scattered off electrons. Two years later, Wolfgang Pauli (1900–1958) published his famous Exclusion Principle, which states that there are no fermion states in which two or more particles share the same quantum numbers. In 1925, Louis de Broglie (1892–1987) proposed that the wave-particle duality is a universal

characteristic of particles in nature rather than just a phenomenon that is observed in light.³³ He claimed that the wave nature of matter would become evident when the magnitude of Planck's constant \hbar could not be ignored. As a consequence, one could observe diffraction patterns from beams of particles other than photons.

Because matter exhibits aspects of both particles and waves, one must modify the tenets of classical physics. Bohr stressed the need for reconciling this wave-particle duality, introducing his concept of "complementarity" in 1927. In order to accomplish this, quantum theory must account for the discreteness of certain physical properties that entered the realm of physics before Bohr's atomic model. Normal modes, for example, are a quantized phenomenon from classical mechanics. Classically, one considers a superposition of such modes to describe the motion of an oscillator, whereas in quantum mechanics one considers an expectation of 'normal modes' (that is, wavefunctions) to describe the system of interest.

The previous year, Erwin Schrödinger (1887–1961) wrote an equation describing the wavefunction of a particle based on the laws of quantum mechanics he had discovered.¹³ This partial differential equation,

$$i\hbar \frac{\partial \psi(r,t)}{\partial t} = H\psi(r,t),$$
 (3)

was similar to the classical equations that describe other types of waves such as those describing sound, light, and (especially) heat. When quantum mechanics was first postulated, most scientsists studying it spent the majority of their effort attempting to solve the Schrödinger equation. Other physicists, including Max Born (1882–1970) and Paul Dirac (1902–1984), extended quantum mechanics further by incorporating phenomena such as

spin.

In 1927, Werner Heisenberg (1901–1976) discovered his Uncertainty Principle, which implies that corresponding to a smaller error in the measurement of a particle's momentum must be a larger one in a simultaneous measurement of the particle's position (and vice versa). For example, if one performs an identical experiment many times in which the position of an electron is measured (with a given momentum), then measurement of the position does not give an identical result for each experiment. A consequence of Heisenberg's principle is that there are compatible variables that can be simultaneously measured and incompatible ones that cannot be. The same year, Clinton Davisson (1881–1958) and Lester Germer conducted experiments on the wave properties of electrons and thereby demonstrated electron diffraction. Also in 1927, Max Born introduced a probabilistic interpretation of wavefunctions ψ . He claimed that the quantity $\|\psi\|^2$ was properly treated as a probability density rather than just as the intensity of a wave. Born's postulate is consistent with the results pertaining to the interference of electrons and photons. The presence of particles leads to interference fringes, which is generated by the wavefunction. At positions for which $\|\psi\|^2$ is large, the probability that the particle is found there is concomitantly large. In the presence of many particles, their distribution is described by the probability density function $\|\psi\|^2$.

Additional discoveries have molded quantum mechanics into its modern form. In 1928, Dirac discovered a relativistic wave equation and predicted the existence of the positron. As quantum mechanics continued to develop, physicists realized that there were many phenomena not directly encompassed in the Schrödinger equation, including electron spin and relativistic effects.¹³ The filling of these gaps led to relativistic quantum mechanics and quantum field theories.

6 Making Sense Out of Quantum Chaos

When given a mystery to solve, one seeks to find the simplest model possible that properly explains the unknown phenomenon. In science as in life, it is beneficial to follow the dictums of Occam's Razor. There will always be debates among scientists as to whether models contain extraneous elements or fail to offer satisfactory explanations, but the basis of simplicity in scientific modelling is one that is almost universally followed. A model must not only explain the desired phenomena, but it must be accessible to as many people as possible subject to that constraint. The success of a model depends not only on its relation to reality but also on its practicality. One can, in principle, incorporate every intricate detail when modelling phenomena, but this serves little purpose if it obscures what is important. Additionally, one also strives to incorporate as many phenomena as possible in such a way as to provide a useful abstraction of the component of the universe in which one is interested. This dichotomy, in fact, is practically an uncertainty principle in and of itself. As one complexifies a model, it (in theory) describes reality more accurately, but it is also simultaneously more difficult to understand and analyze.

Dynamicists have yet to establish a consensus as to what types of behavior constitute quantum chaos. One of the primary goals of the present paper is to offer a classification of the types of quantum chaos as well as an explanation of the behavior and analysis that characterizes each type. In the present paper, we attempt to extend to the chaotic regime the well-established differences between classical and quantum mechanics. Mathematical objects such as wavefunction superpositions are interpreted differently in the two subjects even when the behavior is integrable, so we generalize such distinctions to the case in which a system behaves chaotically. The differences between classical and quantum mechanics in the chaotic regime are a natural extension of those in the integrable regime, but the behavioral consequences of these differences can often be quite profound.

Dynamical systems theory brought about a revolution in deterministic thinking in science just as quantum mechanics fomented a probabilistic revolution. The study of quantum chaos is an attempt to marry these two abstract ways of thinking into a coherent whole in order to describe systems for which both quantum mechanics and nonlinear dynamics are relevant. More specifically, the concept of quantum chaos is an attempt to extend the notions of classical Hamiltonian chaos to the quantum regime. In the present paper, we review a classification scheme for quantum chaos and offer an exposition of the types of behavior described by the term 'quantum chaos.' There are three types of quantum chaotic behavior: "quantized chaos," "semiquantum chaos," and genuine "quantum chaos." Our discussion of quantized chaos is influenced by those in *Chaos in Atomic Physics* and *Chaos in Classical and Quantum Mechanics*, and we mostly follow the work of Porter and Liboff 127, 38–41 in our discussion of semiquantum chaos. We draw our discussion of true quantum chaos from that in *Chaos in Classical in Atomic Physics*.

