Einstein’s Unknown Insight and the Problem of Quantizing Chaos

Chaotic systems were beyond the reach of an ingenious coordinate-invariant quantization scheme developed by Albert Einstein, and to this day, their quantization remains a challenge.

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At the 11 May 1917 meeting of the German Physical Society, Albert Einstein, then a professor at the University of Berlin, presented the only research paper of his career that was written on the quantization of energy for mechanical systems. The paper contained an elegant reformulation of the Bohr–Sommerfeld quantization rules of the old quantum theory, a rethinking that extended and clarified their meaning. Even more impressive, the paper offered a brilliant insight into the limitations of the old quantum theory when applied to a mechanical system that is nonintegrable—or in modern terminology, chaotic. Louis de Broglie cited the paper in his historic thesis on the wave properties of matter, as did Erwin Schrödinger in the second of his seminal papers on the wave equation for quantum mechanics. But the 1917 work was then ignored for more than 25 years until Joseph Keller independently discovered the Einstein quantization scheme in the 1950s. Even so, the significance of Einstein’s contribution was not fully appreciated until the early 1970s when theorists, led by Martin Gutzwiller, finally addressed the fundamental difficulty of semiclassically quantizing nonintegrable Hamiltonians and founded a subfield of research now known as quantum chaos.

Even today, Einstein’s insight into the failure of the Bohr–Sommerfeld approach is unknown to the large majority of researchers working in quantum physics. It seems appropriate, in this centennial of Einstein’s miracle year, to put the achievement of his obscure 1917 paper in a modern context and to explain how he identified a simple criterion for determining if a dynamical system can be quantized by the methods of the old quantum theory.

Motivation

Einstein’s paper was titled “On the Quantum Theorem of Sommerfeld and Epstein.” In his title, Einstein was acknowledging physicist Paul Epstein, who had written a paper relating the Sommerfeld rule to the form of the constants of motion. Epstein’s name has not survived in the context of the Sommerfeld rule, and the quantization condition discussed by Einstein is now referred to as either Bohr–Sommerfeld or WKB (Wentzel-Kramers-Brillouin) quantization.

The 1917 article was written shortly after Einstein completed his groundbreaking work on the quantum theory of radiation in which he introduced the famous A and B coefficients (see the article by Daniel Kleppner, PHYSICS TODAY, February 2005, page 30). Einstein had come back to the quantum theory after focusing intensely from 1911 through 1915 on the theory of general relativity. His deep involvement with general coordinate transformations and curved-space geometry likely motivated him to search for a coordinate-independent formulation of the rules of the old quantum theory.

Einstein begins his paper by saying that for one mechanical degree of freedom the quantization condition is clearly

\[
\int_0^T p \, dq = \int_0^T \frac{dq}{dt} \, dt = n \hbar,
\]

(1)

where \( q \) is a position coordinate, \( p \) is the associated momentum, \( \hbar \) is Planck’s constant, and the time integral is over one period \( T \) of the one-dimensional bound motion. In higher dimensions, bound motion is not necessarily periodic, but for bound separable motion—that is, bound motion for which each coordinate–momentum pair is independent—Sommerfeld had proposed a straightforward generalization:

\[
\int_0^T p_i \, \frac{dq_i}{dt} \, dt = n_i \hbar \quad i = 1, \ldots, d,
\]

(2)

where \( d \) is the number of degrees of freedom, and \( T_i \) is the period of the motion in each of the \( d \) separable coordinates. Einstein comments:

Notwithstanding the great successes that have been achieved by the Sommerfeld–Epstein extension of the quantum theorem for systems of several degrees of freedom, it still remains unsatisfying that one has to depend on the separation of variables . . . because it probably has nothing to do with the quantum problem per se . . . the individual products \( dp_i \, dq_i \) in a system of several degrees of freedom . . . are not invariants, therefore the quantization condition, [equation 2], has no invariant meaning.

He then describes a “small modification” that allows a coordinate-independent formulation of the quantization rules.

