POSTMODERN QUANTUM MECHANICS

Recent progress in semiclassical theory has overcome barriers posed by classical chaos and cast light on the correspondence principle. Semiclassical ideas have also become central to new experiments in atomic, molecular, microwave and mesoscopic physics.

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Postmodern movements are well known in the arts. After a major artistic revolution, and after the "modern" innovations have been assimilated, the threads of premodern thought are always reconsidered. Much of value may be rediscovered and put to new use. The modern context casts new light on premodern thought, which in turn shades perspectives on modernism.

Robert Harris at the University of California at Berkeley coined the term "postmodern quantum mechanics" to describe the keen new interest in semiclassical approximations. These approximations have their roots in the premodern old quantum theory. Semiclassical methods have occupied a niche in the modern era, but lately their evolution has taken a dramatic turn with the confrontation of their nemesis: classical chaos.

It is not widely understood that classical chaos has prevented the broad application of semiclassical ideas and techniques. Semiclassical methods are built on classical trajectories; if these are extremely complex, the semiclassical approximations may become inaccurate, difficult to compute or even ill defined. Chaos kept Bohr, Kramers, Heisenberg and Born from quantizing the helium atom, although they were not aware that chaos was to blame. Among physicists, only Einstein knew that what he called "type B" (chaotic) classical motion would not yield to the old quantization methods. He published a paper pointing this out in 1917, but it was ignored.[1] In the last 10 to 15 years it has been recognized that most classical dynamical systems, including helium, can behave chaotically. What good is a semiclassical theory that cannot handle chaos?

The issue of semiclassical approximations to chaos was confronted for the first time when Martin Gutzwiller[2] derived his semiclassical "trace formula" for the eigenvalues of a chaotic system in 1970. His result reopened the premodern agenda and marked the beginning of the postmodern era.

Theory and experiment interact strongly in the postmodern investigations. The mesoscopic world, caught between classical and quantum behavior, is the focus of much research. Here semiclassical ideas are a necessity. Many new experiments with excited atomic and molecular systems directly probe the realm of high quantum numbers or classically chaotic motion.

The quantum and classical realms are related by the connections that exist between wave phenomena and geometric ray paths. These connections are common to many fields, and essentially identical problems exist in quantum mechanics, optics, acoustics, seismology, oceanography, plasma physics and microwave physics. Some of these fields (for example, optics) far surpass quantum mechanics in the use of geometrical paths as the backbone for understanding. In many areas of wave physics, the geometrical limit has always been regarded simply as a useful approximation to the true wave behavior.

In quantum mechanics, nothing is quite so simple. Controversy surrounds the semiclassical limit. Mathematical questions of wave–ray asymptotics are intertwined with questions of quantum measurement theory, the Copenhagen interpretation, the correspondence principle and even the completeness of quantum mechanics. These issues sharpen the debate but often obscure the technical question of the semiclassical limit to quantum mechanics. Much of the recent controversy is sparked by issues of chaos: Can quantum mechanics give classical chaos as a limiting behavior? Can classical chaos be successfully semiclassically quantized? Are the two questions different? What is "quantum chaos," or does it even exist?[3] In this article we will sidestep the philosophical debate and focus on the issues of useful approximations and physical insight.

When presented with the results of a large quantum calculation, Eugene P. Wigner once said: "It is nice to know that the computer understands the problem. But I would like to understand it, too."[4] It is extremely difficult to visualize or to calculate the movement of a quantum wave in six dimensions, but easy to imagine or calculate trajectories for two electrons moving around a helium nucleus. Unavoidably, we think classically about systems of more than a couple of particles. It would be splendid if most of the physics of such problems could be calculated with classical mechanics and a few rules. That

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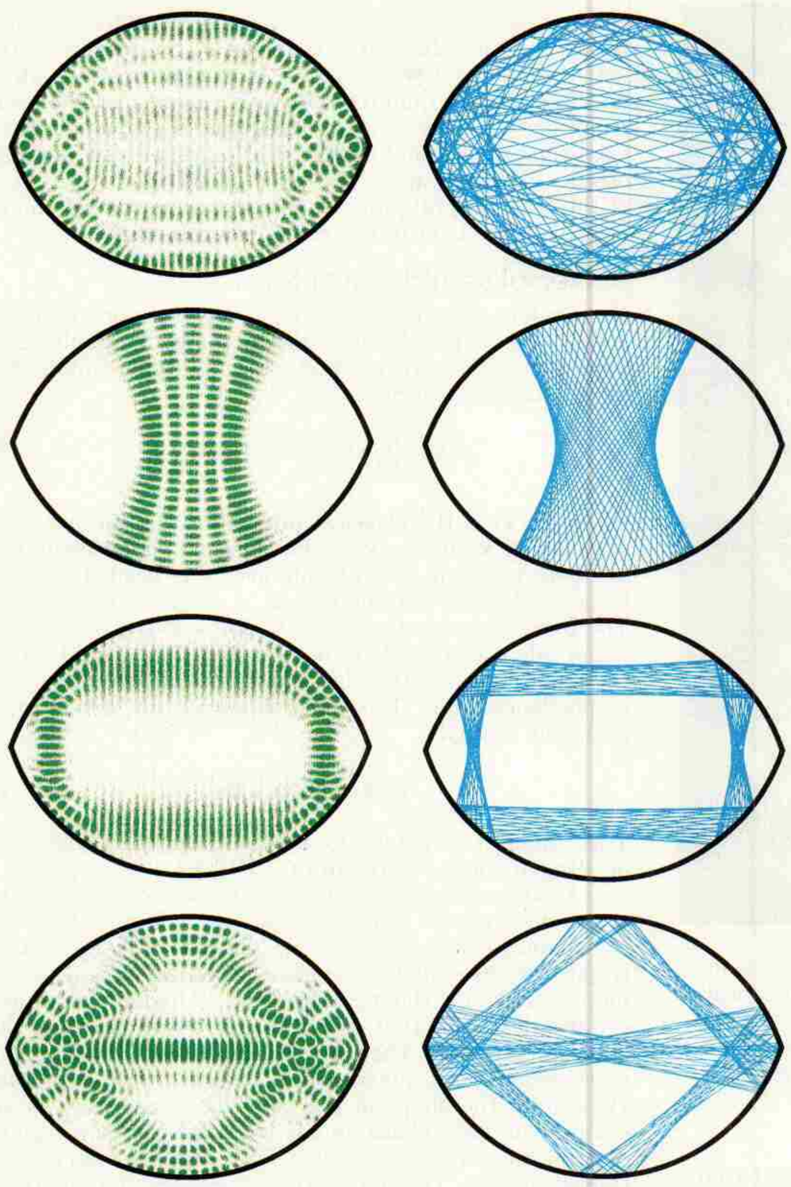


