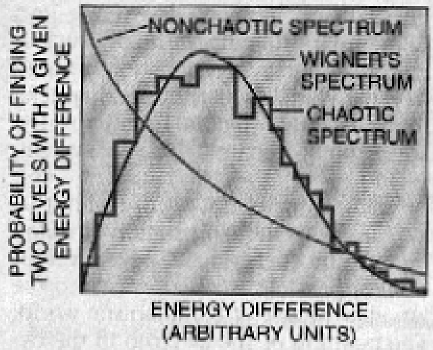


ENERGY SPECTRUM, or distribution of energy levels, differs markedly between chaotic and nonchaotic quantum systems. For a nonchaotic system, such as a molecular hydrogen ion (H_2^+), the probability of finding two energy levels close to each other is quite high. In the case of a chaotic system such as a Rydberg atom in a strong magnetic field, the probability is low. The chaotic spectrum closely matches the typical nuclear spectrum derived many years ago by Eugene P. Wigner.

drogen atom is described by a wave pattern. The electron cannot be pinpointed in space; it is a cloudlike smear hovering near the proton. Associated with each allowed energy level is a stationary state, which is a wave pattern that does not change with time. A stationary state corresponds quite closely to the vibrational pattern of a membrane that is stretched over a rigid frame, such as a drum.

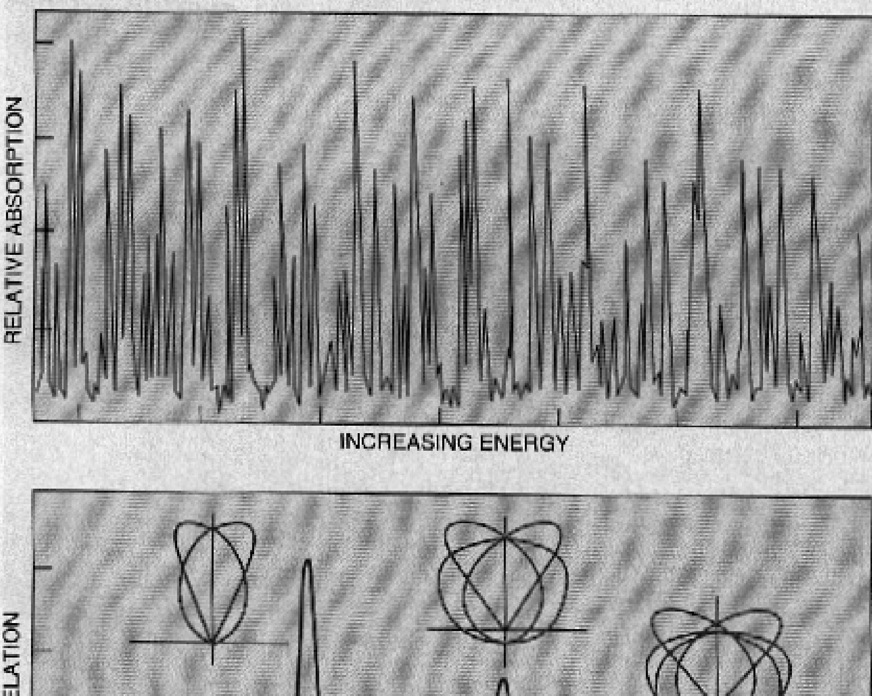
The stationary states of a chaotic system have surprisingly interesting structure, as demonstrated in the early 1980s by Eric Heller of the University of Washington. He and his students calculated a series of stationary states for a two-dimensional cavity in the shape of a stadium. The corresponding problem in classical mechanics was known to be chaotic, for a typical trajectory quickly covers most of the available ground quite evenly. Such behavior suggests that the stationary states might also look random, as if they had been designed without rhyme or reason. In contrast, Heller discovered that most stationary states are concentrated around narrow channels that form simple shapes inside the stadium, and he called these channels "scars" [*see illustration on opposite page*]. Similar structure can also be found in the stationary states of a hydrogen atom in a strong magnetic field [*see illustration on page 79*]. The smoothness of the quantum wave forms is preserved from point to point, but when one steps back to view the whole picture, the fingerprint of chaos emerges.