6.1 Type I: Quantized Chaos

Quantized chaos, also known as "quantum chaology," is the most frequently studied form of quantum chaos. This subject is primarily concerned with bounded autonomous systems with discrete spectra. Quantized chaos concerns the quantization of classically chaotic systems, usually in the semiclassical $(\hbar \longrightarrow 0)$ or high quantum-number regimes. One looks for signatures of classically chaotic systems on the quantum level. In quantizing a chaotic system, one obtains a configuration that though not chaotic in a rigorous sense nevertheless behaves in a intrinsically different manner than an integrable system that has been similarly quantized. Nevertheless, the quantum dynamics of such systems are still affected in a fundamental manner by the fact that their classical counterparts are chaotic. It has been shown, for example, that all atoms and molecules except the hydrogen atom (and related two-body atomic systems) exhibit chaos when treated classically.^{6,20} The quantum dynamics of these systems are not rigorously chaotic, yet their associated waves and energies are strongly influenced by the underlying classical chaos. The reason a quantum-mechanical system so obtained is not rigorously chaotic follows from the discrete nature of its energy spectrum. In classical dynamics, chaotic behavior satisfied boundedness, infinite recurrence, and exponential sensitivity. The properties of boundedness and infinite recurrence can be applied to the quantum regime in a well-defined manner. One might worry that the discrete energy spectrum alters the topology so that one has to be careful about what it means for a "trajectory" (a term we use loosely in the quantum regime) to recur in an infinitesimal neighborhood, but this is not actually a problem, because one can consider things in

a different space, such as by taking Fourier transforms between the position and momentum bases. The concept of exponential sensitity, however, cannot be used directly in the quantum regime, because of the so-called "break time" phenomenon. In classical dynamics, exponential sensitivity refers to the exponentially fast separation of trajectories that began infinitesimally close to each other. If one considers Lyapunov exponents in configuration space, one obtains a time series that increases linearly at first but then tapers off to be roughly constant as "saturation" occurs. 47 In a bounded system, two trajectories can only be separated by a finite distance. In tangent spaces, however, this restriction is no longer present. (The tangent space at a point in a manifold is the set of all tangent vectors at that point.^{1,32}) Time-series plots of Lyapunov exponents in such spaces thus display a linear increase for all time. In the quantum regime, however, one obtains saturation both in configuration space and in the tangent space.³⁵ The saturation in the tangent space referred to as the quantum break-time phenomenon. It is the reason that the concepts of Lyapunov exponents and exponential sensitivity break down in quantum physics. Given that the systems under consideration satisfy boundedness and infinite recurrence rigorously and that there is still exponential sensitivity in some sense, it is not unreasonable to call these systems chaotic even though they are not rigorously so. Nevertheless, we elect not do so, as it is insightful to distinguish this type of behavior from that which is rigorously chaotic. The search for so-called genuine quantum chaos is equivalent to the search for a fully quantized system that is chaotic in a rigorous sense. Defining chaos as deterministic randomness may prove to be very useful in this effort. (With this definition, a system is nonchaotic if the information contained in a system is logarithmically compressed by the algorithms use to compute it. That is, one avoids the use of Lyapunov exponents by comparing the size of information input to the size of information output.)¹⁴

As discussed earlier, the notion of Lyapunov exponents does not directly carry over to the quantum regime. Even in the semiclassical or high quantum number regimes of quantum chaology, one still has problems defining this concept. Nevertheless, it is desirable to have a notion of stability that can be used for these situations. In classical systems, the Lyapnuov exponent is defined as the rate at which the largest eigenvalue of a trajectory grows. When the Lyapunov exponent of a classical trajectory is positive, the associated motion exhibits exponential sensitivity. In computing these exponents, one must consider how fast neighboring trajectories spread apart, which leads to difficulties as discussed above. (Additionally, one no longer has trajectories in the traditional sense.) One may thus define an instability exponent χ related to the eigenvalues of trajectories near periodic orbits. (They are computed in the semiclassical regime for so-called "periodic orbit expansions" and the Gutzwiller trace formula.) These instability exponents are the needed generalization of Lyapunov exponents. We remark that though we use these instability exponents in quantum chaology, there are fundamentally classical objects that are based on the concept of periodic orbits. In order to use classical periodic orbits in quantum mechanics, one must calculate the action integral S over one period and also consider its variation δS . One uses the Bohr correspondence priniple to interest the expression one obtains for δS . Moreover, when a classically chaotic system is quantized, one obtains scars,

which describe the narrow linear regions with enhanced intensity that occur in an eigenstate's intensity pattern.²⁰

Before we indulge ourselves in quantum chaology, let's consider some alternate terminology in the generalization of the notion of classical chaos. In so doing, we introduce the notion of 'quantum billiard chaos,'26 which may also be described in terms of the nodal properties of wavefunctions. This notion of chaos corresponds to quantized chaology as it manifests in quantum billiards. (As we discuss later, this can occur in billiards for which the Helmholtz equation is not globally separable.) It is chaotic in the sense of boundedness, infinite recurrence, and the instability exponents just defined. We earlier generalized the notion of chaos directly to the quantum regime. In this alternate formulation, one retains the classical notion of chaos and instead generalizes one if its component conditions—the idea of exponential sensitivity. Though this procedure is reasonable, we will instead partition quantum chaos into three categories as discussed above, because doing so allows us to discuss quantum chaos for a wider class of systems.

The tools used in the study of quantum chaology include random matrix theory, level dynamics, and periodic orbit expansions. The former comes into play in considering a system's (Hermitian) Hamiltonian matrix H. One defines an "uncorrelated" probability density p(H). That is, separate blocks of H are uncorrelated so that if H is an $n \times n$ matrix, then

$$p(H) = \prod_{i=1}^{n} \prod_{j=i}^{n} p_{ij}(H_{ij}).$$
(4)

For the special case in which n = 2, equation (4) becomes

$$p(H) = p_{11}(H_{11})p_{12}(H_{12})p_{22}(H_{22}). (5)$$

One can show that

$$p(H) = C \exp\left(-A \operatorname{tr}(H^2)\right), \tag{6}$$

where A and C are constants of integration. Related to this is the Wigner distribution

$$P_W(x) = \frac{\pi}{2} x \exp\left(-\frac{\pi}{4}x^2\right). \tag{7}$$

One expects such Wignerian statistics to hold for the spectra of complicated quantum systems with many degrees-of-freedom, in which the associated Hamiltonian is similarly complicated. Wigner statistics P_W are valid only if a system has integral spin and is invariant under an anti-unitary transformation such as time reversal. (An anti-unitary transformation consists of the composition of a unitary transformation with complex conjugation. Among the appropriate complex quantum systems are atoms and atomic nuclei. It has been shown that Wigner's prediction is consistent with experimentally obtained data describing the spacing of energy levels. The hydrogen atom in a strong magnetic field is a "simple" system in which this behavior is observed. The underlying chaotic features of the system cause certain statistical features of the quantum spectrum to obey predictions from random matrix theory.

