Quantum chaos

Roderick V. Jensen

What are the special properties of strongly perturbed quantum systems when the corresponding classical mechanical systems exhibit chaotic behaviour? This is the central question of quantum chaos. Theoretical and experimental studies of highly excited atoms in strong magnetic fields and intense microwave fields have revealed surprising new physical phenomena with far-reaching applications.

> "The classification of the constituents of a chaos, nothing less is here essayed."
>
> Herman Melville
> *Moby Dick*, 1851

IN Melville's time, 'chaos' referred to a state of disorder or confusion. In the past 15 years, the word has been endowed with a new meaning in the lexicon of science and mathematics. Since May's seminal review article[1] in 1976, "*Simple mathematical models with very complicated dynamics*", chaos has emerged as a technical term for the irregular, unpredictable and apparently random behaviour of a wide variety of deterministic dynamical systems such as fluctuating biological populations, cardiac arrhythmias, oscillating electrical circuits, vibrating structures, turbulent fluids and particle orbits in accelerators, plasma fusion devices and the Solar System[2-4]. In turn, this new concept of 'deterministic randomness'[5] has given birth to a rapidly developing interdisciplinary field of research called nonlinear dynamics[6].

My goal here is less ambitious than Melville's stated aim in his well-known treatise on 'chaos'. Although the many new concepts and research methods in nonlinear dynamics and chaos have found widespread applications in the biological and social sciences as well as in the physical sciences and engineering, I will focus here on the classical and quantum mechanical description of strongly coupled and strongly perturbed nonlinear systems in physics. Specifically, I will address the profound and often controversial problem of 'quantum chaos', the question of how quantum systems behave when the corresponding classical systems are chaotic. Extensive theoretical modelling coupled with experimental measurements on physical systems has uncovered a wealth of new physical phenomena at this exciting frontier between the microscopic and the macroscopic world, where the classical theory is chaotic and the quantum theory can be very complicated.

Classical chaos

According to Newton, the behaviour of a mass on the end of spring or a planet orbiting the Sun should be completely described by the differential equations of motion of classical mechanics[7]. If we specify the initial values of the positions and momenta, then the deterministic equations uniquely specify the motion for all times in the future (and the past). But except in rare examples, usually emphasized in physics textbooks, these equations do not have simple analytical solutions.

In general the classical equations of motion are nonintegrable. Although the evolution is deterministic, in most cases we cannot find it without the help of numerical calculations. Worse, numerical studies of the nonlinear classical equations of motion for many model problems, such as two or more coupled, anharmonic oscillators[8], or asteroid orbits periodically perturbed by the gravitational pulls of nearby planets[9], have led to the realization that the time evolution can show 'extreme sensitivity to initial conditions'. Uncertainties or errors in the initial conditions can grow at an exponential rate which is intrinsic, not an artefact of any numerical approximations. Remarkably, this property of nonlinear differential equations was first pointed out by Poincaré[10] at the turn of the century for the classical three-body problem, long before the advent of modern digital computers.

The local instability of motion that leads to this 'extreme sensitivity to initial conditions' is the defining property of chaos in classical systems. The laplacian ideal of perfect predictability in these deterministic systems can only be realized if the initial conditions are known and specified with infinite precision. Any errors grow rapidly, preventing long-time prediction and resulting in behaviour that appears irregular and random[4].

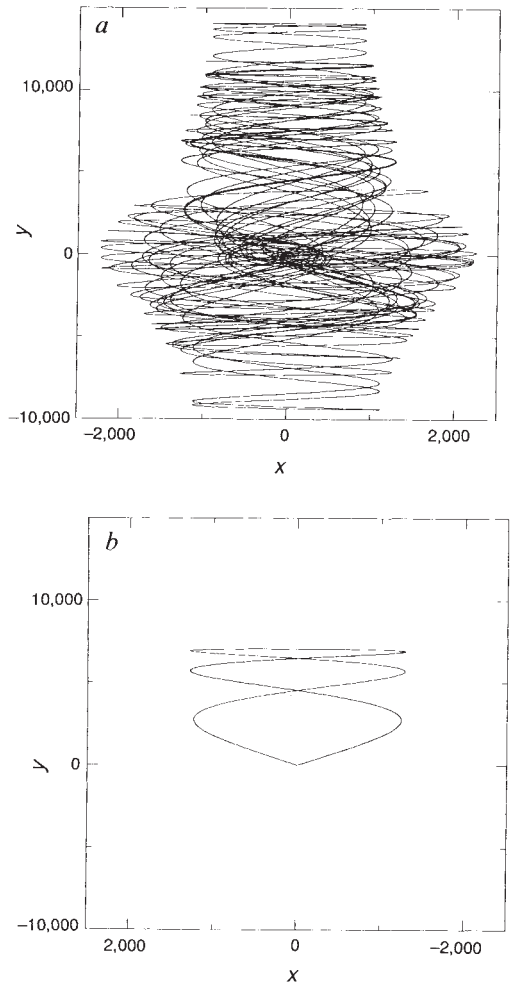

FIG. 1 *a*, A typical chaotic, classical orbit of an electron moving in the two-dimensional potential in equation (1). *b*, For special initial conditions[46] the trajectory can be periodic: the particle moves away from the nucleus at the origin, oscillates because of the force of the magnetic field, and returns to the nucleus where it is reflected backward along its previous path. For strong magnetic fields, however, these regular, periodic orbits are highly unstable. If we displace the trajectory by as little as one part in 10^6, then we get the highly irregular orbit shown in *a*.

To illustrate this concept of deterministic randomness, Fig. 1 shows plots of two different classical trajectories for a particle moving without friction in a two-dimensional potential well[11]

$$V(x, y) = -1/\sqrt{x^2+y^2} + \frac{B^2}{8}x^2 \qquad (1)$$

which corresponds to the effective potential experienced by an electron moving in an attractive Coulomb field and a constant magnetic field, B. If the potential consisted only of the first term representing the Coulomb field or the second term corresponding to a simple harmonic oscillator, then the analytical solutions of the equations of motion could be found in many classical physics texts[7]. But this simple combination of forces often yields irregular, unpredictable, apparently random trajectories such as that shown in Fig. 1*a*. For a slightly different initial condition, corresponding to a change of the starting position by one part in a million, the resulting trajectory (Fig. 1*b*) is completely different. In this case it lies close to one of the infinitely many (but still relatively rare) unstable periodic orbits for this dynamical system.