Einstein quantization

Einstein begins with a point emphasized by Henri Poincaré at the 1911 Solvay Congress: For a dynamical system, \( \sum p_i \, dq_i \) is invariant under coordinate transformations, and
hence the line integral \( \int \mathbf{p} \cdot d\mathbf{q} = \int \mathbf{p} \cdot d\mathbf{q} \) is also invariant. The integral is equal to the phase space action \( S \) of classical mechanics

\[
S(E, \mathbf{r}, \mathbf{r}') = \int_0^t L \, dt' - Et, \tag{3}
\]

where \( L \) is the usual Lagrangian of a mechanical system, \( E \) is the energy, and \( \mathbf{r} \) and \( \mathbf{r}' \) are the final and initial points of the trajectory, which requires a time \( t \) to traverse.

Because \( \nabla S = \mathbf{p}(\mathbf{r}) \), the momentum at \( \mathbf{r} \), one is tempted to regard \( \mathbf{p}(\mathbf{r}) \) as the momentum field of the trajectory, generated by taking the gradient of the function \( S(E, \mathbf{r}, \mathbf{r}') \). As is familiar from electrostatics, the line integral between two points of the gradient of a function is independent of the path taken between the points. As a consequence, all such integrals over a closed loop vanish. However, the “function” \( S \) and its gradient are not single-valued because, as shown in figure 1, typical trajectories for bound motion loop back on themselves and return to a neighborhood of the point \( \mathbf{r} \). Indeed, the neighborhood is typically visited an infinite number of times.

Einstein points out that when the motion has certain properties, which will be specified in the next section, the action \( S \) may be usefully viewed as a function on a \( d \)-torus, the \( d \)-dimensional analogue of a doughnut. On that space, the gradient of the action is single-valued and the momentum field of the trajectory, \( \mathbf{p}(\mathbf{r}) = \nabla S \), is uniquely defined. Nonetheless, the line integral \( \int \mathbf{p} \cdot d\mathbf{q} \) does not vanish for all closed loops on the torus; instead, as Einstein observes, exactly \( d \) independent loops—algebraically independent vectors—give a specific nonzero value to the line integral (see figure 2). The values of the coordinate-invariant integrals depend on the energy of the dynamical system, so by demanding that each such integral be quantized, one arrives at an implicit formula for the quantized energy levels of the system without reference to specific coordinates or to separability of the motion. Thus, Einstein proposes the generalized quantization rule

\[
\oint_{C_i} \mathbf{p} \cdot d\mathbf{q} = nh \quad i = 1, \ldots, d, \tag{4}
\]

where the \( C_i \) are \( d \) independent closed loops of a torus in \( d \) dimensions, and the \( n \) are the quantum numbers associated with the energy levels of the system.

Einstein illustrates his construction with the example of a point mass moving under the influence of a general central force—that is, with a potential energy that depends only on the radial distance from the center—in the plane perpendicular to the particle’s conserved angular momentum. An electron moving around a hydrogen nucleus is an example. Such systems are separable in polar coordinates and could be solved by using the generalized Sommerfeld condition, equation 2; Einstein, however, found them a convenient example to illustrate his approach.

Under the conditions specified in Einstein’s example, any mass with nonzero angular momentum will revolve around the center while oscillating in radial distance between its inner turning radius \( r_i \) and its outer turning radius \( r_o \). As long as the force law is not exactly proportional to \( 1/r^2 \), or \( r \), the mass’s orbit will typically not close on itself: In astronomical terminology, it will precess. Einstein would have been aware of that fact from his work on the relativistic theory of the precession of the orbit of Mercury. As a consequence of the precession, a single orbit will, after many revolutions, define a momentum vector “field” everywhere in the annular region between the inner and outer turning points, as illustrated in figure 2a.