If each of the anti-unitary symmetries is broken, the nearest neighbor statistics are expected to be described by

$$P_U(x) = \frac{32x^2}{\pi^2} \exp\left(-\frac{4x^2}{\pi}\right),\tag{8}$$

where the subscript U stands for 'unitary' since in the present case the system's Hamiltonian is invariant under all unitary transformations. If the

system has half-integral spin and retains anti-unitary symmetry, then all levels of the system are degenerate in the sense of Kramers.²³ The nearest neighbor distribution of energy level spacings between degenerate pairs is given by

$$P_S(x) = \frac{2^{18}x^4}{3^6\pi^3} \exp\left(-\frac{64x^2}{9\pi}\right) \tag{9}$$

where the subscript 'S' stands for 'symplectic'. If all the anti-unitary symmetries are broken, we are again in the case P_U .

The three cases P_W , P_U , and P_S are characterized by the Dyson parameter β , which indicates the degree of level repulsion as $x \longrightarrow 0$. In the three types of statistics above, β takes the respective values 1, 2, and 4 for the probability densities P_W , P_U , and P_S . The matrix elements of the Hamiltonian have a Gaussian distribution and for $\beta = 1, 2, 4$ are invariant respectively under orthogonal, unitary, and symplectic transformations. The random matrix ensembles are given the respective names Gaussian orthogonal ensemble (GOE), Gaussian unitary ensemble (GUE), and Gaussian symplectic ensemble (GSE). In addition to determining the appropriate level statistics, the symmetry class of a given Hamiltonian H also influences physical characteristics such as a system's localization length (which determines how fast wavefunctions decay in a given basis). Additionally, the zeroes of the Riemann ζ -function correspond very closely with the GUE, 19 which leads to the well-known connection between random matrix theory and this famous function.

The concept of level dynamics is also useful in studying the quantummechanical analogs of classically chaotic systems. If a quantum system depends on an external parameter, such as the strength of an externally applied magnetic field, its energy levels depend on that parameter. One may examine the changes in these energy levels as that parameter is adjusted. These so-called *level dynamics* provide useful information about a quantum-mechanical system's underlying chaotic structure. One studies the eigenenergies E_n of a Hermitian Hamiltonian

$$H(\epsilon) = H_0 + \epsilon V \tag{10}$$

as a function of the perturbation parameter ϵ . (The functions H_0 and V are independent of ϵ .) One identifies the eigenenergies E_n with fictitious particles. To derive the equations of motion, one starts with the eigenvalue equation

$$H(\epsilon)|n(\epsilon)\rangle = E_n(\epsilon)|n(\epsilon)\rangle$$
 (11)

and defines the matrix elements

$$V_{nm}(\epsilon) = \langle n(\epsilon)|V|m(\epsilon)\rangle. \tag{12}$$

Assuming that H is invariant under time reversal guarantees that eigenstates and matrix elements are real. The evolution equations of the level dynamics are then

$$\dot{E}_{n}(\epsilon) = V_{nn}(\epsilon),$$

$$\dot{V}_{nn} = 2\sum_{m \neq n} \frac{V_{nm}^{2}}{E_{n} - E_{m}},$$

$$\dot{V}_{nm} = \frac{V_{nm}(V_{nn} - V_{mm})}{E_{m} - E_{n}} + \sum_{l \neq n,m} V_{nl} v_{lm} \left(\frac{1}{E_{n} - E_{l}} + \frac{1}{E_{m} - E_{l}}\right),$$
(13)

which can also be derived from Hamilton's equations. These equations can be solved once the initial conditions at $\epsilon = 0$ are known. Note that the structure of equation (13) is independent of the specific form of the Hamiltonian

H. Moreover, equation (13) shows that the dynamics of energy levels of all Hamiltonian systems can be split into two parts, corresponding to equation (10). (This separation of the Hamiltonian into an unperturbed Hamiltonian H_0 plus a small perturbation ϵV is reminiscent of Melnikov theory.^{18,51}) The characteristics of a given Hamiltonian are used only via the initial conditions. Thus, if the initial conditions are unimportant for a sufficiently large $\epsilon \geq \hat{\epsilon}$, then one can use equilibrium statistical mechanics to compute the statistical properties of the system's energy levels. The methods of level dynamics can be generalized to those of "resonance dynamics." In equation (13), the indices n and m range over the number of dimensions of the relevant Hilbert space \mathcal{H} . These equations preserve the Liouville volume, the energy

$$E = \frac{1}{2} \sum_{n} V_{nn}^2 + \frac{1}{2} \sum_{n \neq m} \frac{|V_{nm}|^2}{(E_n - E_m)^2},$$
(14)

and the total coupling strength

$$Q = \sum_{n \neq m} |V_{nm}|^2, \tag{15}$$

which gives infinitely many first integrals (constants of motion), since increasing the coupling strength ϵ generates an orthogonal transformation in \mathcal{H} whose invariants (including the traces of various operators) stay the same. Moreover, the dynamical system (13) is completely integrable, so that one must understand a system with infinitely degrees-of-freedom and infinitely many constants of motion. In order to do this, one could take the point of view of statistical mechanics. Consider a stationary distribution

$$P = \frac{1}{Z}e^{-\beta E - \gamma Q},\tag{16}$$

where Z is the partition function (a normalization constant). The 'inverse temperature' β and 'chemical potential' γ are determined by prescribing mean values $\bar{E} \equiv \langle E \rangle$ and $\bar{Q} \equiv \langle Q \rangle$. One integrates out the variables V_{nm} to give a distribution of the eigenvalues E_n One obtains a GOE probability distribution in the eigenvalues, which is a bit disturbing because this ensemble now seems to show up in a context sufficiently general that it may not be of much value to the characterization of quantum signatures of classical chaos.²⁰