The problem of quantum chaos

Bohr's correspondence principle[12], which requires that quantum and classical behaviour should coincide for macroscopic systems, might suggest that some vestiges of classical chaos should persist in the quantum theory. For bounded systems, however, neither the quantum wavefunctions nor any observable quantities can show the extreme sensitivity to initial conditions that defines classical chaos. The quantum mechanical energy spectrum is discrete, and the solutions of the Schrödinger equation restrict the quantum dynamics to quasiperiodic behaviour, whereas the corresponding classical dynamics can be fully chaotic.

As a consequence it does not seem possible to define quantum chaos as a property of a quantum system that corresponds to chaos in classical mechanics. Nevertheless, the term quantum chaos is used to refer to the study and description of the properties of quantum systems for which the corresponding classical hamiltonian system is chaotic. In an effort to avoid confusion between the definition of an attribute of a physical system and a field of study, Berry[13] has introduced the term 'quantum chaology' to be synonymous with this usage of 'quantum chaos'.

It may emerge from these studies of quantum chaology that real quantum systems can exhibit true chaos. Indeed, some peculiar theoretical models of unbounded quantum systems (with continuous energy spectra) have been shown to be capable of chaotic dynamics, but these models suffer from unphysical properties such as unbounded, exponential growth of energy and momentum[14]. For realistic, few-body, quantum systems, such as atoms and molecules, it seems that radical changes in the present quantum theory are required for chaotic behaviour[5].

Despite debate over the meaning of the term 'quantum chaos', nearly everyone agrees on the important problems[15]. What is the nature of the classical–quantum correspondence principle for classically chaotic systems? What are the characteristic properties of the energy levels and eigenfunctions for a system of strongly coupled nonlinear oscillators, such as a highly excited polyatomic molecule or a simple hydrogen atom in a strong magnetic field? How does the quantum wavefunction evolve for strongly perturbed nonlinear oscillators such as atoms or molecules in intense electromagnetic fields?

These problems represent an exciting frontier for modern physics and chemistry. Pioneering experiments on highly excited Rydberg atoms in strong magnetic static fields have been made by groups at the University of Bielefeld[16–19] and Massachusetts Institute of Technology[20–22], and in intense microwave fields at the University of Pittsburgh[23,24] and the State University of New York at Stony Brook[25–27]. The classical descriptions of these highly excited electron orbits are chaotic when perturbed by sufficiently strong magnetic and electromagnetic fields. For example, when the Lorentz force on an electron moving in a strong magnetic field competes with the Coulomb binding field[11,28–30], then the typical classical electron trajectory resembles that shown in Fig. 1*a*. Similarly, when the oscillating force due to an applied microwave field becomes comparable to the Coulomb binding field[31], a stroboscopic picture of the classical electron motion in action–angle phase space shows a transition from mostly regular behaviour (Fig. 2*a*) to widespread chaos (Fig. 2*b*). Although the solutions of the Schrödinger equations for these systems cannot satisfy the strict definition of classical chaos, experimental and associated theoretical studies of the quantum chaology for these simple atomic systems have nevertheless revealed a rich variety of new physical phenomena.

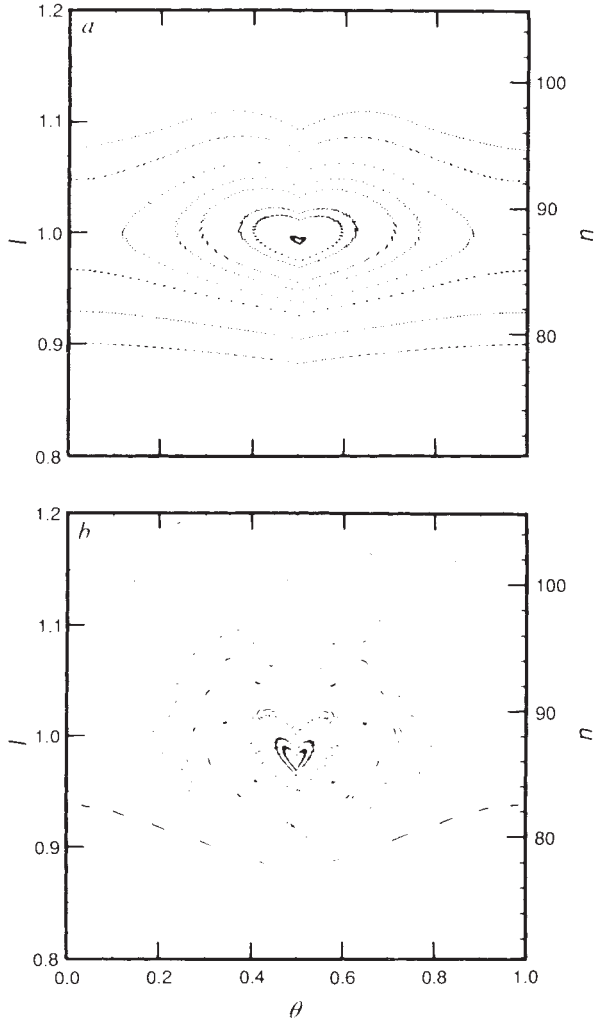

FIG. 2 Poincaré surfaces of section provide a revealing stroboscopic picture of the classical dynamics for a bound electron in a one-dimensional hydrogen atom perturbed by a very intense microwave field. Instead of using the usual position and momentum variables, I have transformed to the more convenient action–angle variables (I, θ) where the action, I, is proportional to the principal quantum number n by the Bohr–Sommerfeld quantization, and the angle variable, θ, is conveniently measured in units of radians/2π. The numerically calculated locations are shown for several classical orbits plotted once every period of the oscillating perturbation. In *a*, the perturbing field is below the threshold for the onset of chaotic ionization and the stroboscopic traces of the classical orbits lie along smooth, regular curves for initial conditions corresponding to highly excited hydrogen atoms with principal quantum numbers between $n=80$ and 100. When the perturbing field is increased above the threshold for chaotic ionization (*b*), many initial conditions lead to highly irregular, chaotic orbits which rapidly ionize. (Reprinted with permission from ref. 33.)