The 'lemon' billiard system, a particle in a lemon-shaped box, is a typical mixed dynamical system, having both chaotic motion (top two images) and quasiperiodic motion (bottom six images). All four distinct types of motion seen in the lemon are shown, in the form of numerically obtained quantum eigenstates (green; $|\psi|^2$ is plotted) and classical orbits (blue). Completely integrable systems (such as a particle in a circular or rectangular box) and completely chaotic systems (such as a particle in a stadium-shaped box) are very rare. Most systems exhibit both types of motion. **Figure 1**

goal seems much closer now. With the chaos barrier coming down, semiclassical ideas are better able to support or suggest new experiments and to lend physical insight into quantum mechanics. Beyond this, semiclassical methods can be the basis of calculations that are computationally out of reach to full quantum approaches.

Eigenvalues and the trace formula

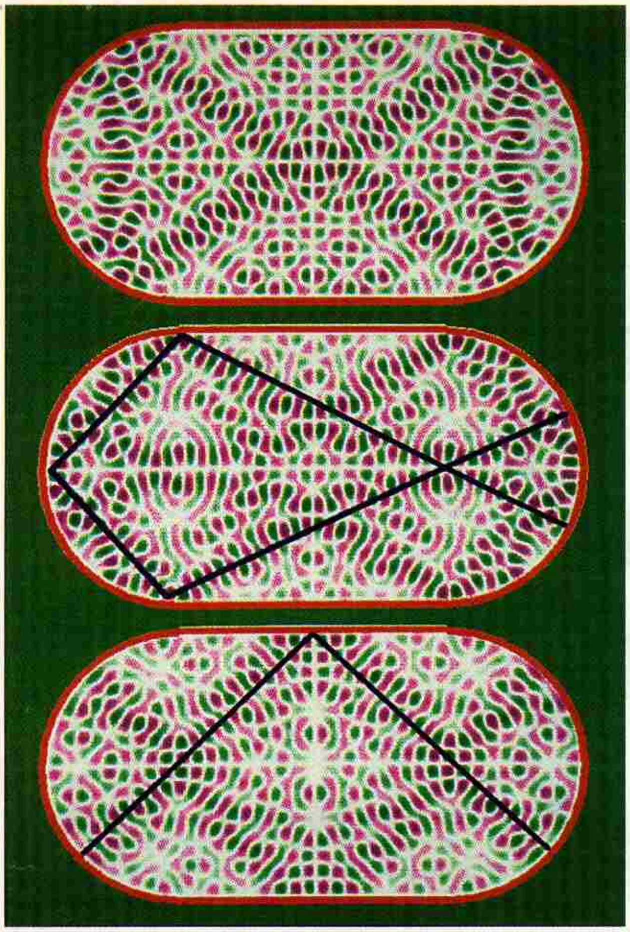
After much effort, the pioneers (Bohr, Kramers, Born and Heisenberg) failed in their attempt to quantize atomic helium. Their problems were fundamental: They neither understood chaos nor had the means to find chaotic trajectories. Helium is chaotic; worse, under classical dynamics it "illegally" ejects an electron (autoionization) for a large fraction of initial conditions. One electron falls closer to the nucleus and to a lower energy than is quantum mechanically allowed, ejecting the other electron. In 1970 Gutzwiller finally did what the pioneers needed to do, namely express the eigenvalues in terms of the periodic orbits.[2] The periodic orbits are the natural extension of the Bohr orbits of the hydrogen atom. For a chaotic system, the periodic orbits are rare, unstable trajectories that return exactly upon themselves. They always exist in a chaotic system and are still infinite in number, though embedded in a much larger sea of chaotic, nonperiodic trajectories.

Gutzwiller had the idea of looking at the trace (the integral over all coordinates) of the energy Green's function, which has simple pole singularities at the eigenvalues E_n. Integrating to obtain the semiclassical version of this trace leaves only the periodic orbit contributions. In the resulting formula, one must sum over all the periodic orbits to find even a single eigenvalue. The trace formula for a particle of mass m and momentum $p = \sqrt{2mE}$ inside a box with arbitrarily shaped walls is

$$g(E) = \sum_n \frac{1}{E - E_n}$$

$$\approx \bar{g}(E) + \frac{1}{i\hbar} \sum_\gamma \sum_{k=1}^{\infty} \frac{m l_\gamma}{p} \frac{\exp(ikpl_\gamma/\hbar - i\pi k \nu_\gamma/2)}{|2 - \mathrm{Tr}(M_\gamma)^k|^{1/2}} \qquad (1)$$

The term $\bar{g}(E)$ is a smooth function giving the mean density of states. The double sum in equation 1 runs over all distinct periodic orbits, labeled by γ, and over k, the number of retracings of each orbit. Each orbit γ has



Typical 'scarred' eigenstates of the stadium billiard. These are plots of ψ for numerically accurate eigenstates. The scars, regions of high amplitude, are generated by periodic orbits, two of which are shown. **Figure 2**

length l_γ, and the integer ν_γ is a phase shift that counts the number of focal points and twice the number of reflections off the walls. The stability matrix M_γ records the sensitivity of the trajectory to changes in initial conditions. If the sum converges (a big if!), the eigenvalues appear as singularities in the sum.

The trace formula is rarely simple to implement. Early attempts to compute enough periodic orbits in equation 1 to give individual eigenvalues found, paradoxically, that the lower energies were easier to obtain and the higher eigenvalues were nonconvergent. This outcome is paradoxical because one expects semiclassical methods to work better at higher energies (the "classical limit"). Also, the series is asymptotic at best and has to be singular at the eigenvalues. Progress has been made using resummation methods, which reorder the terms in the sum in the hope of faster convergence or convergence *per se.* The trace formula is very similar in structure to one of the most studied functions in higher mathematics, the Riemann zeta function. Special means of convergence have been developed for the Riemann zeta function, and "Riemann zeta look-alike procedures" for the trace formula have shown promising convergence.[5] Considerable success also has been achieved by the reordering and regrouping of the terms of the sum in other ways that seem physically rather compelling.[6] Extraction of accurate eigenvalues by examining periodic orbits now appears to be feasible, although most of the results so far are confined to low energies. Indeed the helium atom has finally been quantized directly, using periodic orbit trajectories.[7] Accurate excited-state eigenvalues have been computed from knowledge of relatively few periodic orbits. However, deep questions about the convergence of the trace formula and its modifications remain unanswered. This is still an area of intense effort.