A third tool used in quantum chaology is the study of periodic orbit expansions. In order to pursue this field, it was essential to develop semi-classical methods that worked in the quantum regime. The first procedure to do this was the formalism of periodic orbit quantization.²⁰ The central result of this theory is the Gutzwiller "trace formula." In the semiclassical approximation, only periodic orbits $\{p\}$ contribute in the evaluation of the level density

$$\rho(E) \equiv \operatorname{tr}\left[\delta(E - H)\right]. \tag{17}$$

One finds that the classical approximation $\rho_c(E)$ of the quantum-mechanical trace²⁰ is

$$\rho_c(E) = \frac{1}{i\hbar} \sum_p \frac{T_0}{2\sinh(\chi/2)} \exp\left[i\left(\frac{S}{\hbar} - l\frac{\pi}{2}\right)\right],\tag{18}$$

where E represents energy,

$$T_0(E) \equiv \int \frac{dq_1}{|\dot{q}|} \tag{19}$$

is the primitive period, $\chi(E)$ is the instability exponent, $S(E) = \int pdq$ (integrated over the periodic orbit) is the action integral, and l is the number

of times the stable manifold is oriented in the local p-direction. The superposition of these smooth classical functions yields an approximate spectrum for the quantum-mechanical energy levels. We remark that the above formulation corresponds to a Feynman path integral approach, so that we are integrating in the variable $q \equiv (q_1, q_2, q_3)$ from some initial point q' to some terminal point q''. This formulation has been generalized, but by considering a Green's function (that is, a propagator^{7,42}), even generalized versions of equation (18) reduce to a trace. There are several other similar formulas in the study of quantized chaos, as discussed by Gutzwiller.²⁰ In some situations, for example, it is appropriate to have a hyperbolic cosine function rather than a hyperbolic sine function. One can also study the Riemann- ζ function to gain insight into the trace formula.

There are two ways in which the trace formula can be used to deal with quantum-mechanical problems. It can be applied "forwards" to calculate the level density of a given quantum system based on purely classical input represented by the periods, actions, Lyapnuov exponents, and characteristic parameters of the associated classical periodic orbits. It can also be applied "backwards" if the level density $\rho(E)$ is given. In this usage, information about the periodic orbits is extracted from the level density by a generalized Fourier transform based on the trace formula (since the trace formula is in the form of an eigenfunction expansion). The forward application of the trace formula is considered more difficult, although it has been used successfully on occasion. Gutzwiller, for example, applied the trace formula to a system consisting of electrons with an asymmetric mass tensor moving in a Coulomb potential, ¹⁹ an important problem in semiconductor physics. The forward

transform is considered difficult for three reasons: The number of periodic orbits increases exponentially in a chaotic system, these orbits have to be computed numerically, and the trace formula has convergence issues that have to be circumvented with appropriate summation prescriptions.

In the field of atomic physics, there are many systems whose classical counterparts are chaotic. Perhaps the most famous one is the rotation of a diatomic molecule under the influence of externally applied microwaves.^{6,20} A polar dimer molecule, such as CsI, is located between two plates of a capacitor, which is connected to a pulse generator that periodically charges and discharges the capacitor's two electrodes. This process creates a timevarying, spatially homogeneous electric field, so that the molecule experiences a sequence of electric pulses that couple with its dipole moment. This simple situation is a deterministic one, as we are assuming that there are no random fluctuations. Consequently, given the initial state of the rotating diatomic molecule, one may compute its associated wavefunction for all time.

The above technique captures the essential physical features of a rotating diatomic molecule, but it does not truly explain them. In order to understand the dynamics of the present example, one approximates it by restricting its rotation to a single plane (rather than three-dimensional space) and by ignoring the motion of its center of mass. In this approximation, one treats the rotating diatomic molecule as a $kicked\ rotor$, an example that has become a paradigm of quantum chaology. It has been studied in both a classical and quantum setting.^{6,20} One may treat the classical kicked rotor as a pendulum (or a rotator) that is agitated at equal time intervals with an impulse that varies periodically as a function of the rotor's angular position. The

motion of the rotor is then uniform between kicks, each of which changes the system's angular momentum. As the time interval between agitations becomes smaller, the behavior of the rotor approaches that of an ordinary forced pendulum. This classical system behaves chaotically, and the effects of this behavior are evident in the behavior of its quantum-mechanical cousin.

The study of quantum chaology and its applications remains an active area of research.⁶ Theoretical research addresses its analytical structure as well as the convergence properties of Gutzwiller's trace formula and its derivatives. A major breakthrough occurred in 1986 when Sir Michael Berry observed similarities between the trace formula and certain representations of Riemann's ζ -function. This function has henceforth served as a model for studying the analytical properties of semiclassical trace formulas. There are more fundamental concerns, however, than the convergence of these formulas. Indeed, it has been argued that there may exist a completely bounded chaotic dynamical system whose spectrum (which is both real and discrete) is identical to the imaginary parts of the (nontrivial) zeroes the Riemann ζ -function. The existence of this system would accomplish two important tasks. As a mathematical problem, it would prove the Riemann conjecture that

$$\zeta\left(\frac{1}{2} + iz\right) = 0\tag{20}$$

in the region |Im(z)| < 1/2 only for z with vanishing real part. As a physical system, it would offer important insights regarding the analytical connection between classical chaos and quantum energy levels. Research in applications of quantized chaos include attempts to use the semiclassical methods in this area as a mathematical tool for studying classically chaotic systems. These

methods are currently thought to be much more useful for interpreting quantum spectra and wavefunctions than they are for accurately predicting the spectra of classically chaotic systems.⁶

There is active research in other areas of quantum chaology as well. For example, there have been several recent discoveries concerning the connection between quantized chaos and the three matrix ensembles discussed earlier. Additionally, it is not completely understood why the statistics of random matrix ensembles are so accurate in describing how classical chaos induces universal fluctuations in energy levels. Other topics of current interest include diffraction and refraction corrections in semiclassical procedures. Some scientists are also studying whether the presence of chaos in a system can increase tunnelling. In this context, a wave would tunnel between two islands in a chaotic sea. It has been surmised that the presence of chaos would increase the tunnel splitting of energy levels by several orders of magnitude. Lastly, quantum chaology in dimensions greater than two is virtually unexplored. The methods in this subject are only expected to be accurate to order \hbar^2 independent of dimension, although this has not been shown rigorously. The extension of quantum chaology to higher dimensions should nevertheless prove quite fruitful.