For example, measurements and calculations of the spectra of hydrogen atoms in strong static magnetic fields[28–30] have revealed relationships between the statistics of the energy level spacings and the predictions of the random matrix theory of nuclear physics[32]. In addition, detailed investigations of the electron dynamics in a hydrogen atom exposed to strong electromagnetic fields have shown how the quantum dynamics can mimic the classical chaos for limited times[33–34] and how quantum interference effects can suppress the chaotic classical dynamics by localizing the wavefunction[35–37] through a mechanism related to Anderson localization in solid-state physics.

Moreover, theory and experiment for both systems have exposed the importance of 'scarred' wavefunctions which are highly correlated with unstable classical periodic orbits[38]. Even though the classical description of the electron motion in a highly excited hydrogen atom in an intense microwave field or in a strong magnetic field may be fully chaotic, many quantum wavefunctions nevertheless seem to cling to the remnants of regularity represented by these unstable periodic orbits.

Highly excited atoms in strong magnetic fields

The Zeeman splitting of atomic energy levels by magnetic fields[39] has traditionally been a proving ground for new theoretical ideas and approximations in the development of quantum mechanics. For weak and moderate magnetic fields, the splitting is well described by quantum perturbation theory[40]. For example, in moderate magnetic fields the electron energy levels in hydrogen atoms have the regular sequence (Fig. 3*a*) that is predicted by the theory of the quadratic Zeeman effect[41]. In large magnetic fields, however, where the magnetic forces on the electron become comparable to the Coulomb binding fields, the conventional tools of quantum perturbation theory break down and the energy levels become 'irregular', as shown in Fig. 3*b*. This transition from regular to irregular spectra, as the corresponding classical system goes from regular to chaotic, was first conjectured by Percival[42] and Zaslavsky[43] in the 1970s, although this conclusion was presaged by Einstein[44] in 1917 when he remarked on the difficulty of assigning quantum numbers to the energy levels in nonintegrable systems.

For ground-state atoms this transition occurs for astronomically large fields ($\sim 10^4$ Tesla) which can only be realized in white dwarf and neutron stars. But as the Coulomb binding fields decrease rapidly as $1/n^4$ with increasing principal quantum number n, this new parameter regime where the classical mechanics is chaotic and the quantum spectrum is complex can be readily achieved using highly excited atoms with principal quantum numbers ranging from $n = 30$ to 40 in laboratory fields of 4–6 T. As a consequence, the energy spectrum of highly excited hydrogen atoms has emerged as an important model problem in this new field of quantum chaos.

Because of the complexity of the irregular energy spectrum for hydrogen atoms in strong magnetic fields (Fig. 3*b*) and for other model quantum systems that are classically chaotic, the spectra were first analysed with statistical methods that had been previously developed to characterize the complex, irregular energy-level spectra of excited nuclei[28–30]. Because the precise coupling between strongly interacting nucleons is not known and is presumed to be complicated, it was simply assumed that the statistical properties of the nuclear energy-level spacings would be indistinguishable from the distribution of eigenvalues of large matrices with randomly chosen matrix elements[32]. This random matrix theory predicts that the probability distributions for the spacings, s, of adjacent energy levels should be well approximated by the Wigner–Dyson distribution $P(s) \approx s \exp(-s^2)$, which provides an excellent description of the spacings of the measured energy levels in excited nuclei[32].

Although there are no unknown or random elements in the hamiltonians for these classically chaotic systems, the statistics of the energy-level spacings for these systems also agreed remarkably well with the specific predictions of the random matrix theory. This striking result suggests that the quantum dynamics of the strongly interacting nucleons in excited nuclei may share many features with the much simpler hydrogen atom in a strong magnetic field[32]. Nuclear physicists have been greatly interested by these results, and some have even proposed that these statistical properties of the energy distributions should form the definition of quantum chaos[32]. But this statistical 'structure' in energy-level spacings is only one of the many interesting properties of quantum systems that are classically chaotic.

The first experiment on highly excited atoms in strong magnetic fields to indicate that there was even more interesting structure in the spectrum than that described by the statistical theories were done by Garton and Tompkins[45] in 1969. They measured the photoabsorption spectrum by exposing barium atoms in strong magnetic fields to different wavelengths of light. When the photon energy of the light matched the excitation energy for a highly excited state, the production of excited states could be detected. Although the distribution of energy levels was expected to resemble well-stirred spaghetti (like the pattern shown in Fig. 3*b*), these experiments produced one of the first surprises of the quantum description of classically chaotic

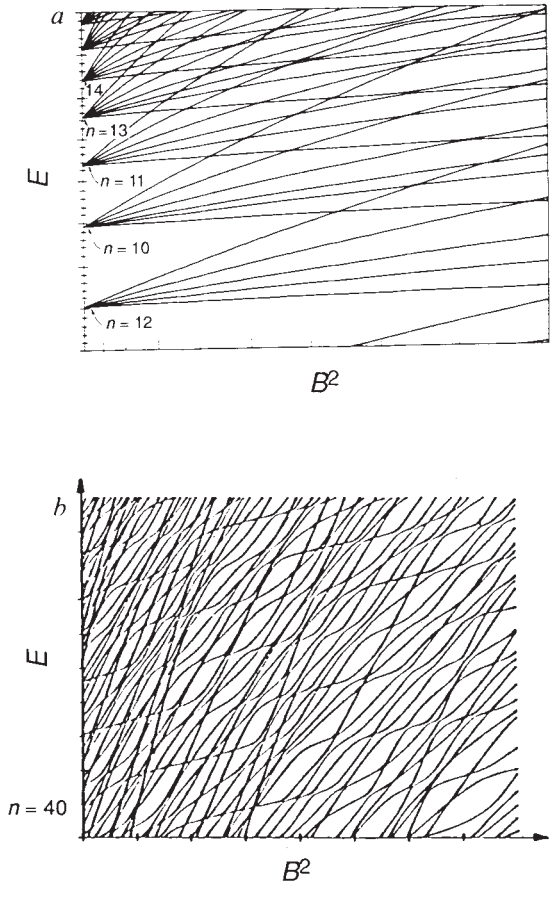

FIG. 3 The discrete, quantum-mechanical energy levels of a hydrogen atom in an external magnetic show a well studied symptom of 'quantum chaos'[28–30]. When the magnetic forces on the electron are much weaker than the Coulomb forces (*a*), the low-lying energy levels of the hydrogen atom with $n = 10 - 16$ in static magnetic fields have a regular spacing which increases with B^2 as predicted by the theory of the quadratic Zeeman effect. (This figure was provided by D. Kleppner.) *b*, For highly excited atoms with $n \geq 40$, magnetic fields of 5–6 T strongly perturb the electron energy levels. The classical dynamics in the combined Coulomb and magnetic fields is chaotic, and the calculated and measured spectra show irregular patterns resembling well stirred spaghetti. (Reprinted with permission from ref. 74.)

systems by exhibiting regular modulations of the photoabsorption cross section as a function of energy[45].