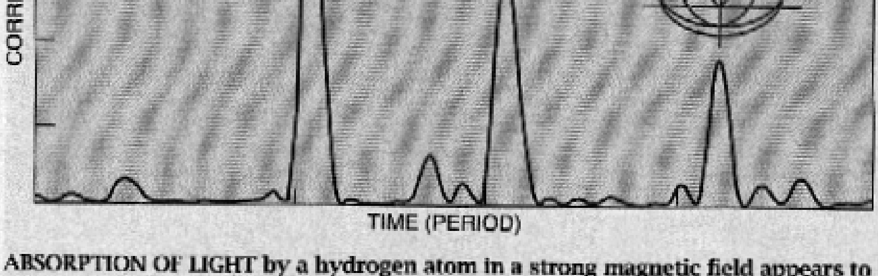
It is possible to connect the chaotic signature of the energy spectrum to ordinary classical mechanics. A clue to the prescription is provided in Einstein's 1917 paper. He examined the phase space of a regular system from box R and described it geometrically as filled with surfaces in the shape of a donut; the motion of the system corresponds to the trajectory of a point over the surface of a particular donut. The trajectory winds its way around the surface of the donut in a regular manner, but it does not necessarily close on itself.

In Einstein's picture, the application of Bohr's correspondence principle to find the energy levels of the analogous quantum mechanical system is simple. The only trajectories that can occur in nature are those in which the cross section of the donut encloses an area equal to an integral multiple of Planck's constant, h (2π times the fundamental quantum of angular momentum, having the units of momentum multiplied by length). It turns out that the integral multiple is precisely the number that specifies the corresponding energy level in the quantum system.

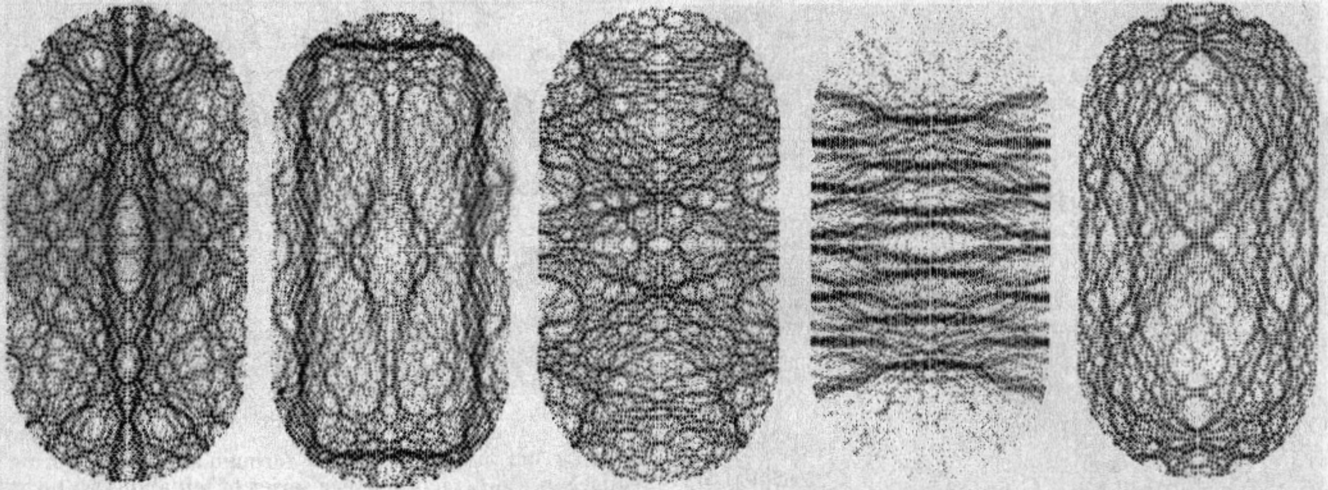
Unfortunately, as Einstein clearly saw, his method cannot be applied if the system is chaotic, for the trajectory does not lie on a donut, and there is no natural area to enclose an integral multiple of Planck's constant. A new approach must be sought to explain the distribution of quantum mechanical energy levels in terms of the chaotic orbits of classical mechanics.

Which features of the trajectory of classical mechanics help us to understand quantum chaos? Hill's discussion of the moon's irregular orbit because of the presence of the sun provides a clue. His work represented the first instance where a particular periodic orbit is found to be at the bottom of a difficult mechanical problem. (A periodic orbit is like a closed track on which the system is made to run; there are many of them, although they are isolated and unstable.) Inspiration can also be drawn from Poincaré, who emphasized the





ABSORPTION OF LIGHT by a hydrogen atom in a strong magnetic field appears to vary randomly as a function of energy (*top*), but when the data are analyzed according to the mathematical procedure called Fourier analysis, a distinct pattern emerges (*bottom*). Each peak in the bottom panel has associated with it a specific classical periodic orbit (*red figures next to peaks*).



PARTICLE IN A STADIUM-SHAPED BOX has chaotic stationary states with associated wave patterns that look less random than one might expect. Most of the states are concentrated around narrow channels that form simple shapes, called scars.

general importance of periodic orbits. In the beginning of his three-volume work, *The New Methods of Celestial Mechanics*, which appeared in 1892, he expresses the belief that periodic orbits "offer the only opening through which we might penetrate into the fortress that has the reputation of being impregnable." Phase space for a chaotic system can be organized, at least partially, around periodic orbits, even though they are sometimes quite difficult to find.