Inspection of the orbit reveals that the momentum vector has exactly two possible values at each point in the allowed region. They correspond to the opposite values of the radial momentum that occur when the orbit passes through the point heading outward or inward. A different initial condition for the trajectory, as long as the angular momentum is unchanged, would define the same vector field, so the double-valued field is unique. Now, Einstein says, one can just as well regard the red vectors of figure 2a as living on the top surface of a doughnut and the blue vectors as lying on the bottom surface (see figure 2b). That is, one can think of the momentum as being single-valued on a torus. Given the force law and conserved angular momentum, one can calculate the momentum field everywhere on the torus and hence can compute any loop integral of the type that appears in equation 4. Note here a crucial point: In the Sommerfeld rule, the integrations follow a trajectory, but the loop integrals of equation 4 may be evaluated along any convenient set of independent loops.

For the central-force case considered by Einstein, one of the loop integrals is particularly simple. Consider a loop that, on the figure-2a annulus, travels around the center in a circle just outside the inner turning radius. The momentum \( \mathbf{p} \) must be purely azimuthal on that loop because the radial momentum is zero at the turning radius. By choice, \( d\mathbf{q} \) is azimuthal so the loop integral is just \( p(2\pi r) = 2\pi L \), where \( L \) is the angular momentum of the motion. Equation 4 says that quantization is achieved by setting \( 2\pi L = nh \). In other words, \( L = nh \), the familiar Bohr rule for the quantization of angular momentum for an arbitrary central force law. The second loop integral will quantize the energy of the motion and its precise form will depend on the particular force law.

**The remarkable insight**

Based on what I’ve discussed to this point, Einstein’s paper can be regarded as an elegant improvement on the Bohr–Sommerfeld quantization rules, but not necessarily as a work containing a deep physical insight. In the fourth section of his paper, however, Einstein elucidates the na-
The latter case, the momentum an infinite number of different momentum directions. In example. He then remarks type (b) passes through an infinite number of different momentum directions, and an orbit of figure

Einstein quantization rule, equation 4 in the text, requires that the momentum integrated around each of two independent loops on the torus yields an integer times Planck's constant h. The figure indicates two appropriate loops, labeled C1 and C2.

A modern perspective
To clarify the relationship between Einstein's type (a) and type (b) motion and what is now called regular and chaotic motion, one can turn to dynamical billiards, which are paradigms for the study of classical and quantum chaos. A billiard is a 2D region of space in which a point mass moves freely between perfectly reflecting walls. The dynamics are completely determined by the shape of the boundary and the law of specular reflection.

In the central-force example that Einstein considered,
angular momentum is conserved. A billiard with the same property is the circular billiard of radius $R$. In principle, if a particle in the circular billiard were launched with precisely the right angle of incidence to the boundary, it would execute a closed periodic orbit. For example, a particle launched at 45° to the boundary would produce a square-shaped orbit. But it would be practically impossible to start a particle with an appropriate angle of incidence—in technical terms, closed periodic orbits have zero measure in phase space. Generic “quasiperiodic” orbits fill an annular region between the boundary and an inner caustic as shown in figure 3a. Each quasiperiodic orbit passes in exactly two directions through any neighborhood in the allowed region of motion, just as in the central-force example presented earlier. Thus, the circular billiard can be quantized, rather accurately in fact, by the method developed by Einstein and refined by Keller as detailed in the next section.

By way of contrast, consider trajectories in the so-called stadium billiard shown in figure 3b: All initial conditions except a set of zero measure lead to chaotic motion. Figure 3b indicates that every neighborhood is traversed in an infinite number of directions; the billiard allows only Einstein’s type (b) motion. Based on the theory of the Hamiltonian transition to chaos developed in the 1940s, 1950s, and 1960s by Andrei Kolmogorov, Vladimir Arnold, Jürgen Moser, and others, a generic billiard such as the quadrupole shown in figures 3c and 3d exhibits a mixture of regular and chaotic motion. Some initial conditions lead to type (a) motion and others to type (b), a situation called mixed dynamics. For mixed dynamics, the subset of quantum levels corresponding to regular motion can be quantized by the Einstein method, now known as the Einstein-Brillouin-Keller or EBK method. The subset corresponding to the chaotic region of phase space cannot be quantized by any analytic method, although techniques do exist for finding the contribution of the chaotic states to the density of states and other related quantities. A well-established technique known as the Weyl expansion shows that, to leading order in the system size, the same density of quantum energy levels exists for classically chaotic systems, such as the stadium billiard, as for integrable systems, such as the circular billiard. Therefore, the question arises: Why can’t the chaotic levels be found by some version of the Bohr–Sommerfeld approach? Einstein’s insight will reappear as the answer to this question.