Because of the enormous number of quantum levels spanned by these early experiments, it was difficult to resolve the fine structure of the spectrum, let alone individual quantum levels. Higher-resolution measurements of photoabsorption in strong magnetic fields of highly excited hydrogen atoms[16-19] and of highly excited lithium atoms[20-22] provided a detailed picture of the rich and intricate structure of the spectrum. For example, Fig. 4*a* shows the measured photoabsorption spectrum for hydrogen atoms in a strong, 5.96-T magnetic field. The graph shows the laser-excitation probability from an $n = 2p$ state to high-lying Rydberg states with principal quantum numbers $n >$ 60 for laser photon energies $E < E_{IP}$ and into free-electron resonance states for $E > E_{IP}$, where E_{IP} is the ionization potential. This complex spectrum, representing the contributions of millions of individual energy levels, does not seem obviously regular. If, however, we plot the Fourier transform of this photoabsorption spectrum as a function of energy, then we find distinct peaks as a function of time, as shown by the dotted curve in Fig. 4*b*. For example, the original Garton-Tompkins oscillations correspond to a characteristic time, 2/3 the classical gyro-period of a free electron in the magnetic field, which gives rise to the largest peak in Fig. 4*b*. Many more peaks are clearly visible.

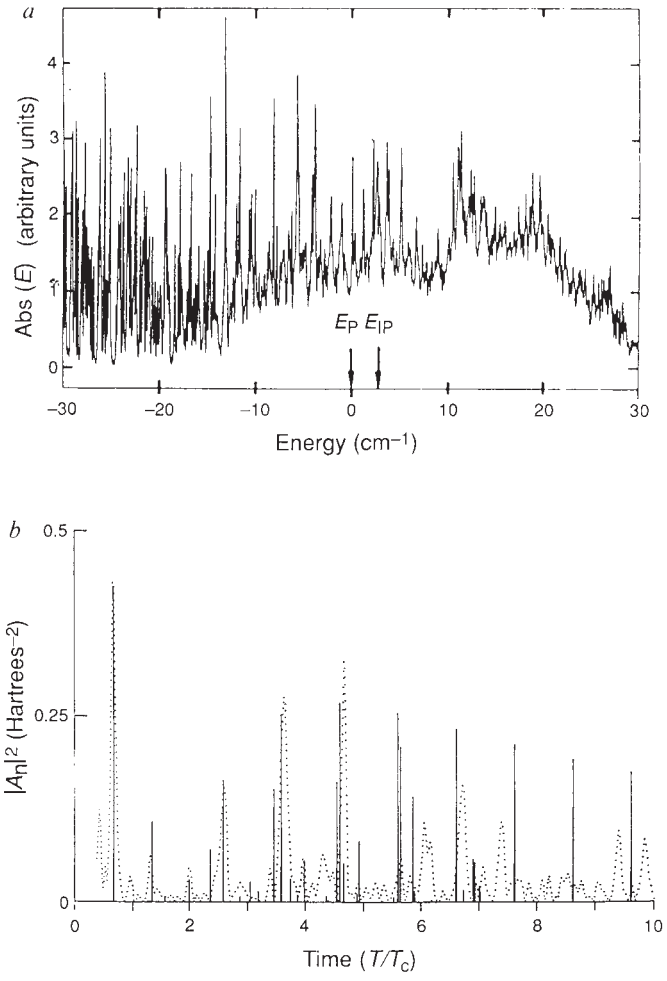

FIG. 4 *a*, The photoabsorption spectrum for a hydrogen atom in a strong, 5.96-T magnetic field as a function of laser energy for transitions near the ionization potential E_{IP}, which is shifted slightly above 0 in the presence of the strong magnetic field. If the experiment had unlimited resolution, then the spectrum for $E < E_{IP}$ would consist of an infinite sequence of sharp peaks located at the transition energies in the strongly perturbed atom and the heights of the peaks would provide a measure of the transition probability. This 'stick' spectrum is smoothed because of the finite experimental resolution and the natural line widths of the ionizing states for $E > E_{IP}$. Although this complex spectrum seems to have little structure, the reader may still discern a few Garton-Tompkins oscillations[16] with period ~10 cm^{-1} on the right side of the figure. (Reprinted with permission from ref. 18.) *b*, The Fourier transform of the photoabsorption spectrum in *a* (dotted curve), compared with semiclassical theoretical predictions based on the contributions from short periodic (or closed) orbits in the classical description of a highly excited hydrogen atom in a strong magnetic field. The locations of the peaks in the Fourier transform, which represent regular modulations of the quantum photoabsorption spectrum, correspond to the periods of these short orbits measured in units of the classical gyro-period of a free electron in the static magnetic field, T_c. (Reprinted with permission from ref. 46.)

Extensive theoretical work[18,19,28-30] has now shown that the characteristic times for these regular oscillations in the 'irregular' spectrum correspond to the periods of short, usually unstable, periodic orbits in the classical description of electron motion in combined magnetic and Coulomb fields, such as that shown in Fig. 1*b*. The solid lines in Fig. 4*b* indicate the results of theoretical calculations of the photoabsorption spectrum based on the contributions of interfering wavefunctions that propagate along the directions of these unstable classical orbits[46]. Moreover, additional high-resolution measurements of photoabsorption by lithium atoms in strong magnetic fields[21,22] show that these regular features in the spectrum associated with unstable classical periodic orbits clearly persist for positive energies where the typical classical electron trajectories are not only highly unstable but are not even bound.