In 1970 I discovered a very general way to extract information about the quantum mechanical spectrum from a complete enumeration of the classical periodic orbits. The mathematics of the approach is too difficult to delve into here, but the main result of the method is a relatively simple expression called a trace formula. The approach has now been used by a number of investigators, including Michael V. Berry of the University of Bristol, who has used the formula to derive the statistical properties of the spectrum.

I have applied the trace formula to compute the lowest two dozen energy levels for an electron in a semiconductor lattice, near one of the carefully controlled impurities. (The semiconductor, of course, is the basis of the marvelous devices on which modern life depends; because of its impurities, the electrical conductivity of the material is halfway between that of an insulator, such as plastic, and that of a conductor, such as copper.) The trajectory of the electron can be uniquely characterized by a string of symbols, which has a straightforward interpretation. The string is produced by defining an axis through the semiconductor and simply noting when the trajectory crosses the axis. A crossing to the "positive" side of the axis gets the symbol +, and a crossing to the "negative" side gets the symbol –.

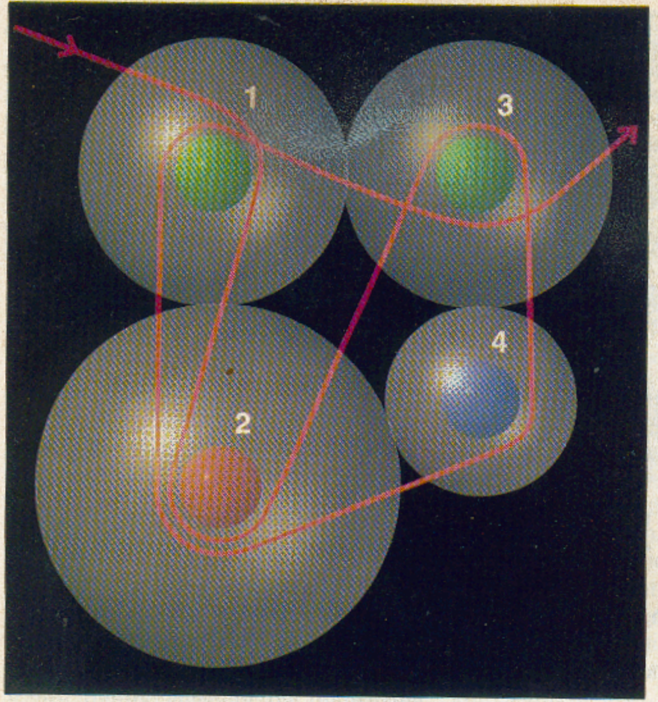
A trajectory then looks exactly like the record of a coin toss. Even if the past is known in all detail—even if all the crossings have been recorded—the future is still wide open. The sequence of crossings can be chosen arbitrarily. Now, a periodic orbit consists of a binary sequence that repeats itself; the simplest such sequence is (+ –), the next is (+ + –), and so on. (Two crossings in a row having the same sign indicate that the electron has been trapped temporarily.) All periodic orbits are thereby enumerated, and it is possible to calculate an approximate spectrum with the help of the trace formula. In other words, the quantum mechanical energy levels are obtained in an approximation that relies on quantities from classical mechanics only.

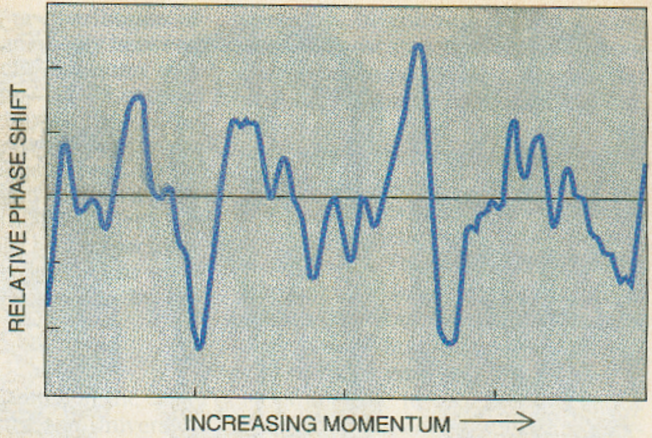
The classical periodic orbits and the quantum mechanical spectrum are closely bound together through the mathematical process called Fourier analysis [see "The Fourier Transform," by Ronald N. Bracewell; SCIENTIFIC AMERICAN, June 1989]. The hidden regularities in one set, and the frequency with which they show up, are exactly given by the other set. This idea was used by John B. Delos of the College of William and Mary and Dieter Wintgen of the Max Planck Institute for Nuclear Physics in Heidelberg to interpret the spectrum of the hydrogen atom in a strong magnetic field.

