Semiclassical Construction of Chaotic Eigenstates

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It has been a long-standing problem to understand the eigenfunctions of a system whose classical analog is strongly chaotic. We show that in some cases the eigenfunctions can be constructed by purely semiclassical calculations.

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As Bohr discovered the correspondence principle, he quickly found that it could only be put forth for systems with as many independent classical constants of the motion as degrees of freedom [1]. Hence, fully or even partially chaotic systems were beyond the realm of the "old quantum theory." Helium, with its unstable dynamics, was not to be explained despite the preoccupation of Bohr, Kramers, and others. By 1917, Einstein [2] had already understood the geometry of semiclassical quantization and pointed out the fundamental reason why Bohr's still developing correspondence principle would not be extended. After quantum theory was finally introduced, interest in its correspondence to classical mechanics waned for some time. In just the last few years and after much effort, significant progress on the semiclassical quantization of chaotic systems has accelerated [3]. Nevertheless, the question remains unresolved to what extent semiclassical theory can reproduce chaotic spectra [4], and can predict eigenstates and explain their structure. The eigenstates remain much less well studied than the spectrum. Among the limited results there is Berry's statistical hypothesis of Gaussian random behavior [5], and the prediction and observation of eigenfunction scarring by the least unstable, short periodic orbits [6]. In this Letter we show that, at least in some cases, a complicated eigenstate of a strongly chaotic system can be extremely well approximated by purely semiclassical construction.

Classical mechanics emerges from quantum mechanics in a singular limit [7]. This is summarized by the statement that the two limits, vanishing Planck's constant, $\hbar \to 0$, and long time, $t \to \infty$, are noncommuting—they cannot legitimately be interchanged. The problem is that the order of these limits gets reversed when extracting individual eigenstates from semiclassical dynamics [8].

A natural, straightforward semiclassical eigenfunction calculation starts with the energy Green's function

$$G(\mathbf{q},\mathbf{q}';E)=\langle \mathbf{q}|\frac{1}{E-\hat{H}}|\mathbf{q}'\rangle=\sum_j \frac{\Psi_j(\mathbf{q})\Psi_j^*(\mathbf{q}')}{E-E_j}. \quad (1)$$

In the second form $\Psi_j(\mathbf{q})$ is an eigenstate of energy E_j. The semiclassical approximation of $G(\mathbf{q},\mathbf{q}';E)$ expresses it as a sum over all trajectories of energy E starting at $\mathbf{q}'$ and ending at $\mathbf{q}$. An eigenstate is found by fixing $\mathbf{q}'$ to some arbitrary point, letting E tend to E_j (say, $E_j+i\epsilon$), and repeating the trajectory sum for each member of a collection of $\mathbf{q}$. For each value $\mathbf{q}$, the semiclassical energy Green's function leads to a divergent sum over an infinite set of classical orbits. Even if the sum is somehow cut off self-consistently, it also typically happens that many of the contributions are individually singular due to caustics (the generalization of turning point or focusing singularities).

Conceptually, it is advantageous to begin the attack on this problem from the time domain. Recent work has demonstrated the computability, the long-time accuracy, and the utility of semiclassical propagation in highly chaotic systems [9]. It has also explained why it functions better than previously imagined, even in the face of seemingly reasonable counterarguments [10]. Consider an eigenstate $\Psi_j(\mathbf{q})$. It can be projected from a propagating state $\Phi(\mathbf{q};t)$ by simple Fourier transform (ignoring an irrelevant overall constant),

$$\Psi_j(\mathbf{q})=\int_{-\infty}^{\infty} d\mathbf{q}\exp(iE_jt/\hbar)\Phi(\mathbf{q};t). \quad (2)$$

The propagation of $\Phi(\mathbf{q};0)$ can be expressed as

$$\Phi(\mathbf{q};t)=\int_{-\infty}^{\infty} d\mathbf{q}'\,G(\mathbf{q},\mathbf{q}';t)\Phi(\mathbf{q}';0), \quad (3)$$

where $G(\mathbf{q},\mathbf{q}';t)=\langle \mathbf{q}|\exp(-i\hat{H}t/\hbar)|\mathbf{q}'\rangle$ and $\hat{H}$ is a quantum Hamiltonian. The fundamental approximation is to replace $G(\mathbf{q},\mathbf{q}';t)$ with a semiclassical version, $G_{sc}(\mathbf{q},\mathbf{q}';t)$ (the semiclassical or Van Vleck–Gutzwiller propagator) [11],

$$G(\mathbf{q},\mathbf{q}';t)\approx G_{sc}(\mathbf{q},\mathbf{q}';t)=\left(\frac{1}{2\pi i\hbar}\right)^{d/2}\sum_j\left|\mathrm{Det}\left(\frac{\partial^2 S_j(\mathbf{q},\mathbf{q}';t)}{\partial\mathbf{q}\,\partial\mathbf{q}'}\right)\right|^2\exp[iS_j(\mathbf{q},\mathbf{q}';t)/\hbar-i\pi\nu_j/2]. \quad (4)$$