Quantum 'scars' of classical orbits

Although the solutions of the time-dependent Schrödinger equation for this bounded quantum system cannot exhibit the local instability of chaotic classical trajectories, like the one shown in Fig. 1*a*, the eigenfunctions and eigenvalues nevertheless seem to be strongly correlated with the more regular classical periodic orbits, like the one in Fig. 1*b*. This remarkable property of the quantum description of classically chaotic systems was strikingly demonstrated in a simple model problem known as the 'stadium billiard'[38]. Figure 5*a* shows a typical classical trajectory of a particle moving without friction on a billiard table shaped like a stadium. This model system can be rigorously proven to be fully chaotic. Although there is a dense set of periodic trajectories, they are all unstable.

The quantum description is equivalent to solving for the electromagnetic modes in a cavity or the vibrations of a drumhead of this shape[47]. In spite of the irregular classical dynamics, many of the quantum eigenfunctions (or normal modes of vibration) have surprising structure with high amplitude along short, unstable periodic orbits. For example, Fig. 5*b* shows a contour map of the probability amplitude for a highly excited eigenstate of the stadium. Heller[38], who first observed these structured eigenstates in numerical calculations of the eigenfunctions of the stadium billiard, described them as having 'scars' of the classical periodic orbits, and provided theoretical arguments for the constructive quantum interference responsible for their appearance.

These 'scarred' wavefunctions were subsequently found in other classically chaotic quantum systems: they exist in the model systems corresponding to smooth molecular potentials[48], in numerically calculated wavefunctions for hydrogen atoms in strong magnetic fields[49] and in experimental measurements of the eigenmodes of microwave cavities with walls shaped like classically chaotic billiards[50]. The scars seem to be ubiquitous in quantum descriptions of classically chaotic systems, and this has important implications. In particular, the existence of these highly structured wavefunctions suggests that a reinterpretation of the correspondence principle is necessary, at least in this intermediate regime between the microscopic quantum and macroscopic classical worlds. For example, because of this 'localization' of some of the quantum wavefunctions to the vicinity of classical periodic orbits, statistical theories that are

applicable to the ergodic, classical systems may fail for the quantum.

Theoretical research into the mathematical connection between the classical periodic orbits and the spectral oscillations and scarred wavefunctions using the elaborate, semiclassical periodic orbit theory of Gutzwiller[51], which is based on the Feynman path-integral formulation[52] of quantum mechanics, is now beginning to bear much fruit. For example, using the unstable periodic orbits of the highly chaotic motion of two classical electrons orbiting the helium nucleus, Ezra *et al.* have succeeded in doing a semiclassical calculation of the energy levels of doubly excited states of helium atoms[53]. This striking illustration of the classical–quantum correspondence for classically chaotic systems finally provides the solution of a 70-year-old problem[54] which had originally led to the demise of the old Bohr–Sommerfeld quantum theory in the 1920s.

Microwave ionization of excited atoms

Einstein's 1905 theory of the photoelectric effect[55] stated that the ionization of an atom exposed to electromagnetic radiation requires the absorption of a photon with the right frequency (or energy) to make the transition from a bound state to the continuum. As a consequence, photoionization is expected to depend very sensitively on the radiation frequency but not on the intensity. But in 1974, Bayfield and Koch[23] reported a remarkable result from their experiments on microwave ionization of highly excited hydrogen atoms with principal quantum numbers near $n = 66$. They found that the ionization depended strongly on the intensity of the radiation and only weakly on the frequency. When the microwave fields were below a critical threshold, no ionization occurred. When the microwave fields exceeded a critical threshold, corresponding to 10–20% of the Coulomb binding field for these highly excited states, the atoms were rapidly ionized.

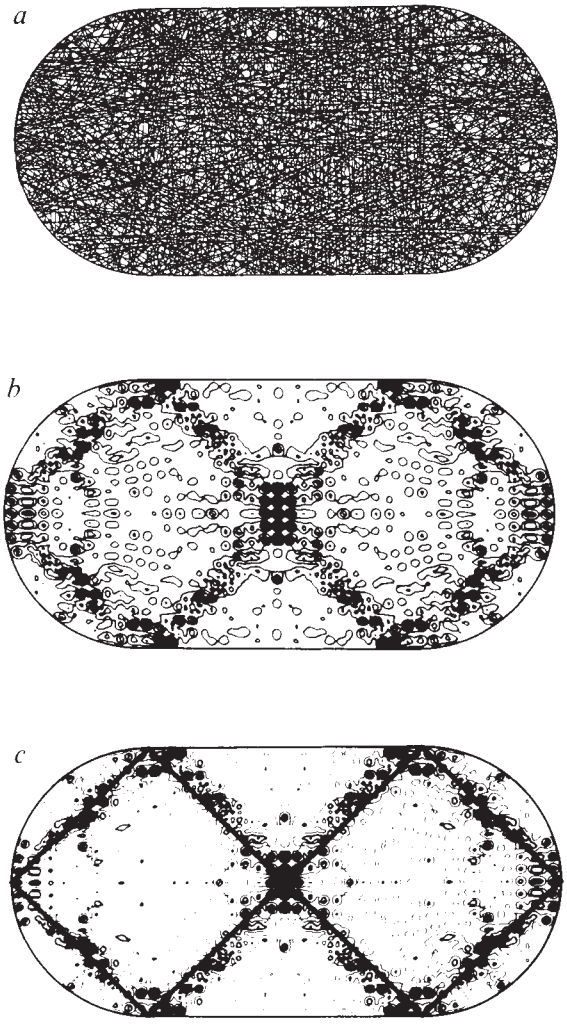

FIG. 5 *a*, Typical, chaotic classical trajectory for a 'stadium billiard'. Ten thousand bounces are shown of a highly irregular orbit, which never repeats and eventually will uniformly (ergodically) cover the area enclosed by the stadium walls. In stark contrast, highly excited quantum eigenfunctions often show regular structures that restrict the probability for finding the particle to bands along some of the unstable, periodic orbits in the stadium. A topographic map of one of these 'scarred' wavefunctions is shown in *b*, and the guiding unstable periodic orbit is superimposed in *c*. (Reprinted with permission from ref. 38.)