**Keller’s modification**

Einstein’s work preceded the Schrödinger equation by eight years, and Einstein had no way of knowing that his quantization condition was essentially a means to find the eigenvalues of a wave equation. I have found no record that he reconsidered his approach after the wave equation was discovered.

For motion in a single dimension, the Bohr–Sommerfeld quantization rule can be derived by using the WKB ansatz familiar from undergraduate quantum mechanics. Specifically, one inserts into the 1D Schrödinger equation a wavefunction of the form

$$\psi(x) = A(x) e^{i \int_{x_0}^{x} p(x') dx'} + B(x) e^{-i \int_{x_0}^{x} p(x') dx'},$$

where $p(x) = \sqrt{2m(E - V(x))}$ is the local momentum in the potential $V(x)$, which is assumed to be slowly varying, and $x_0$ is a classical turning point of the potential. By insisting that the wavefunction be single-valued, one obtains the Bohr–Sommerfeld quantization condition, equation 1. Use of the so-called connection formula yields a corrected condition that includes the zero-point energy.

The EBK quantization formula may be viewed as arising from a higher-dimensional version of the WKB
For the simple case of the circular billiard, one needs only two terms in equation 6. Moreover, the two amplitudes are equal, \( A_1 = A_2 = A(x, y) \), and so one needs to determine the three functions \( S_1, S_2, \) and \( A \). The condition that the wavefunction vanish on the boundary implies that \( kS_1 = kS_2 = \pi \) there (the waves destructively interfere) and that the rays \( \nabla S \), speculatively reflect into the rays \( \nabla S_2 \). Figure 4 displays functions \( S_1 \) and \( S_2 \) that satisfy the stated requirements.

The final condition on the wavefunction is that it be single-valued. That requirement will not be met for an arbitrary value of the wave vector \( k \); it will only hold true if

\[
k \oint_C \nabla \cdot d\mathbf{q} = 2\pi n_i + \pi/2 m_i,
\]

which is the Einstein quantization condition with a small modification on the right-hand side—an additional phase shift that is an integer multiple of \( \pi/2 \). In 1958, Keller derived equation 7 from the equation-6 ansatz without any knowledge of Einstein’s 1917 paper.

The additional phase shift is due to leakage of the wavefunction into classically forbidden regions. It is independent of the value of the quantum number \( n \), and depends only on the number of turning points—that is, encounters with a caustic or boundary—in the real-space projection of the loop \( C \). Of course, Einstein could not have anticipated the correction since it arises from the failure of semiclassical theory near a turning point. In sum, Einstein’s topological quantization condition, with Keller’s minor improvement, is correct in the limit of short wavelength, if solutions of the WKB/EBK form exist.

The failure of EBK

Where is the problem of chaotic motion lurking in the EBK procedure? It is hidden in a very subtle place: The sum in equation 6 must have a finite number of actions \( S_i(x, y) \). But, as discussed in the caption of figure 4, if the motion is on a billiard that generates only Einstein’s type (b) motion, then the number of terms in any would-be EBK solution is infinite; no solution of the equation-6 form can be constructed. If the billiard generates a mixture of type (a) and type (b) motion, as for the quadrupole billiard shown in figure 3, then EBK solutions can be found, but some perfectly good solutions of the Schrödinger equation are not of the EBK form.

The EBK expansion seems innocent enough: Why does it sometimes fail and sometimes succeed? The reason is that the EBK procedure assumes that the wavefronts move in straight lines for distances much larger than the wavelength. That assumption goes into the derivation of the Hamilton–Jacobi and continuity equations once the EBK ansatz is inserted into the Schrödinger equation.