In this expression, the sum over j is for all trajectories connecting $\mathbf{q}'$ to $\mathbf{q}$ in time t, d is the number of degrees of freedom, the prefactor involving the determinant plays the role of the square root of a classical probability, and the phase is determined by the classical action $S_j(\mathbf{q},\mathbf{q}';t)$ and the count of conjugate points (like focal points), ν_j. $S_j(\mathbf{q},\mathbf{q}';t)$ is

specified by the time integral of the Lagrangian $\mathcal{L}$

$$S_j(\mathbf{q},\mathbf{q}';t) = \int_0^t dt' \mathcal{L}$$

$$= \int_0^t dt' \{\mathbf{p}(t')\cdot\dot{\mathbf{q}}(t') - H(\mathbf{p}(t'),\mathbf{q}(t'))\} \quad (5)$$

along the jth classical path (H is the classical Hamiltonian corresponding to $\hat{H}$).

The specific forms of Eqs. (2)–(5) were chosen because we presume that the configuration space representation is the most natural and intuitive for the present purposes. However, practical evaluation of Eq. (3) may be more efficient and/or accurate by decomposing $\Phi(\mathbf{q};t)$ on a convenient intermediate basis. Let

$$\Phi(\mathbf{q};t) = \sum_k \langle \mathbf{q}|k\rangle\langle k|\Phi(t)\rangle . \quad (6)$$

The semiclassical approximation is then applied to the collection of $\langle k|\Phi(t)\rangle$ and the functions $\langle \mathbf{q}|k\rangle$ are presumably known.

With the choice of a coherent state basis and initial state, the techniques of [10] can be taken over almost without modification. It was shown there that the infinite set of orbits contributing to a particular $\langle k|\Phi(t)\rangle$ could be organized into a finite set of subgroups, each collection responsible for building a topologically distinct wave front. The sum of these wave fronts gives the full dynamics. Within each subgroup, the orbits are all very similar. Each member orbit can be approximated by expanding the local classical motion about a representative orbit. In this way each wave front is associated to one such orbit and its stability parameters. Because of the exponential instability of chaos, a natural choice for the set of representative orbits is the so-called "heteroclinic orbits." They lie at the intersections of the stable and unstable manifolds emanating from within the local phase space associated to $|k\rangle$ and $|\Phi\rangle$, respectively. For a more complete description of these heteroclinic orbit summations, see [10]. A salient feature of this approach is that, although caustics lead to inaccuracies, they no longer generate infinities (which would make it impossible to proceed).

The same arguments that explain the long-time fidelity of semiclassical methods also predict a time scale for its breakdown [10]. In approximating $\Psi_j(\mathbf{q})$, it is desirable to restrict the integral of Eq. (2) to the time domain where the propagated state is well represented. Of the many ways to accomplish this, we usually apply a Gaussian damping of the integrand, or, occasionally, end the integration abruptly so there is an effective cutoff time τ. In so doing, there are no longer infinite divergent sums to worry about as in the energy Green's function. Unfortunately, it is almost always the case that we are forced to use an even smaller τ because with present techniques the exponential proliferation of orbits in the developing chaotic dynamics bogs us down before the approximation itself is found to fail.

If τ were to greatly exceed the Heisenberg time, $t_H = h/D$, D being the mean level spacing, we should expect to resolve most if not all the eigenstates having appreciable overlap with $\Phi(\mathbf{q};0)$. This is far from the present state of the art and the semiclassical approximation is expected, in general, to break down before the Heisenberg time [10]. It may still be possible to project a few of the eigenstates if an initial, localized $\Phi(\mathbf{q};0)$ happens to have a few strong, well separated (in energy) eigenstate overlaps. Thus, the best conditions prevail if $\Phi(\mathbf{q};0)$ is selected as a Gaussian wave packet placed on a strongly scarring, short periodic orbit. By choosing various $\Phi(\mathbf{q};0)$ on a number of different such orbits, many different states may emerge. The selectivity of the initial state is crucial, allowing shorter time dynamics to capture the essence of some subset of the eigenstates. An approach more in the spirit of periodic orbit theory, where use is not made of this selectivity, is certainly much more difficult technically and may also break down because of its necessary reliance on longer time dynamics where the approximation is