As the photon energy was only ~1% of the energy required to ionize these atoms, this novel ionization mechanism was presumably a high-order multiphoton process (one hundred photons or more). A quantum mechanical, time-dependent perturbative treatment of this system was not feasible because both the magnitude of the perturbation and the numbers of photons were large. In fact, the first successful theoretical description of these results was provided in 1978 by Leopold and Percival[56], who used the large quantum numbers in the experiment to justify a classical treatment of the Bohr atom in the oscillating electric field. By numerically solving the classical equations of motion they showed that the classical theory predicted ionization in good agreement with experiment.

The physical mechanism responsible for the classical ionization is the onset of chaos in this strongly perturbed nonlinear oscillator. In the absence of the perturbation, the classical equations of motion are integrable, and the bound electron motion is confined to a Kepler ellipse like the orbit of a planet about the Sun. But when the microwave perturbation is applied, the Kepler ellipse begins to wobble, precess and elongate, and when the perturbation exceeds a sharp threshold the electron escapes and the atom is ionized. For example, Fig. 2 illustrates this transition from regular, bounded motion to chaotic ionization in a one-dimensional classical model of a hydrogen atom in a strong oscillating field as the field is increased from below (Fig. 2*a*) to above (Fig. 2*b*) the threshold for widespread chaos.

Further confirmation[25] of this chaotic ionization mechanism was provided by experimental measurements of the threshold fields for the onset of microwave ionization over a wide range of excited states of hydrogen with principal quantum numbers from $n = 32$ to 90. Figure 6 shows a comparison of the experimental thresholds with the numerically calculated classical and quantum thresholds for the onset of chaotic ionization[31,33,34] in a one-dimensional model of the experiment. The threshold microwave fields, F, for the measured onset of ionization are plotted in scaled atomic units, n^4F, against the scaled microwave frequency, $n^3\Omega$, for many different initial quantum states and two different microwave frequencies, 9.9 and 36 GHz. For both frequencies, the classical predictions for the onset of chaotic ionization are in remarkably good agreement with the quantum ionization thresholds (both experimental and theoretical) as long as the microwave frequency, Ω, is less than the Kepler orbital frequency, $1/n^3$ in atomic units. These results clearly indicate that, although quantum mechanics cannot satisfy the strict definitions of classical chaos, the quantum dynamics may nevertheless mimic the chaotic classical ionization, at least on the limited timescales of these experiments.

For higher frequencies, $n^3\Omega > 1$, the classical and quantum thresholds start to diverge. This apparent breakdown of the correspondence principle was theoretically predicted by Casati *et al.*[37] who argued that the chaotic classical ionization should be suppressed by quantum interference effects related to the mechanism of Anderson localization in solid-state physics. As in the previous example of highly excited atoms in strong magnetic fields, these novel results for the interaction of intense

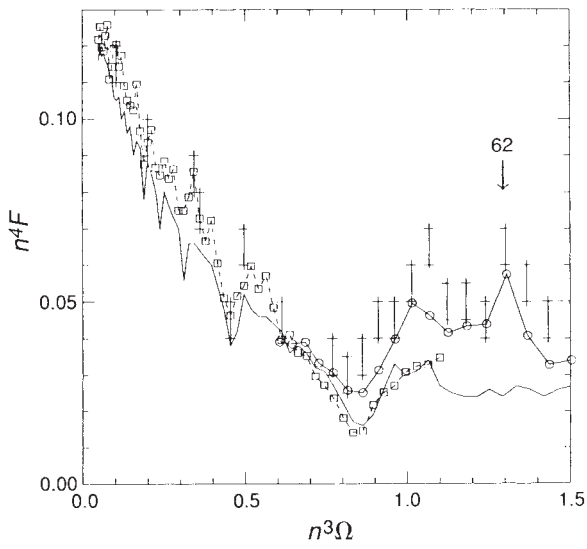

FIG. 6 Experimental measurements of the threshold microwave fields for the onset of ionization in scaled atomic units, $F_0 = n^4F$, are plotted as a function of the scaled microwave frequency, $\Omega_0 = n^3\Omega$, for highly excited hydrogen atoms with principal quantum numbers $n = 32$ to 90, exposed to a 9.92-GHz field[25] (□) and a 36 GHz field[26] (○). Each experimental data point indicates a different initial quantum state. For $\Omega_0 < 1$ these experimental results are in very good agreement with the classical predictions of the onset of chaotic ionization (solid curve) and the (less accurate) quantum calculations (crosses with large error bars) for a one-dimensional model of the experiment[33]. For higher scaled frequencies, $\Omega_0 > 1$, the experimental thresholds continue to show good detailed agreement with the quantum calculations but at fields much larger than the classical thresholds. The arrow indicates the initial state, $n = 62$, that is stabilized by the excitation of the 'scarred' wavefunction shown in Fig. 7. (Reprinted with permission from ref. 60.)

electromagnetic fields with matter demand a careful reassessment of the correspondence principle.

In particular, for this time-dependent problem, the classical–quantum correspondence depends on a timescale known as the 'break-time', t_B which is roughly determined by the energy-level spacing of interacting quantum states, $\Delta E \propto 1/t_B$, through the Heisenberg uncertainty principle[35–37]. Roughly speaking[57], for short times $t < t_B$, the quantum system cannot recognize the discrete nature of the interacting quantum states with typical energy spacing ΔE, and the quantum evolution of observable quantities such as the expectation of position and momentum may be well approximated by classical dynamics. For longer times, the quantum discreteness of the coupled states requires that the quantum evolution of observables be quasiperiodic rather than chaotic.

For experiments at low scaled frequencies ($n^3\Omega < 1$ in Fig. 6), many quantum states are strongly coupled by multiphoton processes of all orders, so the effective ΔE is small and the classical theory is a good approximation on the short timescales of the experiment. For higher frequencies, however, a dynamical selection rule restricts the coupling to relatively few quantum states that are close to resonance for single photon excitations[58,59]. This reduction in the density of coupled states decreases the break-time so that quantum interference effects can inhibit the classical chaotic ionization on the timescales of the experiment.