Experimental work on such spectra has been done by Karl H. Welge and his colleagues at the University of Bielefeld, who have excited hydrogen atoms nearly to the point of ionization, where the electron tears itself free of the proton. The energies at which the atoms absorb radiation appear to be quite random [*see upper part of bottom illustration on opposite page*], but a Fourier analysis converts the jumble of peaks into a set of well-separated peaks [*see lower part of bottom illustration on opposite page*]. The important feature here is that each of the well-separated peaks corresponds precisely to one of several standard classical periodic orbits. Poincaré's insistence on the importance of periodic orbits now takes on a new meaning. Not only does the classical organization of phase space depend critically on the classical periodic orbits, but so too does the understanding of a chaotic quantum spectrum.

So far I have talked only about quantum systems in which an electron is trapped or spatially confined. Chaotic effects are also present in atomic systems where an electron can roam freely, as it does when it is scattered from the atoms in a molecule. Here energy is no longer quantized, and the electron can take on any value, but the effectiveness of the scattering depends on the energy.

Chaos shows up in quantum scattering as variations in the amount of time the electron is temporarily caught inside the molecule during the scattering process. For simplicity, the problem can be examined in two dimensions. To the electron, a molecule consisting of four atoms looks like a small maze. When the electron approaches one of the atoms, it has two choices: it can turn left or right. Each possible trajectory of the electron through the molecule can be recorded as a series of left and right turns around the atoms, until the particle finally emerges. All of the trajectories are unstable: even a





TRAJECTORY OF AN ELECTRON through a molecule during scattering can be recorded as a series of left and right turns around the atoms making up the molecule (*left*). Chaotic variation (*above*) characterizes the time it takes for a scattered electron of known momentum to reach a fixed monitoring station. Arrival time varies as a function of the electron's momentum. The variation is smooth when changes in the momentum are small but exhibits a complex chaotic pattern when the changes are large. The quantity shown on the vertical axis, the phase shift, is a measure of the time delay.

minute change in the energy or the initial direction of the approach will cause a large change in the direction in which the electron eventually leaves the molecule.

The chaos in the scattering process comes from the fact that the number of possible trajectories increases rapidly with path length. Only an interpretation from the quantum mechanical point of view gives reasonable results; a purely classical calculation yields nonsensical results. In quantum mechanics, each classical trajectory of the electron is used to define a little wavelet that winds its way through the molecule. The quantum mechanical result follows from simply adding up all such wavelets.

Recently I have done a calculation of the scattering process for a special case in which the sum of the wavelets is exact. An electron of known momentum hits a molecule and emerges with the same momentum. The arrival time for the electron to reach a fixed monitoring station varies as a function of the momentum, and the way in which it varies is what is so fascinating about this problem. The arrival time fluctuates smoothly over small changes in the momentum, but over large changes a chaotic imprint emerges, which never settles down to any simple pattern [*see right part of illustration above*].

A particularly tantalizing aspect of the chaotic scattering process is that it may connect the mysteries of quantum chaos with the mysteries of number theory. The calculation of the time delay leads straight into what is probably the most enigmatic object in mathematics, Riemann's zeta function. Actually, it was first employed by Leonhard Euler in the middle of the 18th century to show the existence of an infinite number of prime numbers (integers that cannot be divided by any smaller integer other than one). About a century later Bernhard Riemann, one of the founders of modern mathematics, employed the function to delve into the distribution of the primes. In his only paper on the subject, he called the function by the Greek letter zeta.

The zeta function is a function of two variables, x and y (which exist in the complex plane). To understand the distribution of prime numbers, Riemann needed to know when the zeta function has the value of zero. Without giving a valid argument, he stated that it is zero only when x is set equal to $1/2$. Vast calculations have shown that he was right without exception for the first billion zeros, but no mathematician has come even close to providing a proof. If Riemann's conjecture is correct, all kinds of interesting properties of prime numbers could be proved.

The values of y for which the zeta function is zero form a set of numbers that is much like the spectrum of energies of an atom. Just as one can study the distribution of energy levels in the spectrum, so can one study the distribution of zeros for the zeta function. Here the prime numbers play the same role as the classical closed orbits of the hydrogen atom in a magnetic field: the primes indicate some of the hidden correlations among the zeros of the zeta function.

In the scattering problem the zeros of the zeta function give the values of the momentum where the time delay changes strongly. The chaos of the Riemann zeta function is particularly apparent in a theorem that has only recently been proved: the zeta function fits locally any smooth function. The theorem suggests that the function may describe all the chaotic behavior a quantum system can exhibit. If the mathematics of quantum mechanics could be handled more skillfully, many examples of locally smooth, yet globally chaotic, phenomena might be found.

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