Intuitively, one can think of the EBK solutions as consisting of a sum of waves that superpose to form a standing wave. The number of waves in the superposition is independent of wavelength, and each superposing wave locally looks like a plane wave—that is, it has straight wavefronts on the scale of the wavelength. But there is no reason to expect that all of the solutions to the Schrödinger equation will satisfy that smoothness condition; only for certain very special billiard shapes are all solutions smooth in that sense. Those special shapes are precisely those, such as the circular billiard, with only type (a) motion.

For any two billiard shapes with the same area, there exist, to leading order, the same number of standing-wave patterns. But many of those patterns are not smooth in the EBK sense; their wavefronts bend and twist on the scale...
of a wavelength. Those are the chaotic solutions and they must be found numerically. Figure 5 shows an example of such a solution. In fact, the numerical solutions essentially come from superposing a number of smooth waves that grows inversely with the wavelength. The results are “turbulent” standing-wave patterns, such as the one shown in the figure. The fraction of chaotic solutions is just the fraction of phase space in which Einstein’s type (b) motion occurs.

**Einstein’s insight redux**

The 1917 paper of Einstein’s was cited during the 1920s by such luminaries as de Broglie and Schrödinger. Indeed, Schrödinger commented in his initial work on the wave equation:

> The framing of the quantum conditions [in Einstein’s 1917 paper] is the most akin, out of all the earlier attempts, to the present one.

Many early quantum texts also cited Einstein’s 1917 work. But nothing indicates that anyone understood the difficulty Einstein had identified, that of quantizing chaos. The paper then appears to have been forgotten for roughly 25 years, until Keller cited it in connection with his own independent derivation of the quantization rule. Keller relates that he heard of the Einstein paper from Fritz Reiche at New York University. Reiche had previously succeeded Einstein as a professor at the University of Berlin. Keller’s works in the late 1950s and early 1960s do not mention the potential problem with type (b) motion and give the impression that the method presented is of general applicability, though in later publications Keller makes the limitations of the method clear.4

Ian Percival reintroduced the physics community to Einstein’s work in a 1973 paper emphasizing that a generic system should have regular and irregular (chaotic) levels.5 Percival coined the term Einstein-Brillouin-Keller quantization for equation 7, the corrected form of Einstein’s condition. By 1971, although he was unaware of Einstein’s work, Gutzwiller had come to understand that it is not possible to use a Bohr–Sommerfeld type of quantization to deal with chaotic systems. He introduced an entirely new semiclassical approach that abandoned the attempt to find individual chaotic states. Instead, his approach yielded an equation to calculate the density of states of a chaotic system from knowledge of the unstable periodic orbits of the system.6 Much beautiful work has gone into refinements of Gutzwiller’s approach, which has been successfully applied to systems in atomic and condensed matter physics.

Gutzwiller’s work showed that despite the absence of a Bohr–Sommerfeld or EBK quantization scheme for chaotic systems, strong classical–quantum correspondences exist even in chaotic systems. Those correspondences have inspired a new interdisciplinary field of quantum physics, unhappily known as quantum chaos theory. The name is unfortunate because linear quantum systems don’t exhibit exponential sensitivity to initial conditions—the hallmark of classical chaos. Nonetheless, the search for semiclassical approximations and classical insights into “chaotic” quantum systems is a lively and useful endeavor that has flourished now for over three decades.7

Although Einstein’s antipathy to certain aspects of modern quantum theory is well known, there appears to be a renewed appreciation this year of his seminal contributions to quantum physics. With his introduction of the photon concept in 1905, his clear identification of wave–particle duality in 1909, his founding of the quantum theory of radiation in 1917, and his treatment of the Bose gas and its condensation in 1925, Einstein laid much of the foundation of the theory. He commented to Otto Stern, “I have thought a hundred times as much about the quantum problems as I have about general relativity.
We should add to his list of illustrious achievements another advance, modest on the scale of his genius, but brilliant by any other standard: the first identification of the problem of quantizing chaotic motion.

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References