High-scaled-frequency experiments[24,26] have confirmed this prediction that the quantum system tends to be more stable against ionization than the classical. But the quantum excitation still seems to fluctuate considerably depending on the experimental parameters. For example, Fig. 6 shows that the quantum state with $n = 62$ is much harder to ionize than $n = 61$ or $n = 63$. Theoretical work on the physical mechanisms responsible for this striking fluctuation in the quantum transport again illustrates the important role of scarred wavefunctions. Specifically, Jensen *et al.*[60] showed that this enhanced stabilization in the quantum calculations is due to the selective excitation of a quantum wavefunction that is highly localized to the vicinity of an unstable periodic orbit in the classical phase space. A topographic map of this scarred wavefunction is superimposed on the corresponding classical phase space in Fig. 7. The quantum probability for this state is strongly peaked near an unstable periodic orbit and its associated stable and unstable manifolds. In contrast, the wavefunctions excited from $n = 61$ and $n = 63$ are extended throughout the chaotic region of the classical phase space in Fig. 7 and therefore ionize more readily.

Applications and new directions

Quantum mechanics has traditionally (and very successfully) dealt with problems involving weakly interacting or weakly perturbed microscopic systems. Strongly coupled or strongly perturbed systems in atomic, molecular, solid-state, nuclear and elementary particle physics represent a new and difficult regime for quantum mechanics, requiring new theoretical as well as experimental methods.

In the past six years, theoretical and experimental investigations of hydrogen atoms in intense microwave fields or highly excited hydrogen and lithium atoms in strong magnetic fields have been the principal focus of much of the research in quantum chaos. Despite the relative simplicity of these physical systems, remarkable and unexpected properties of strongly perturbed quantum systems have appeared which have required a careful reassessment of our understanding of the classical–quantum correspondence principle. For example, the chaotic ionization of highly excited hydrogen atoms has shown how the quantum

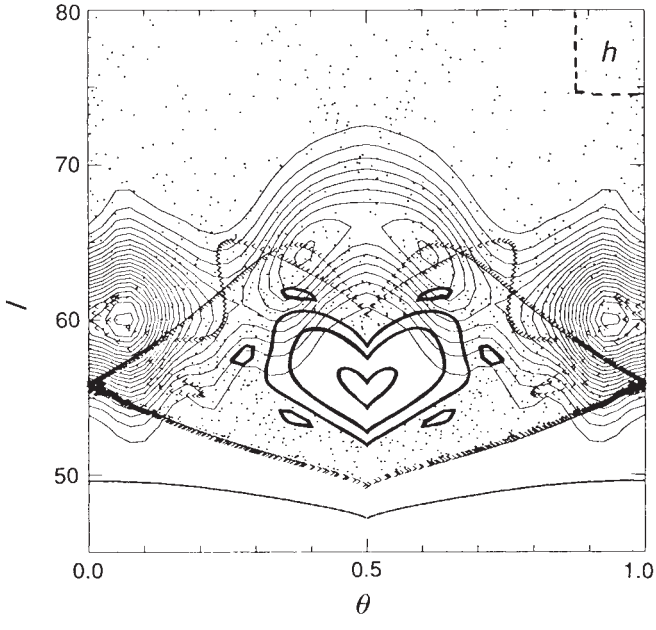

FIG. 7 A topographic map (light lines) of the highly localized, 'scarred' wavefunction that is responsible for the anomalous stability of $n = 62$ is superimposed on the corresponding classical Poincaré surface of section (dots and heavy lines) similar to those shown in Fig. 2. For the more experienced quantum chaologist, the relative size of Planck's constant for these experimental parameters is indicated in the upper right-hand corner, and the lines of arrows indicate the classical stable and unstable manifolds emanating from the unstable periodic orbit centred at $l = 56$ and $\theta = 0, 1$. (Reprinted with permission from ref. 60.)

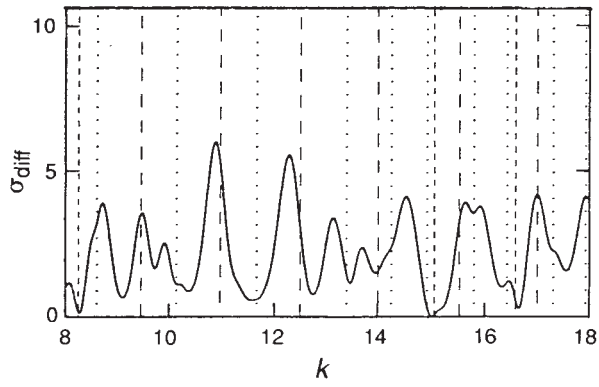

FIG. 8 The differential cross-section for the two-dimensional, elastic scattering of a plane wave from three perfectly reflecting discs, plotted as a function of incident wavenumber k. This scattering cross-section is only weakly correlated with the real parts of the resonance energies, indicated by the vertical broken lines, because the widths of the resonances are comparable to or greater than their separation. In this regime the irregular fluctuations of the scattering cross-section are reminiscent of the Ericson fluctuations in neutron scattering from heavy nuclei[63], the conductance fluctuations in small solid-state devices[69,71] and the large fluctuations in the quantum transport measured by the threshold fields for microwave ionization for $n^3\Omega > 1$ in Fig. 6. (Reprinted with permission from ref. 67.)

dynamics can mimic the chaotic classical dynamics for limited times[31,33,34] and the high-frequency stabilization of these Rydberg atoms has revealed the important role of quantum interference effects in localizing the quantum wavefunction[35–37], in close analogy with the mechanism of Anderson localization in solid-state physics. In addition, experimental measurements and theoretical calculations of the energy-level spectrum of highly excited atoms in strong, static magnetic fields have shown that the irregular spectrum for this simple quantum system with chaotic classical dynamics has the same statistical laws as the much more complicated and poorly understood spectrum of excited nuclei[32]. Finally, experiments on both physical systems have shown quantum wavefunctions that seem to have scars[49,60] associated with unstable classical periodic orbits embedded in the chaotic classical phase space.

The lessons learned from these studies of single hydrogen atoms in strong fields promise to have many important applications in different areas of physics and chemistry. For example, in nuclear physics a realistic model of the low-lying collective states of nuclei[61] (which is chaotic in a classical limit) has been found to have statistical distributions of energy-level spacings and transition amplitudes that are similar to those for the chaotic hydrogen atoms in strong magnetic fields. Moreover, in atomic physics it has been suggested[62] that the quantum mechanical scarring of unstable periodic orbits may provide a mechanism for the suppression of ionization of ground-state atoms in super-intense laser fields.