Universal semiclassical form

Eigenvalues are important, but a spectrum or an eigenstate, for example, depends also on quantum amplitudes. Semiclassical approximations to quantum amplitudes have a universal form,

$$\psi(\mathbf{x}) = \sum_n \sqrt{P_n(\mathbf{x})}\,\exp(\mathrm{i}\varphi_n(\mathbf{x})/\hbar) \qquad (2)$$

where $P_n(\mathbf{x})$ is the classical probability for the nth way of reaching $\mathbf{x}$, and $\varphi_n(\mathbf{x})$ is the classical action along the nth path reaching $\mathbf{x}$. The sum over n is needed because in general there may be $0, 1, 2, \ldots$ ways of reaching $\mathbf{x}$. The Born interpretation, namely that $\psi(\mathbf{x})$ is a probability amplitude, dictates that the wavefunction should go as the square root of the classical probabilities in the correspondence limit. The phase is always an "action integral," for example,

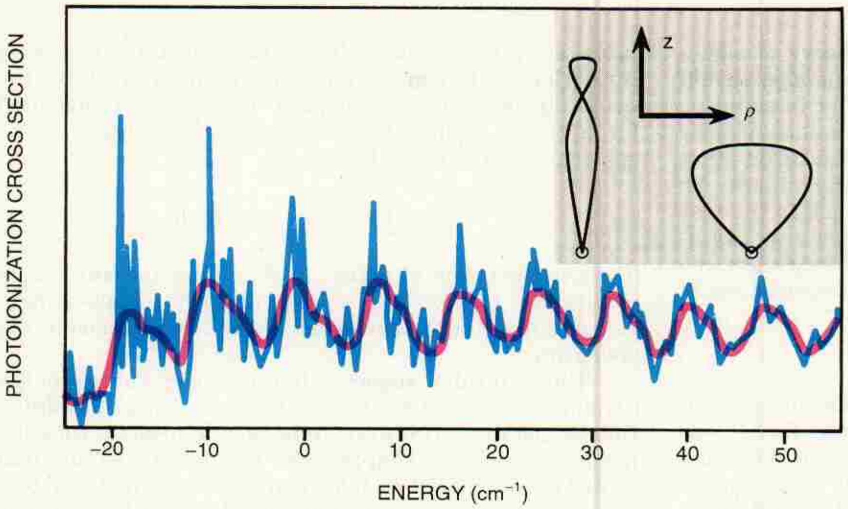
$$\varphi_n(\mathbf{x}) = \int \mathbf{p}_n(\mathbf{x}')\cdot \mathrm{d}\mathbf{x}' \qquad (3)$$

This integral amounts to accumulating the phase of de Broglie waves, since $|\mathbf{p}(\mathbf{x}')| = h/\lambda(\mathbf{x}')$.

As an example, consider a point particle confined to a two-dimensional lemon-shaped box. Figure 1 shows the quantum eigenstates (left) and the classical orbits (right) for three distinct types of classical quasiperiodic motion and one chaotic trajectory. Hidden dynamical symmetries exist that are revealed easily through the classical motion. They are called hidden because the more complicated quasiperiodic motion is not at all obvious from the shape of the box. The lemon box is an example of "soft" chaos, by far the most common type of dynamical system, possessing both regular motion and chaotic motion. The chaotic trajectories are characterized by extreme sensitivity to initial conditions.

Figure 1 shows clear examples of the universal formula, equation 2. The wavefunction is large only where trajectories go. Each of the independent rays reaching a given point gives a term in equation 2. The nodal pattern results from two to eight distinct terms in the sum, depending on how many ways the trajectory visits a given position. Wherever there are several distinct directions of rays, a wild nodal pattern results. Regions of classical buildup of probability, particularly at the focal points, or "caustics," show quantum buildup as well. (The classical–quantum correspondence is just as strong for the usual textbook circular or rectangular box, but the existence of analytic quantum solutions in those cases makes the classical approach seem superfluous.)

The trajectory is the scaffolding on which semiclassical approximations to the wavefunction are built. The quasiperiodic motion and the corresponding semiclassical wavefunctions are all part of the conventional theory having its roots in the old quantum theory and standard semiclassical approximations. The accurate, numerically determined eigenstates corresponding to the quasiperiodic motion show almost perfect correspondence with the trajectories. The trajectories are quasiperiodic and have two constants of the motion ("actions"), corresponding to



Photoionization cross section of a hydrogen atom in a strong magnetic field in the chaotic regime. Medium- and low-resolution spectra (blue and red curves, respectively) clearly exhibit structure, which was ascribed to the returning orbits sketched in the inset. The direction of the magnetic field is along *z*. The energy zero is at the energy of ionization. (Adapted from ref. 14.) **Figure 3**

the direction along and the direction transverse to the channels in which the trajectories choose to move. This property allows an assignment of two quantum numbers to those eigenstates, corresponding to the two classical actions.