6.2 Type II: Semiquantum Chaos

Semiquantum chaos concerns systems with both classical and quantum subsystems. It can arise, for example, in the form of the dynamic Born-Oppenheimer approximation,⁵ which shows up commonly in the study of mesoscopic and chemical physics. This adiabatic approximation arises naturally in systems that may be expressed as the coupling of slow and fast sub-

systems. In the Born-Oppenheimer scheme, chaos may occur in both the classical (slow) and quantum (fast) subsystems, although considered separately, neither of those regimes is necessarily chaotic. The first step in the Born-Oppenheimer approximation is to quantize the fast (electronic) subsystem. The second step is to quantize the nuclear (slow) subsystem. If, however, the electronic energy levels are too close together, the Born-Oppenheimer approximation breaks down, as the electronic and nuclear subsystems are nonadiabatically coupled. When this occurs, one treats the nuclear degrees-of-freedom as classical variables, thereby obtaining a semiquantal regime in which a classical system is coupled nonadiabatically to a quantum one. It is this nonadiabatic coupling that produces semiquantum chaos in the resulting system, which is sometimes called a semiclassical quantization.^{34,50}

One may mathematically abstract numerous systems that exhibit semiquantum chaos as quantum billiards with vibrating boundaries.^{5,6,27,38–41,50} Such systems are not necessarily expressible *precisely* as vibrating quantum billiards, but such billiards serve as a useful toy model in that that they capture many of the features of molecular systems. It is in this abstract context that we discuss the notion of semiquantum chaos.

Quantum billiards describe the motion of a point particle of mass m_0 undergoing perfectly elastic conditions in a bounded domain of mass $M \gg m_0$ in a potential V. The particle's motion is described by the Schrödinger equation with Dirichlet boundary conditions. One defines the "degree-of-vibration" (dov) of a billiard as the number of boundary dimensions that vary with time. If the boundary is time-independent, the billiard is said to have zero dov. The one-dimensional vibrating billiard and the radially vi-

brating spherical billiard have a single dov, and the rectanglular billiard with time-varying length and width has two dov. The dov of a quantum billiard are its classical ("nuclear") degrees-of-freedom. A zero dov quantum billiard exhibits only integrable behavior if it is globally separable.⁴¹ (A quantum billiard is globally separable if the geometry of the billiard is one in which the Helmholtz equation is globally separable.) Two simple ways in which global separability is violated are when a quantum billiard has a concave boundary component and when a billiard is geometrically composite, although it is believed that global separability may be violated in other ways (such as with a quantum billiard whose boundary is a quartic ellipse), by analogy with known non-integrable classical billiards. When global separability is violated in a quantum billiard, the observed behavior is "chaotic" in the sense of quantum chaology. Billiards with concave boundary components, for example, share many of the properties of Anosov diffeomorphisms.³ Composite quantum billiards such as the stadium billiard (whose boundary consists of two semi-circles joined by a pair of straight lines) have also been shown to exhibit chaotic behavior. 22,30 In globally separable, zero dov quantum billiards, however, one expects to observe primarily quasiperiodic behavior, analogous to the Asteroids example discussed earlier. (One must be careful with the term "quasiperiodic" in the quantum regime just as one is with the notion of chaos. Essentially, one is looking at the quantization of what was a quasiperiodic regime in the classical situation.) The easiest example to visualize is that of a zero dov rectangular quantum billiard. Imagine that the boundary acts as a mirror, so that there are imaginary billiards adjoining the actual one on each of its four sides. Modulo translation, one then recovers the same situation,

as we described earlier when we discussed motion on a 2-torus. If a wave hits a side of the billiard, the reflection in the mirror behaves just as the motion in the Asteroids example. Under perfect reflection, the angle of incidence equals the angle of reflection, and so perfectly reflected trajectories have the same features as trajectories on a 2-torus with respect to periodicity and quasiperiodicity. Although a stationary, globally separable quantum billiard is necessarily integrable, we remark that the Toda lattice is an example of a dynamical system that is integrable but not separable.^{20,28}

Consider an s dov quantum billiard. The total Hamiltonian of the system is given by

$$H(a_1, \dots, a_s, P_1, \dots, P_s) = K + \sum_{j=1}^s \frac{P_j^2}{2M_j} + V,$$
 (21)

where a_1, \dots, a_s represent the time-varying boundary components and the kinetic energy (which corresponds to the quantum-mechanical Hamiltonian of the particle confined within the billiard) is given by

$$K = -\frac{\hbar^2}{2m} \nabla^2. \tag{22}$$

A two-term superposition of the nth and qth states (that is, a two-term Galërkin projection^{18,49}) is given by

$$\psi_{nq}(x,t) \equiv \alpha_n A_n(t) \psi_n(x,t) + \alpha_q A_q(t) \psi_q(x,t), \tag{23}$$

where the complex amplitudes $A_j(t)$ are time-dependent because the system has time-dependent boundary conditions. Linear equations with such nonlinear boundary conditions thus lend themselves to analysis via Galërkin methods just like nonlinear partial differential equations such as the Navier-Stokes and nonlinear Schrödinger equations. The present problem is of a

type known as a *free-boundary problem*, in which one does not know a priori the shape of the domain.¹⁵ It is well-posed by the specification of Dirichlet boundary conditions, an initial radius a(0), and initial momentum P(0), and initial amplitudes $A_i(0)$.