Another exciting direction is the extension of these new ideas to irregular, or chaotic, scattering processes[63]. Conventional quantum collision theory requires that the collisions be weak (so that perturbation theory can be applied) or that the collisions be very slow (adiabatic approximation) or fast (sudden approximation). If the collisions of electrons on atoms, atoms on molecules, molecules on surfaces, neutrons on nuclei or pions on protons are neither weak, nor slow, nor fast, then the scattering process may be very complex and difficult to describe. In the course of such a scattering event a collision complex is formed, the constituents rattle around, and the pieces fly apart. Chemists have already shown that the quantum description of this classically chaotic process can exhibit intricate interference associated with the unstable periodic orbits in the collision complex, reminiscent of the scars in bounded atomic systems[64–66]. Moreover, it has been shown that fluctuations in the collision cross-sections for electromagnetic waves in curved waveguides[67,68] (shown in Fig. 8) and for electrons in mesoscopic solid-state devices[69] obey the same statistical laws found empirically for the scattering of neutrons from compound nuclei[63].

Like the oscillations of the photoabsorption spectrum of hydrogen atoms in strong magnetic fields and the fluctuations in the threshold fields for the microwave ionization of highly excited hydrogen atoms for $n^3\Omega > 1$, these so-called Ericson fluctuations[63] in the scattering cross-sections seem to be intimately related to the classical properties of unstable periodic orbits. Many experimental and theoretical studies of these interconnections between classical and quantum physics are in progress[63–69]. For example, detailed comparisons of the classical, semiclassical and quantum theories with experimental measurements of the simplest inelastic and reactive atom–molecule collisions $D + H_2$ have recently been announced[70]. In solid-state physics the efforts to fabricate smaller and smaller electronic devices have led to the discovery that electron scattering in 'mesoscopic' wires with widths smaller than 1 μm produces 'universal conductance fluctuations', which are 'random' reproducible variations in the resistance or conductance of the wire[71]. These fluctuations even arise when the wires are so small that the electron collides only with the curved boundary of the wire[69]. As a final illustration, it has also been suggested that the scattering cross-sections of elementary particles, such as pions on protons, may exhibit Ericson fluctuations[72] due to the strong many-body interaction of the quark constituents. Since asymptotic freedom was discovered in the mid-1970s, most experimental emphasis has been on high-energy scattering, where the quarks are weakly coupled and perturbation theory can be applied[73], so this last extension of quantum chaos to the farthest boundaries of modern physics remains to be explored. □

Roderick Jensen is in the Department of Physics, Wesleyan University, Middletown, Connecticut 06457, USA.

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The structure of the *E. coli recA* protein monomer and polymer

Randall M. Story, Irene T. Weber* & Thomas A. Steitz

Department of Molecular Biophysics and Biochemistry, and Department of Chemistry and Howard Hughes Medical Institute at Yale University, New Haven, Connecticut 06511, USA

The crystal structure of the *recA* protein from *Escherichia coli* at 2.3-Å resolution reveals a major domain that binds ADP and probably single- and double-stranded DNA. Two smaller subdomains at the N and C termini protrude from the protein and respectively stabilize a 6_1 helical polymer of protein subunits and interpolymer bundles. This polymer structure closely resembles that of recA/DNA filaments determined by electron microscopy. Mutations in *recA* protein that enhance coprotease, DNA-binding and/or strand-exchange activity can be explained if the interpolymer interactions in the crystal reflect a regulatory mechanism *in vivo*.

THE *recA* protein (recA) has a pivotal role in homologous DNA recombination and DNA repair in *E. coli* and other eubacteria. The gene encoding recA was first shown in 1965 to be essential for genetic recombination and resistance to ultraviolet irradiation[1]. The 352-residue protein[2,3] encoded by this gene has a remarkable range of activities *in vitro* (for reviews, see refs 4–6). RecA protein alone catalyses the central steps of recombination: the pairing and strand exchange of homologous DNA molecules.

RecA protein polymerizes cooperatively and nonspecifically on DNA to form a helical filament that is the active species in the DNA-strand exchange and repressor-cleavage reactions. Filaments are formed by rapid polymerization 5′ to 3′ on single-stranded DNA or duplex DNA possessing a single-stranded gap[7]. Stable binding to duplex DNA is also observed, but this process is slow at neutral pH (ref. 8). Formation of active recA filaments requires ATP or an analogue such as ATP-γ-S[9]. Such filaments can then specifically bind homologous duplex DNA and promote a strand-exchange reaction[10]. They can also induce the cleavage of lexA (which leads to the SOS response[11]), umuD[12] and the repressor proteins of λ and other phages, binding these proteins and stimulating their intrinsic ability to self-cleave[13], thereby acting as a 'coprotease'.

Image reconstructions of electron micrographs have provided a low-resolution structure of the recA protein filament bound to single- or double-stranded DNA[14,15]. These filaments have a pitch of 85–100 Å, 6.1–6.2 monomers per turn, and a distinct polarity. The DNA in recA/DNA filaments is extended by ~150% relative to B-form DNA, and unwound to ~18.6 nucleotides (or base pairs) per turn[16]. The stoichiometry of binding is three nucleotides (or base pairs) per recA monomer[17]. Geometrical constraints require that the DNA must lie near the centre of the helical filament[14]. In the absence of DNA, recA protein exists in various states of aggregation, including pure protein polymers[18]. These polymers have a shorter pitch than the active recA/DNA filaments (~70 Å); refs 19, 20), but under certain conditions, such as high salt, they assume the higher pitch and have the ATPase and coprotease activities normally associated with the recA/DNA filament[21,22].

For a full understanding of recA protein function we need details of the structure of the recA filament because of its importance in recA activity. We have established and refined at 2.3 Å resolution the crystal structure of the recA protein that forms a recA polymer in the crystal. This polymer closely resembles the low-resolution structure of recA/DNA filaments seen in the electron microscope, and contains an extensive interface between subunits. The study of recA structure and function has been complicated by the interrelatedness of the

* Present address: Department of Pharmacology, Thomas Jefferson University, Philadelphia, Pennsylvania 19107, USA.