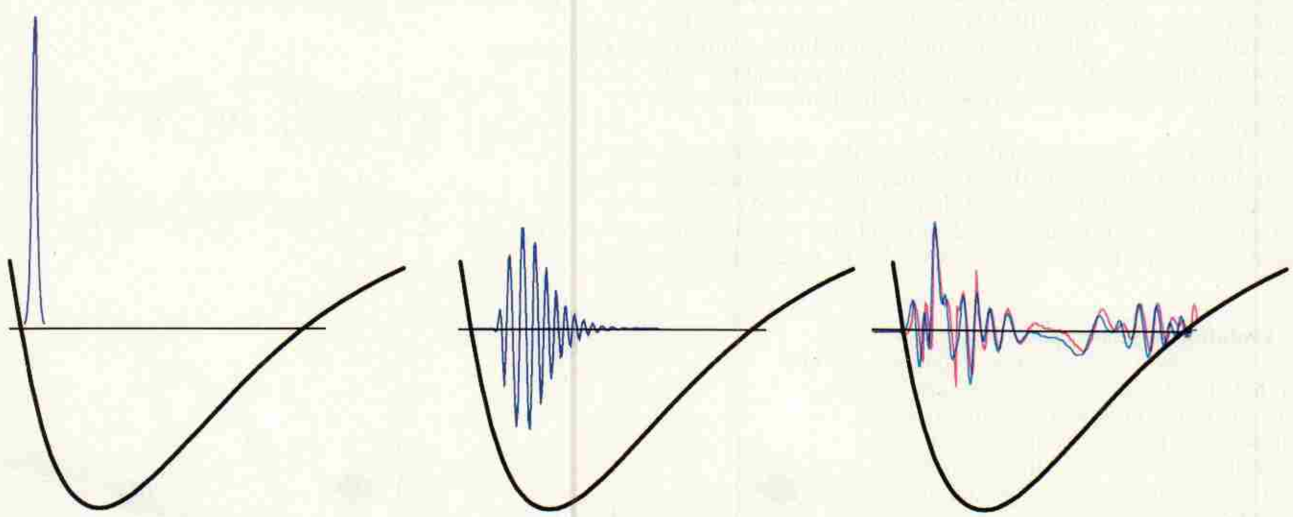
Chaotic eigenstates and scars

We haven't considered the chaotic trajectory (figure 1, top right). The eigenstate corresponding to it also was determined accurately by numerical methods. The chaotic trajectory passes through a given location with a continuous range of momenta instead of a finite set. In this case the universal formula is not on solid ground, because there are infinitely many terms. Worse, the quantization condition requiring phase coherence upon repeated revisitation of the same region cannot be arranged. The frustration of semiclassical theory in the case of chaotic motion is evident. The quasiperiodic motion quantizes beautifully, but neighboring chaotic motion in the same system has no theory.

It is still not known to what extent eigenstates can be understood from a semiclassical analysis. The deepest issues in semiclassical theory are at stake. In principle, the dynamics over infinitely long times is needed to determine an eigenstate completely. Semiclassical approximations are predicted to break down well before the time–energy uncertainty principle allows the eigenstates to be resolved from one another. This difficulty gets worse at higher energy. In spite of this, an accurate high-energy semiclassical wavefunction was recently successfully constructed from strongly chaotic motion,[8] as we discuss below. This accomplishment represents a milestone, but semiclassical construction of eigenstates in general remains a doubtful prospect.

About 20 years ago, Michael Berry made a conjecture about the eigenstates of chaotic systems. Extending the ideas of regular motion and equation 2 to hard chaos, he suggested that the eigenstates of chaotic systems are governed by *random* sums of infinitely many terms in equation 2, corresponding to the infinitely many ways a trajectory accesses a given region for a chaotic system.

Accurate numerical calculations tend to support Berry's conjecture, but there is a caveat: Some eigenstates have regions of high amplitude, called "scars," near certain classical periodic orbits.[9] As we have just seen,



Quantum and semiclassical time evolution (red and blue curves, respectively) of an initially Gaussian wavepacket in a Morse potential. From left to right the times are $t = 0$, $t = 0.1$ and $t = 6.0$, where $t = 1$ is the mean period of one oscillation. Note that the Gaussian becomes delocalized after a few classical periods (the evolution is past the "Ehrenfest" regime) but the semiclassical propagation still works well (right). **Figure 4**

periodic orbits play a large role in the theory of eigenvalues, so a corresponding role in the eigenstates should not come as a surprise. Periodic orbits differ in stability, the property that governs how far a similar, nearby trajectory moves away in one period. Periodic orbits that are not too unstable cause scarring. (See figure 2.) Eugene Bogomolny[10] and Berry[11] added much to the scar theory by quantifying the appearance of scars in coordinate and phase space, respectively. The scars are the most noticeable features in the otherwise confused sea of amplitude in chaotic eigenstates.

The importance of time

We have discussed eigenvalues and eigenstates so far. The great bulk of the work in semiclassical theory has been in the energy domain, with an emphasis on eigenvalues. One can, however, argue that the time domain is more fundamental, since it contains the stationary states with no further constructions. Moreover, explicitly time-dependent experiments are proliferating, providing further motivation for studying the time-domain theory. Other experiments, although not time dependent, are best understood in the time domain because their essential physics is of short duration.

The hydrogen atom in a magnetic field is a beautiful problem of atomic physics, intermediate between hydrogen and helium in difficulty. For a wide range of magnetic field strengths and the energies of the atom, this dynamical system is a typical case of soft chaos, approaching hard chaos for certain ranges. Measurements of direct absorption spectra show oscillatory structure in the cross section even above the ionization threshold; the origin of these features is not immediately obvious. Building on early experimental results of William Garton and Frank Tomkins,[12] Karl Welge and coworkers[13,14] published beautiful spectra and a semiclassical theory of the system in 1986, attracting many new converts to the field. Harald Friedrich, Dieter Wintgen, John Delos and Meng Li Du[15] furthered the connection between the carefully remeasured spectral features and the periodic orbits of the classical hydrogenic electron in a magnetic field. (See figure 3.)

This problem is best understood semiclassically. Indeed, some low-lying energy levels were successfully predicted from the Gutzwiller trace formula using very few periodic orbits. Along with another modified Coulomb system, the so-called anisotropic Kepler problem,[16] this was one of the early successes of the Gutzwiller trace formula.

However, the essential physics of the striking quasi-Landau oscillations in the spectrum involves short-time motion of the electron as it leaves the vicinity of the nucleus and then returns.[17] The spectrum can be represented as the Fourier transform of the autocorrelation function $\langle\varphi|\varphi(t)\rangle$, where $|\varphi\rangle$ is the nonstationary state consisting of the ground eigenstate multiplied by the usual dipole coupling. The state $|\varphi(t)\rangle$ is $|\varphi\rangle$ propagated for a time t under the full atomic Hamiltonian. The spectrum $\varepsilon(\omega)$ is given by[18]

$$\varepsilon(\omega) = \int \exp(\mathrm{i}\omega t)\, \langle\varphi|\varphi(t)\rangle\, \mathrm{d}t \qquad (4)$$

The *low-resolution* structure in the Welge measurements is thus due to *short-time* motion of $|\varphi(t)\rangle$. Time-domain features in $\langle\varphi|\varphi(t)\rangle$ correspond to distinct patterns in the spectrum.