For now, we specialize to the case of one dov, in which only a single boundary dimension varies in time. Porter and Liboff have shown⁴¹ that a two-state superposition consisting of the nth and qth states exhibits chaotic behavior if and only if the quantum numbers corresponding to stationary dimensions of the billiard's boundary are the same in both states. This result, which manifests in observed coupling behavior in the electronic states of polyatomic molecules, 36,50 is easily extended to any finite-term superposition by considering the terms pairwise. The result then states that there must exist one pair of states that satisfies the above condition. In the vibrating spherical quantum billiard, for example, a pair of states has to have the same angular momentum quantum numbers l and m for chaotic behavior to occur. (This result is proven using separability and orthogonality conditions of the Helmholz differential operator. These conditions are not surprising, because the rotational symmetry of the system is invariant under radial vibrations.

In an integrable two-term superposition state of a one *dov* quantum billiard, the equations of motion are

$$\dot{a} = \frac{P}{M},\tag{24}$$

$$\dot{P} = -\frac{\partial V}{\partial a} + \frac{\lambda}{a^3},\tag{25}$$

where $\lambda \equiv 2 (\epsilon_1 |C_1|^2 + \epsilon_1 |C_2|^2)$, and C_1 and C_2 are constants such that $|C_1|^2 + |C_2|^2 = 1$. (The energy parameter λ is necessarily positive because $\epsilon_i > 0$ and the $|C_i|^2$ correspond to probabilities.) A special case of this configuration is obtained by considering a single eigenstate.

Equation (25) has been studied numerically in the context of the bifurcations that can occur when one considers different potentials V.³⁸ In particular, one observes only saddle-center bifurcations (and generalizations thereof). Either all the equilibria are centers or—for sufficiently small energies λ —some of them are centers and others are saddle points (depending on the form of the potential). Saddle connections in this system have been studied to some extent using continuation methods, although there is room for quite a bit more research in this area.

In the chaotic case, the equations of motion take the form

$$\dot{x} = -\frac{\omega_0 y}{a^2} - \frac{2\mu Pz}{Ma},\tag{26}$$

$$\dot{y} = \frac{\omega_0 x}{a^2},\tag{27}$$

$$\dot{z} = \frac{2\mu Px}{Ma},\tag{28}$$

$$\dot{a} = \frac{P}{M},\tag{29}$$

and

$$\dot{P} = -\frac{\partial V}{\partial a} + \frac{2[\epsilon_+ + \epsilon_-(z - \mu x)]}{a^3},\tag{30}$$

where x, y, and z are Bloch variables,² a represents a displacement, P is its conjugate momentum, M is the mass of the billiard, $m_0 \ll M$ is the

mass of the confined particle, $\mu > 0$ is the coupling coefficient between the two eigenstates, $V \equiv V(a)$ is the potential in which the billiard resides, $\omega_0 \equiv (\epsilon_2 - \epsilon_1)/\hbar$, $\epsilon_{\pm} \equiv (\epsilon_2 \pm \epsilon_1)/2$, and ϵ_1 and ϵ_2 (where $\epsilon_2 \geq \epsilon_1$) are the energies of the two eigenstates.³⁸ The bifurcation structure of this system of equations is a generalization of that observed in the integrable case in the sense that only generalized saddle-center bifurcations can occur. As before, pairs of stable and unstable directions bifurcate to the center manifold as the energy of the system is increased. Additionally, there is evidence of saddle connections for this chaotic case.

For the one-dimensional vibrating quantum billiard, Blumel and his coauthors 5,6 considered a two-term superposition state that they computed to have a coupling coefficient $\mu=3/4$. They computed Liapunov exponents to show expontial divergence (and hence chaos) in this case. However, for given parameter values and initial conditions, one can tell whether the configuration is chaotic simply by examining the associated Poincaré maps. This, of course, does not *prove* rigorously that the configuration is chaotic. Nevertheless, it corresponds to the canonical application of KAM theory to engineering and the physical sciences, so we consider this a sufficient demonstration of chaotic behavior in the present context. Figures 2 and 3 display chaotic behavior in the classical variables, and Figure 4 shows chaos in the quantum-mechanical Bloch variables. Classical Hamiltonian chaos in the positions and momenta lead to quantum-mechanical wave chaos in the normal modes, whereas chaos in the Bloch variables corresponds to chaos in the quantum probabilities. 41

The single dov quantum billiard that has been analyzed most extensively

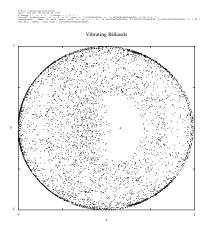


Figure 4: An example of chaotic behavior in the Bloch variables in a vibrating quantum billiard.

is the vibrating sphere,²⁷ although the one-dimensional vibrating billiard was studied earlier.^{5,6} One finds that the coupling coefficient μ depends on the geometry of the system (as well as what quantum states one considers), but that the general behavior of the system is typified by the fact that only a single boundary variable is time-dependent. Even though the vibrations of a sphere occur in \mathbb{R}^3 , only the radial dimension of the billiard actually depends on time. Other single dov quantum billiards include the radially vibrating cylinder, the longitudinally vibrating billiard, and the rectanglar billiard in which either the length or width (but not both) depends on time.

One can generalize the above notions to quantum billiards with two or more dov. Two examples of such quantum billiards are the rectangular billiard in which both length and width are permitted to vibrate⁴⁰ and the cylindrical billiard with both radial and longitudinal vibrations. The latter

may be useful as a model for carbon nanotubes or quantum wires. The theorems cited above can be generalized, although these generalizations require further study.