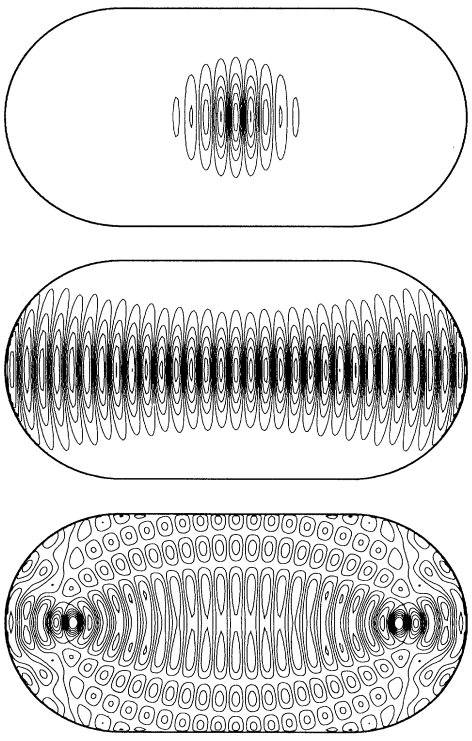

FIG. 1. The symmetric coherent state pictured on top has been chosen such that 15 wavelengths span the horizontal axis of the stadium. The free particle motion contribution (zero-bounce dynamics) to an even-even eigenstate, $\Psi_j(\mathbf{q})$, at energy $E_j = 297.12$ (about the 320th state) is shown in the middle. The contribution after one reflection from the wall is on the bottom. There are ten equally spaced contours drawn. E_j is the same for all the figures.

increasingly suspect.

We emphasize that the calculation of $\Psi_j(\mathbf{q})$ can be done in an entirely semiclassical way. For example, it is not necessary to have any prior knowledge of E_j. The norm of the projected semiclassical state grows much faster with τ for an energy "on resonance" than it does off. This is one method of obtaining the E_j. Alternatively, the interesting energy values can be located semiclassically by Fourier transform of $\langle\Phi(\mathbf{q};0)|\Phi(\mathbf{q};t)\rangle$ giving its spectrum which can be studied to select the best energies.

We demonstrate the existence of "semiclassical chaotic" eigenstates by construction with the Bunimovich stadium billiard. The system is a particle in a stadium shaped enclosure undergoing specular reflection off the walls. It is completely chaotic [12] and has proven quite useful in many chaos studies. In Fig. 1, we illustrate the Fourier transformed contribution of the pictured initial state $\Phi(\mathbf{q};0)$ motion (forward and backward in time) to the state $\Psi_j(\mathbf{q})$. The shortest time dynamical feature of the coherent state placed inside the stadium (upper plot) is its free particle motion toward the walls (zero-bounce dynamics). The projection of the spreading of the wave packet and its simple dynamics is easily seen in the middle plot. As the waves reach the wall, they are reflected back, leading to the one-bounce dynamical contribution seen in the lower part of Fig. 1. The continuing sum of these functions is the semiclassical eigenstate. At this energy, by three-bounce dynamical times, the essential state has emerged. Figure 2 shows its appearance. Two versions are given. On top is a cumbersome, but direct **q**-state calculation. Below is the result where an intermediate plane wave basis was used (it runs nearly 1000 times faster). They compare favorably, but the **q**-state version shows a few isolated almost singular points, whereas the plane wave version has delocalized differences (due to the representation dependence of handling caustics). Finally, in Fig. 3, we compare the semiclassical ten-bounce state (above) with the actual eigenstate (below). The remarkable precision of the semiclassical approximation is clearly seen. Indeed, the overlap of the unit normalized pair is 0.95.

For this eigenstate, the overlaps with the n-bounce states uniformly increase as a function of n (if even and odd n are grouped separately) as far as our calculation is carried. Surprisingly by only five bounces the overlap is already 0.895. It would be interesting to know how closely the overlap approaches unity with time before it levels off, or, worse yet, even decreases with the addition of the later dynamics. The closer to unity, the more insignificant the effects unaccounted for by the approximation. Most important is the diffraction that occurs when a wave impinges on the joint between the straight edge and semicircular boundaries. Are some eigenstates diffraction free whereas others concentrate its effects?