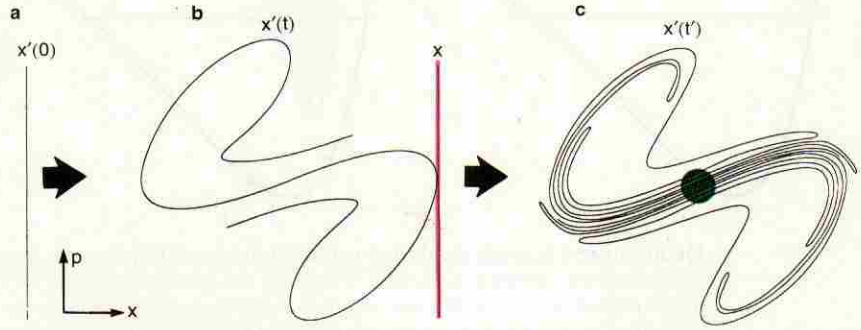
These results suggest that one can calculate the dynamics of $|\varphi(t)\rangle$ directly from the time domain, avoiding the eigenstates. However, to do so one needs a time-dependent semiclassical approach. The oldest postquantum semiclassical theory is John van Vleck's time-dependent semiclassical Green's function, introduced in 1928. It has been relatively neglected except as a route to the stationary-state results. The realization of the full potential of the van Vleck Green's function is one of the promising new developments in semiclassical theory.

Recall that the *quantum* propagator $G(x,x';t)$ takes amplitude from x' to x in time t. The classical analog of this is constructed by way of the universal formula, equation 2. The classical analog starts with all the trajectories at x' at time $t = 0$. They have all possible momenta, corresponding to the infinite quantum uncertainty in momentum for a position state. The trajectories fan out in all directions with all speeds for $t > 0$. The classical probability needed for equation 2 is simply the classical density of trajectories arriving at x by a given route; different routes to the same x each merit a term in equation 2. The action integral is computed for each trajectory; this becomes the phase. The picture is one of a swarm of trajectories carrying amplitude and phase around with them. They interfere destructively or constructively and collectively build the wavefunction. As complicated as this may seem, it is vastly simpler than the exact Feynman path integral construction of the propagator. The trajectories are the scaffolding for semiclassical stationary states and for semiclassical dynamics.[19]

The van Vleck Green's function is

$$G^{\mathrm{sc}}(x,x';t) = \left(\frac{1}{2\pi\mathrm{i}\hbar}\right)^{1/2} \sum_j \left|\frac{\partial^2 S_j(x,x')}{\partial x\,\partial x'}\right|^{1/2} \exp\left(\frac{\mathrm{i}S_j(x,x')}{\hbar} - \frac{\mathrm{i}\nu_j\pi}{2}\right)$$

$$= \left(\frac{1}{2\pi\mathrm{i}\hbar}\right)^{1/2} \sum_j \left|\frac{\partial p'}{\partial x}\right|_{x'}^{1/2} \exp\left[\frac{\mathrm{i}S_j(x,x')}{\hbar} - \frac{\mathrm{i}\nu_j\pi}{2}\right] \qquad (5)$$



Evolution in phase space of a classical distribution under chaotic dynamics. **a:** Initial distribution $x'(0)$ corresponding to a definite position x' and all possible momenta. **b:** Early folding of $x'(t)$. The position x (red) shows the location of a caustic singularity. **c:** The folding and winding due to chaotic dynamics over a longer time. The green disk has area $\hbar$ and corresponds to a localized state in a "safe" zone away from area-$\hbar$-violating regions at the ends of loops. **Figure 5**

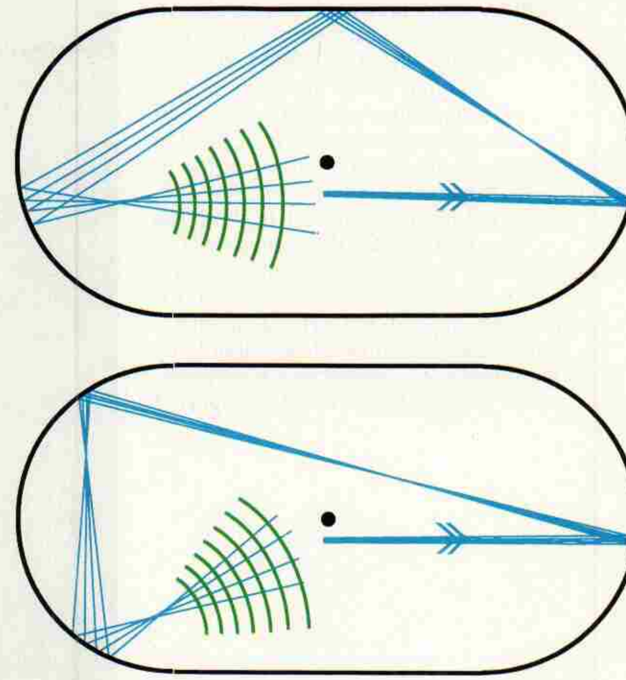
The action

$$S_j(x,x') = \int_0^t dt' \,[\,p(t')\,\dot{x}(t') - H(p(t'),x(t'))\,] \qquad (6)$$

is the usual integral of the classical Lagrangian $L = p(t')\dot{x}(t') - H(p(t'),x(t'))$ over the jth classical path from x' to x. The sum is over all trajectories that connect x' to x in time t. The term $-i\nu_j\pi/2$ is the Maslov–Gutzwiller phase. The integer ν_j increases by 1 whenever the classical trajectory connecting x' to x meets a focal point, or caustic, where $\partial^2 S_j(x,x')/\partial x\,\partial x'$ diverges. Although there were precedents to this Green's function in related contexts, Gutzwiller gave the crucial phase correction ν_j to the van Vleck expression, without which it would be useless.

Certainly one impediment to the use of the van Vleck–Gutzwiller Green's function has been the apparently forbidding task of evaluating it. For each time t and separately for each pair of points x and x' we must find all trajectories connecting those points. One of the exciting recent developments is the realization that this is too pessimistic a perspective. Much more efficient algorithms exist. One direct approach is to run a grid of trajectories and use interpolation, accounting for essentially all relevant classical paths. Successive times $t + \delta t$ are built upon the prior time t by a single integration step.