Before we proceed to the third type of quantum chaos, it is important to discuss what is meant when we say that vibrating billiards exhibit quantum chaotic behavior when the coupling coefficient μ is nonzero. What exactly constitutes such behavior and why should one care about it? We formulated the chaotic configuration of single dov quantum billiards as a five-dimensional dynamical system: the displacement a and conjugate momentum P are classical variables, and the Bloch variables x, y, and z are quantum-mechanical variables—as they are obtained from the probabilities $|A_n|^2$ and $|A_q|^2$. Another way to formulate this system is to use action-angle variables, which gives one classical degree of freedom coupled to a single quantum-mechanical one.⁵⁰ In each interpretation, we treat the dynamical equations as a classical subsystem coupled to a quantum one. The chaotic behavior in the (a, P)-plane represents wave chaos, as the position a is an argument of the individual wavefunctions ψ_n and ψ_q . Additionally, chaos on the Bloch sphere (equivalently, in the quantum-mechanical action and angle) represents chaos in the quantum probabilities. Therefore, both manifestations of the observed chaotic behavior have interpretations that go beyond classical Hamiltonian chaos. Moreover, the observed chaotic amplitudes along with chaotic waves give us a chaotic superposition of chaotic normal modes. This is a hallmark of semiquantum chaos.

Vibrating quantum billiards, though an idealized mathematical model, bear import as simple manifestations of semiquantum chaotic behavior. They

are important for other-more practical-reasons as well. They may be used to describe nonadiabatic coupling in polyatomic molecules. Such behavior is relevant, for example, in the study of Jahn-Teller systems. 50,54 In the present context, chaotic configurations of a one dov quantum billiard are analogous to a diatomic molecule with two electronic states (of the same symmetry) coupled nonadiabatically by the single internuclear vibrational coordinate.⁵⁰ The former gives the quantum degrees-of-freedom, while the latter produces the classical ones. (This situation is easily generalized to ones with three or more electronic states. Additionally, the radially vibrating spherical quantum billiard captures features of particle behavior in the nucleus⁵² and as a simplistic representation of the quantum dot nanostructure.²⁹ The vibrating cylindrical billiard may be used as a model for the quantum wire, another microdevice component.⁵³ More importantly, it may also prove useful as a model of carbon nanotubes. Additionally, other geometries of vibrating quantum billiards may have similar applications in mesoscopic physics. That is, they may be used as models of various chemical nanostructures, as they describe the nanomechanical (electronic-vibronic) coupling that can occur in such devices.³⁶ Moreover, vibrating quantum billiards generalize Enrico Fermi's bouncing ball model of cosmic ray acceleration.^{4,28} Finally, when some compounds are placed into liquids, one obtains solvated electrons that may be described as oscillating billiard systems. 45,46 With such a wide array of possible application, vibrating quantum billiards are a very versatile model. They provide a simple illustration of semiquantum chaos, they generalize a toy model of Enrico Fermi, and they have already been shown to be relevant to areas of nuclear, chemical, and mesoscopic physics.

There remains much to be studied about semiquantum chaos in vibrating billiard systems. For example, one may analyze Galërkin projections with more than two terms (in which the Bloch sphere is generalized) and quantum billiards with two and three dov. A quantum billiard with three dov (such as a rectangular prism billiard with vibrating length, width, and depth) may also exhibit Arnold diffusion and cross-resonance diffusion, because the Hamiltonian (classical) subsystem has a number of degrees-of-freedom equal to the number of dovs of the billiard. These problems may also be studied using action-angle coordinates, in which the number of degrees-of-freedom of the system is more readily apparent. Future work also includes the study of other geometries, such as the two dov cylindrical quantum billiard and billiards with concentric geometries (such as spheres or disks) whose inner and outer radi both oscillate. Note, in particular, that this latter example removes the assumption of convexity and may also lead to a generalization of the notion of dov. Another effect to incorporate is that of rebound from the collisions of particles with the billiard's boundary. Additional work to be done includes further studies of bifurcations in vibrating quantum billiards as well as an analysis of coupled vibrating quantum billiards, which is important because quantum dots are often coupled in arrays of various geometries in laboratory settings. It may also be fruitful to extend the analysis of vibrating quantum billiards to a relativistic setting as well as to studying multiple-particle vibrating quantum billiards. Finally, the Galërkin method discussed briefly in the present paper may also be useful for analyzing nonlinear Schrödinger equations, because linear partial differential equations with nonlinear boundary conditions are similar in several respects to nonlinear partial differential

equations.

Semiquantum chaos may be considered in other settings as well. The fact that such systems exhibit exponential sensitivity in their quantum subsystems (represented by the fact that the Bloch variables behave chaotically) is a hallmark of the traditional notion of chaos in a semiquantal setting.^{6,41} We remark that quantum chaos is a type of 'wave chaos.' This generalization is nominal in terms of 'type I' quantum chaos, as it make little difference whether a system is quantum-mechanical or classical when one is studying spectra or wave manifestations of ray dynamics in classical wave systems in areas such as acoustics, optics, and electrodynamics. However, when applying this generalization to the semiquantal regime, it is important to note that for classical wave systems, having a classical boundary is no longer an approximation. This shows that 'type II' wave chaos exists in nature. Such waves have been studied in classical electrodynamics.

It would be fruitful to apply the methods that have been used in the study of semiquantum chaos to nonlinear Schrödinger equations, which can be used to describe optical waves in certain media as well as superfluid hydrodynamics. Recall, however, that in quantum mechanics, the classical boundaries used in the present analysis are in truth an approximation. The nuclear degrees-of-freedom (represented by the oscillating components of the billiard boundary) may be quantized, resulting in a purely quantum (though higher-dimensional) system. The effect of such a quantization on semiquantum chaotic systems has not been completely resolved, although every previous attempt has produced an example of quantized chaos. In particular, quantizing the walls of a vibrating quantum billiard leads to a higher-dimensional

system that properly falls under the heading of quantized chaos.

6.3 Type III: True Quantum Chaos

Bounded, fully quantized systems that exhibit exponential sensitivity and infinite recurrence are genuinely quantum chaotic. (Semiquantum chaos describes exponential sensitivity in the semiquantal regime; systems in this regime consist of classical subsystems coupled with quantum mechanical ones, so they are not fully quantized.) Quantum chaology describes quantum signatures of classically chaotic systems. This regime is fully quantal, but the "chaos" observed cannot exhibit exponential sensitivity, as we discussed earlier. Indeed, the existence of systems that are quantum chaotic in the above, stronger sense remains an open question. From our previous discussion, we note that the energy spectrum of such a system cannot be fully discrete. Otherwise, such a system could not display exponential sensitivity.