A one-dimensional example illustrates a valuable point. If we launch a narrow wavepacket $|\varphi(0)\rangle$ in an anharmonic oscillator, Ehrenfest's theorem tells us that it will (for a limited time) follow a classical trajectory (x_t, p_t) in the sense $\langle\varphi(t)|x|\varphi(t)\rangle \approx x_t$ and $\langle\varphi(t)|p|\varphi(t)\rangle \approx p_t$. The wavepacket remains localized for a time we call the Ehrenfest time, after which it becomes delocalized over all of the potential accessible to it. One might expect that the semiclassical approximation would break down after the Ehrenfest time, but this is far from the case, as figure 4 shows.[19]



Two groups of trajectories leaving with very similar initial conditions in a stadium return to the starting point by different paths. Each group carries wave amplitude and corresponds to a term in equation 2. These are two of the more than 30 000 "echoes" whose return contributes to the later values of the autocorrelation function shown in figure 8. **Figure 6**

Oil on troubled waters

As mentioned above, caustics occur at divergences of

$$\frac{\partial^2 S_j(x,x')}{\partial x\,\partial x'} = \left(\frac{\partial x}{\partial p'}\right)_{x'} \qquad (7)$$

A divergence is caused by trajectories piling up at certain values of x after they leave x'. A phase space picture is very helpful. A vertical line at x' corresponds to the initial classical distribution $x'(0)$, that is, all possible momenta at a single position. (See figure 5a.) After some time the trajectories have spread out to many places, but there are caustics at certain values of x where loops or folds form and the density of trajectories diverges. More specifically, a caustic occurs at x if the vertical line at x is tangent to the curve $x'(t)$. (See figure 5b.)

The divergences of the Green's function would appear to be a major problem. The semiclassical Green's function blows up at the divergences, but the quantum Green's function is finite. In their pioneering study of semiclassical propagation, Berry and coworkers noted that the divergences grow in number until almost no region is free of them.[20] The problem is much worse for chaotic systems, because the number of divergences grows exponentially fast. This growth was widely thought to lead to the demise of semiclassical propagation on a disappointingly short time scale.

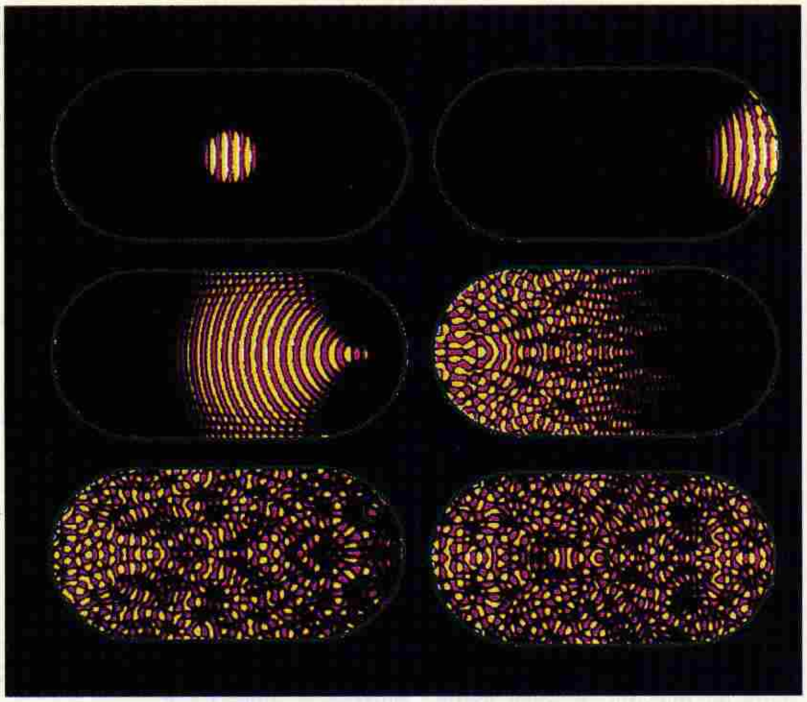
A fortunate circumstance saves semiclassical propagation from the divergences. The Green's function itself is normally not needed; instead, it is applied to smooth states $\varphi(x)$ to move them forward in time. The use of a smooth wavefunction $\varphi(x)$ with the badly behaved Green's function is like pouring oil on troubled waters: The Green's function singularities disappear, replaced by much more benign errors. The semiclassical van Vleck Green's function $G^{sc}(x,x';t)$ is used by exact analogy to the quantum propagator:

$$\varphi(x,t) \approx \int_{-\infty}^{\infty} G^{sc}(x,x';t)\,\varphi(x',0)\,dx' \qquad (8)$$

In this way classical trajectories from various initial locations x', weighted by the amplitude $\varphi(x',0)$, guide the moving wavefronts of $\varphi(t)$.

The smoothing of the Green's function singularities is done in amplitude space, not as a palliative but as a necessity. Smooth states are localized in phase space to zones of area h. They can easily dodge error-prone regions, as figure 5c shows. The green disk representing the smooth state in phase space is out of harm's way by being far from the ends of loops in $x'(t')$. The loops cause errors when they enclose area less than $\hbar$, as they must if they are approached too closely.

Now we can understand the time-dependent semiclassical treatment of the hydrogen atom in a magnetic field: The trajectories leave the region of the nucleus and groups of them later return. The wave $\varphi(x,t)$, guided by the trajectories, does the same. If the wave returns, there will be a recurrence, an increase in the correlation function $\langle\varphi|\varphi(t)\rangle$, at a time governed by the classical



Evolution of a localized wavepacket in the stadium billiard system, computed numerically. The initial Gaussian, pictured in the first frame, has a momentum corresponding to 30 wavelengths stretching across the horizontal axis. From left to right, top to bottom, the images are for $t = 0$, 0.4, 0.8, 1.6, 3.2 and 6.4, where 1 is about the time required for the wavepacket to traverse the stadium horizontally. After a few bounces the wavefunction is completely delocalized. The dynamics is nonetheless almost all describable by time-dependent semiclassical methods. (Adapted from ref. 24.) **Figure 7**

trajectories. This will appear in the spectrum as oscillatory structure spaced proportionally to the inverse time of return.

Chaos: The demise of semiclassical dynamics?

The smoothing effect is a big help, but it is not enough to fix all the problems of the semiclassical approach. Chaos complicates matters by creating exponentially many new ways to get from x' to x as time increases, and these new ways necessarily cause stretching and folding in the phase space distribution. (See figure 5.) This creates two new difficulties, one fundamental, one practical. The fundamental problem is that the narrow folds may enclose area less than $\hbar$. This feature is a red flag in semiclassical theory, one that the "oil" cannot really fix. For areas less than $\hbar$ there is a breakdown of the stationary-phase evaluation of integrals that are at the heart of the theory.

The practical problem is the task of enumerating all the trajectories. Fortunately the trajectories often naturally divide into groups with similar histories. One can approximate each group by expanding the local classical motion about a representative orbit. The sum over individual trajectories then becomes a sum over far fewer groups, each one guiding an independent wavelet. The sum of all these wavelets yields the semiclassical approximation to the full dynamics. However, the groups visit any region by a staggering number of topologically distinct paths as time evolves, so eventually even the number of groups becomes a problem.

It is very instructive to see how these wavelets develop for a stadium-shaped box, a system known to be completely chaotic. In figure 6 we see two groups of rays emanating from very similar initial conditions near the center of the stadium. After three bounces both sets have returned, but by topologically distinct paths. As in all chaotic systems, small differences between trajectories have been rapidly amplified. Each group carries with it a wavelet, which will contribute amplitude to a recurrence, that is, a growth in the correlation function $\langle\varphi|\varphi(t)\rangle$. The returning wavelets are separate terms in equation 2.

An acoustical version of the stadium has almost the same physics. Imagine shouting in a certain direction in a stadium-shaped room. The correlation function amounts to listening for echoes. The earliest returning echoes can only have bounced off one or two walls, but very shortly thereafter the number of distinctly different paths leading to echoes is staggering. Labeling the walls (top, side, bottom, side) 1 through 4, a path is distinct if the sequence of bounces (for example, 1-2-3-2-3-1-4) is new. After just 10 bounces there are roughly 100 000 approximately equally important distinct paths for echoes. Clearly each of the separate subechoes has to be extremely feeble. Can the process of following the echoes by such ray tracing be meaningful under such conditions? Here we face the semiclassical crisis of confidence.

One view of the crisis is that as time increases, the initial shift of position or direction required to distinguish one set of returning rays from another is microscopic, perhaps one ten-thousandth of a wavelength. It would seem that the rays can no longer be used to construct the semiclassical propagation if classical details on a scale much smaller than a wavelength are important. The other side of the same coin is that any phase space cell the size of Planck's constant is bent and folded into pieces seemingly insignificant on the scale of Planck's constant. This happens in a short time dubbed the "log time," because if $\hbar$ is made smaller the time to reach supposedly ruinous folding only gets longer as $\log(1/\hbar)$. Until very recently, it was widely believed that semiclassical approximations would break down on this time scale. If that is true, it is hard to see why the energy space results such as the trace formula should work, because the Fourier transform from time to energy implies they depend on long-time propagation.

Fortunately these worries are ill posed and ill founded. The right question to ask is, How much has the semiclassical phase (action) changed between different returning wavelets? There is a simple rule: Trajectories leaving from very similar initial conditions and returning to very similar final conditions at the same time need to have phases that differ by at least one radian, or else the usual rules of semiclassical approximations break down. In a billiard system this means path lengths differing by approximately one wavelength divided by 2π or greater. As time increases, even microscopic differences in initial conditions get amplified and can lead to large path length differences before the trajectories return. Amazingly, strong chaos may *help* the semiclassical approximation by amplifying such differences or, equivalently, by building large loops in phase space. Detailed analysis along these lines shows that the breakdown happens at times much longer than the log time. The breakdown time goes algebraically in $\hbar$, not logarithmically.[21]

Chaos in the stadium

The stadium has played a large role in the study of classical chaos and its effect on quantum mechanics. Now it is playing an experimental role as well. Recently, a mesoscopic stadium-shaped chamber has been constructed[22] for the study of conductance fluctuations as a function of magnetic field. The stadium has also been the subject of microwave cavity experiments.[23]

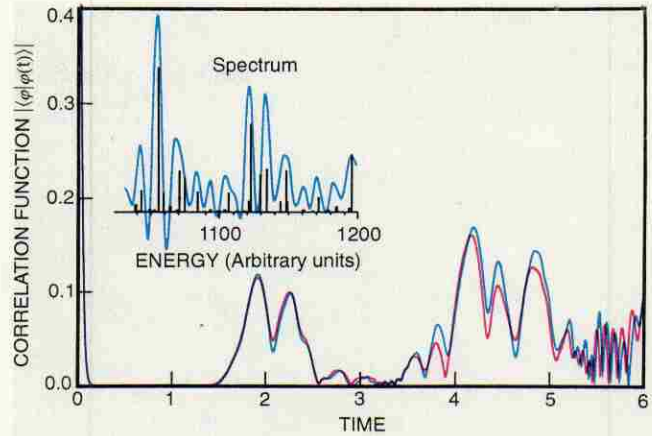
Figure 7 shows the time evolution of a *smooth* nonstationary wavepacket in a stadium.[24] The wavepacket was computed accurately by numerical means at times $t = 0.4$, 0.8, 1.6, 3.2 and 6.4 (where 2 is about the time it takes the center of the wavepacket, bouncing horizontally, to make a round trip). The rapid breakup of the packet is evident; the Ehrenfest time (time required for wavepacket breakup) is less than 1. The log time is around $t = 2$.

Figure 8 shows the quantum and semiclassical results[24] we obtained for the correlation function $\langle\varphi|\varphi(t)\rangle$ for the wavepacket $|\varphi(0)\rangle$ shown in figure 7. Long after the log time, the results hold up well. By $t = 6$ the number of contributing paths was about 30 000 and growing exponentially. In short, we ran out of computer time. No significant breakdown of the semiclassical propagation had taken place.

We get the spectrum by taking the Fourier transform of the correlation function. The inset of figure 8 shows the semiclassical result along with the numerically determined exact spectrum. The semiclassical spectrum is remarkably accurate and resolves the spectrum to nearly the mean spacing; only classical mechanics was used to generate it! Eigenvalues in the neighborhood of the 1000th are given accurately. The finite resolution of the semiclassical spectrum results from our cutting off the Fourier integral at $t = 6$, where the correlation function was doing well. This implies that if more classical detail had been followed past $t = 6$, even finer resolution would have been obtained.

Because of the benefits of using smooth states and the more optimistic fold analysis, we find that while chaotic dynamics increases the complexity of the semiclassical constructions, the accuracy is good for times much longer than the log time. In the acoustical case, adding all 30 000 feeble echoes gives the correct sound amplitude after all.