The following example has been proposed as a *possibility* of such a quantum chaotic system. Most scientists do *not* consider it an example of such, although it is certainly a very interesting system. Consider a spin 1/2 particle passing through a chain of two different magnets (types A and B), sequenced according to the following recursion formula:

$$M_{n+1} = M_n \circ M_{n-1}, \quad M_0 = A, M_1 = B,$$
 (31)

where the symbol \circ denotes the operation of appending one chain of magnets to another. For example, $M_2 = M_1 \circ M_0 = BA$, $M_3 = M_2 \circ M_1 = BAB$, and $M_4 = M_3 \circ M_2 = BABBA$.

In general, the chain of magnets (which, in principle, can be constructed in laboratory settings) induces spin precession. The propagator U of a spin

1/2 particle satisfies the recursion relation

$$\hat{U}_{n+1} = \hat{U}_n \hat{U}_{n-1} \tag{32}$$

and can be parametrized by

$$\hat{U}_n = e^{-i\alpha_n \sigma_z} e^{-i\beta_n \sigma_y} e^{-i\gamma_n \sigma_z},\tag{33}$$

where σ_x , σ_y , and σ_z are the Pauli spin matrices.⁴²

We follow Blümel and Reinhardt and consider the special case in which the magnetic field of each of the magnets is aligned along the y-axis. It follows that the propagator \hat{U}_n represents a rotation by angle β_n . This leads to to following recurrence relation for β :

$$\beta_{n+1} = \beta_n + \beta_{n-1} \pmod{2\pi}. \tag{34}$$

For the initial conditions $\beta_0 = \beta_1 = 1$, we recover the Fibonacci sequence.⁴³ Defining $b_n \equiv \beta_n/2\pi$, one obtains the above recursion relation mod 1, which can be written as the map $Q: \vec{w}_n \mapsto \vec{w}_{n+1} =$

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \pmod{1},\tag{35}$$

where the vector $\vec{w} \equiv (b_n, b_{n-1})$. The map (35) is very similar to the Anosov map³ $C: \vec{w}_n \mapsto \vec{w}_{n+1} =$

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}, \tag{36}$$

whose chaotic properties are well-known. The map Q shares many of the properties of the Anosov diffeomorphism. For example, it possesses a stretching direction $\vec{v}_1^{(Q)}=(1,g)$ with a corresponding eigenvalue $e_1^{(Q)}=\bar{g}>1$ that

has a positive Lyapunov exponent. The mapping Q thus exhibits exponential sensitivity and chaotic behavior just like the Anosov diffeomorphism. The quantum dynamics of spin 1/2 particles in the given magnetic chain are thus argued by Blümel and Reinhardt to be truly chaotic.⁶ The sequence of rotation angles $\beta_n \pmod{2\pi}$ is consequently also chaotic.

If the spin 1/2 particles are prepared in a pure spin state polarized in the +z direction, the corresponding occupation probability in the $+|z\rangle$ state after the nth section is given by $\cos^2(\beta_n)$, so the population in the $+|z\rangle$ state must be chaotic as well. Measuring this occupation probability provides an experimental test for the occurrence of quantum chaos in the present system.

Additional issues are involved, which raises doubt as to whether one should consider this system a genuinely quantum chaotic one. For a given n, the magnetic chain is not chaotic because of the unitarity of quantum mechanics, as there is no exponential instability for fixed n. Instead, chaos occurs as a function of the discrete variable n. Moreover, one must consider the length of the apparatus required to observe the quantum chaotic behavior described above. It is well-known that the Fibonacci sequence diverges exponentially, so the number of magnets increases exponentially with n. Therefore, the action of this chain of magnets is equivalent to free motion of a particle on a ring whose position is measured at the end of exponentially growing time intervals. This provides an alternate means of understanding this example. Because of the exponential increase in the length of the magnet chain, the "physical flight time" it takes for particles to go through the actual apparatus also grows exponentially in n. However, if the magnets are exponentially close in n, then the "natural flight time" grows linearly, and

the magnet chain would consequently also be chaotic with respect to this temporal variable. Tranforming to the rest frame of the moving beam particles, the quantum-mechanical description of a spin 1/2 particle traversing the chain of magnets is equivalent to the quantum description of a stationary spin 1/2 particle perturbed by a sequence of external field pulses.

Note finally that the dynamics of the case with aligned magnetic fields is the only one that has been investigated thus far. Additionally, this system of Fibonacci magnets is considered to be a genuinely quantum chaotic by only a handful of scientists. Other candidate systems have been proposed,⁸ but the existence of chaotic behavior (in the traditional sense) in fully quantized systems remains an open question. Nevertheless, there are some clues concerning where to look. In order to have a chance at representing the Holy Grail of quantum chaos, a system must be (spatially) bounded, finite-particle, undriven, and fully quantum with a spectrum that is not discrete.¹⁴

7 Conclusion

The fields of nonlinear dynamics and quantum mechanics have both achieved their share of attention in popular culture. Each has been a part of a scientific revolution. For example, the notion of quantum mechanics brought an important probabilistic interpretation to science, and the advent of dynamical systems theory showed that determinism did not imply solvability. The study of quantum chaos, which has been increasingly scrutinized in recent years, is an effort to marry these two subjects. In the present paper, we discussed the historical evolution and some principle ideas of both subjects. We then divided quantum chaos into three behavioral subclasses

and discussed several examples, methods, and results in each of these areas.

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Figure Captions

- Figure 1: A separatrix that occurs in an integrable configuration of a vibrating quantum billiard in a double-well potential. Trajectories inside the separatrix behave qualitatively differently from those outside the separatrix.
 - Figure 2: An example of hard Hamiltonian chaos.
 - Figure 3: An example of soft Hamiltonian chaos.
- Figure 4: An example of chaotic behavior in the Bloch variables in a vibrating quantum billiard.