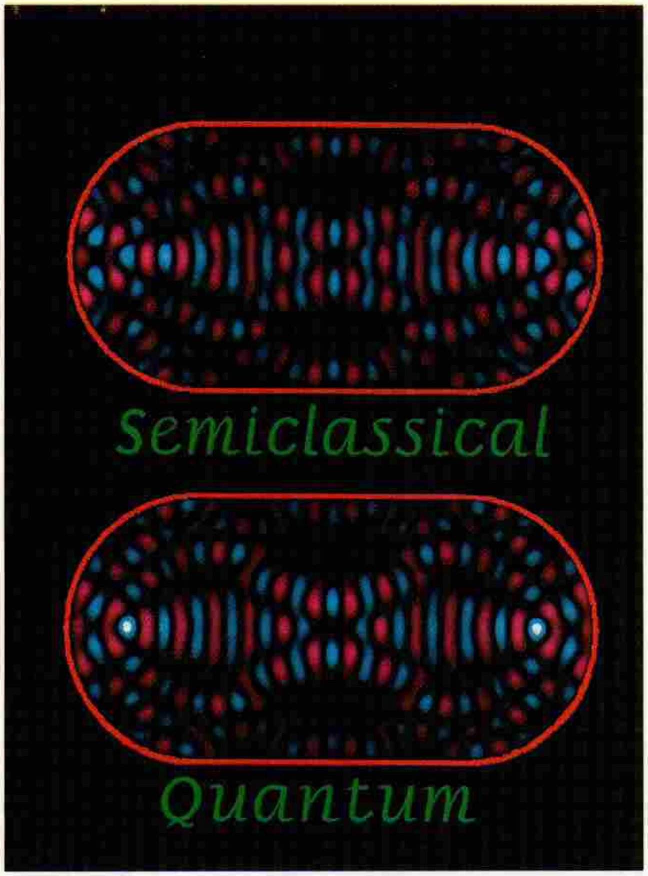
Is there a paradox here, in that 30 000 extremely small zones in phase space are contributing to an accurate result? The key point is to recognize that the uncertainty principle is a one-way street: While it is true that quantum mechanics cannot *resolve* structures finer than $\hbar$ in size, it is quite possible to construct quantum mechanics from thousands of pieces of data within each Planck cell. The matter is no more profound than a blurry photograph. The blurred image cannot be used to construct a sharp one, but the sharp image can certainly give the correct blurred one. In fact, infinitely many different sharp photographs give the same blurred one. Current research is exploiting this idea; it may not be necessary to calculate the exact classical dynamics, or its full complexity, to get an accurate approximation to quantum mechanics. This is one implication of the "cycle expansion" for the eigenvalues,[6,7] which uses "pseudo-orbits" (collections of subtly related classical orbits) to speed or even induce convergence in the trace formula.



Autocorrelation function $C(t) = \langle\varphi|\varphi(t)\rangle$ for the system shown in figure 7, computed using quantum and semiclassical evolution (red and blue curves, respectively). Inset shows the spectrum obtained by taking the Fourier transform of $C(t)$ (blue) and the numerically determined exact spectrum. (Adapted from ref. 24.) **Figure 8**

When does semiclassical propagation become inaccurate? There is no single answer to this question, even for a given system. The time of breakdown can vary dramatically depending on the location of the initial state to be propagated. All "classically forbidden" processes are by definition absent from an approach based purely on ordinary classical trajectories. These processes go under the names of diffraction, tunneling and localization, although the distinctions between them are not always well defined. In the time domain, the wavefunction starts out exact by definition. Accuracy is expected to deteriorate with time, due to all the accumulated effects of the classically forbidden processes. For billiard systems (disks, stadiums and so on) breakdown can squarely be blamed on diffraction. In the stadium, the biggest source of diffraction is the joints between the straight walls and the circular sections. By examining the accumulation of the diffracted amplitude, it is possible to show that the time scale for breakdown is not logarithmic in $\hbar$ but follows a power law. For the stadium, it goes as $\hbar^{-1/2}$. While this is good news compared with the log time, it bodes ill for the determination of individual eigenstates as $\hbar \to 0$. The reason is that the density of states goes as $\hbar^{-2}$, so the breakdown will occur before the eigenstates can be resolved.

Nevertheless, it is possible to go further and attempt to construct a semiclassical eigenstate from the chaotic trajectories. This is another watershed. Figure 9 shows the exact and semiclassical eigenfunctions obtained from the Fourier transform of a propagated wavepacket similar to the one shown in figure 7. The energy was chosen to match one of the peaks in the packet's semiclassical spectrum.[8] The normalized overlap between the exact



A quantum eigenstate and its semiclassical approximation for the chaotic stadium billiard. The normalized overlap between the two states is approximately 0.96. (Adapted from ref. 8.) **Figure 9**

and approximate states is approximately 0.96. The semiclassical eigenfunction is surprisingly accurate considering the intricate and delicate interferences taking place in its construction. Could it be that the mathematical arguments about the breakdown of semiclassical theory are still far too pessimistic?

The Holy Grail?

Beginning about 20 years ago, Berry focused attention on the dilemmas of semiclassical theory by defining its Holy Grail: quantization of classical chaos. The recent quantization of the helium atom[7] and the construction of the spectra and semiclassical eigenstates directly from chaotic classical trajectories mean the grail is much nearer. However, too many questions remain about convergence and errors of the procedures to say that the grail has been found.

There is no doubt that the agenda of the old quantum theorists is active again, after a long hiatus caused by classical chaos. At first people were unaware of chaos and the problems it can create. Later, those problems may have been overestimated. We have learned that chaos poses no devastating threat, but it adds complexity to the classical mechanics. Enumerating the periodic orbits for the trace formula or the groups of returning (but not necessarily periodic) orbits for a correlation function is difficult for long orbits. Simplifying that complexity is a major challenge. The analogy with a blurry photograph may provide a clue. There ought to be a simplest sharp photograph (set of effective rays) that gives substantially the correct blurred one. This approach is a major area of research.

The normal sorts of threats to semiclassical methods (diffraction and tunneling) will take center stage as chaos *per se* recedes in importance. Effects such as diffraction may be too important to be safely ignored, or may even be the essence of the problem. Still, it is amusing to note that the concepts of diffraction and tunneling only exist relative to classical mechanics as a baseline! Classical ideas pervade quantum mechanics. It is good to know how far they can really take us.

Most importantly, many applications to physical systems lie ahead. If semiclassical methods are really worthwhile, the best understanding of many atomic, molecular, nuclear and mesoscopic processes and properties will be in terms of classical mechanics and semiclassical amplitudes.

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We thank our coworker Miguel Sepúlveda for many helpful discussions and William P. Harter for a critical reading of the manuscript.

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