Although the overlap of the approximate and exact eigenstate increases uniformly as longer time dynamics is incorporated semiclassically, the developing eigenstates do not behave so simply. It is typical for many of the features, especially those of a secondary nature away from the main scar, to appear, fade away, and reappear

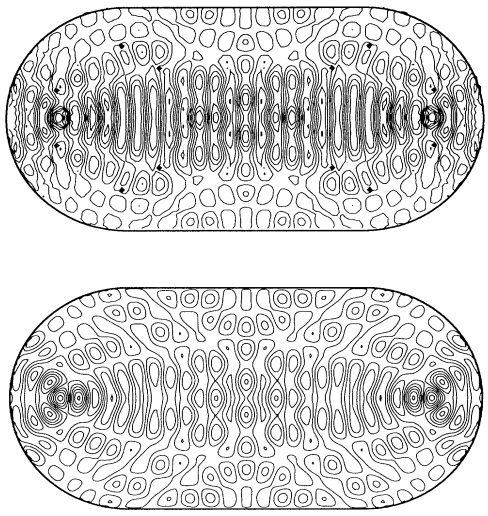

FIG. 2. The quality and difficulties encountered depend somewhat on the basis used. Above, a direct **q**-state basis calculation of the three-bounce dynamics is contoured. Below is its plane wave counterpart. The eigenstate (see Fig. 3) is already emerging. The ten contours are spaced equally, but are set below the very narrow nearly singular points found in the upper drawing.

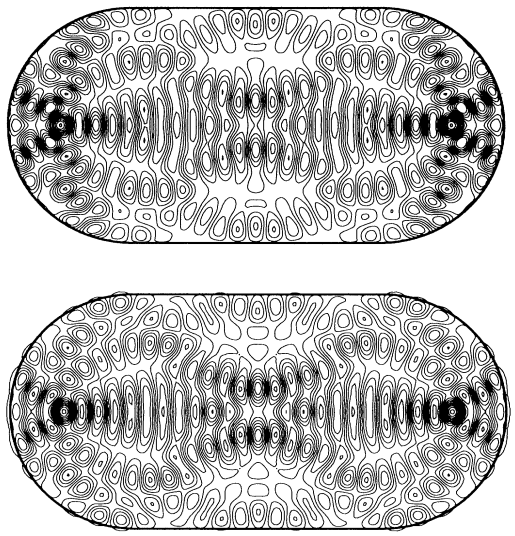

FIG. 3. Shown on top is the semiclassical state that includes all the dynamics up to ten bounces. Below is the eigenstate it is approximating. The 13 contours are equally spaced and placed at exactly the same levels for both states (the states were normalized to unity first).

at later times. In relation to Fig. 3, the effect of the long orbits is to fine tune the peak energy, reinforce the main scar, and fill in the secondary structure more accurately. The relative importance of the roles played by the short and long orbits, respectively, needs to be explored for a sampling of the eigenstates.

We consider our techniques to be in their infancy and believe that further improvements are very probable. Our incorporation of the dynamics is still, in a sense, rather pedestrian. Ten-bounce dynamics only gives access to times of about 2.5 to 3.0 tracings of the horizontal bouncing periodic orbit and requires about 10^6 orbits. This is about half the Heisenberg time at E_j where $t_H = 5.5$. If the dynamics were followed to t_H, approximately 10^{15} orbits would enter the full calculation. It is clear that there is far less information than this in the propagation of $\Phi(\mathbf{q};t)$. Progress in this direction could potentially result in great simplifications.

We have shown by construction that at least some chaotic eigenstates are essentially semiclassical in nature. This is quite puzzling, almost paradoxical. Current indications of the validity of semiclassical theory imply that eigenstates should be impossible to obtain semiclassically in the $\hbar \to 0$ limit. On the other hand, semiclassical methods are supposed to fail in the opposite regime (extreme quantum limit). Is it that somehow this does not exclude the possibility of an intermediate regime where some eigenstates are mostly semiclassical or are the estimates of the time scale of semiclassical breakdown still too pessimistic? It would also be interesting to know what fraction of the eigenstates in a local energy domian could be similarly obtained, especially since no diffraction effects have been incorporated, though they certainly exist in the dynamics. Can states that are not heavily scarred be found and thus be semiclassical in this sense? Independently of the resolution of these questions, the techniques herein developed will allow us to advance beyond the present theory of eigenstate scarring, develop a more complete view of chaotic eigenstates, and dissect the contributions that coherently add to build an eigenstate. We are pursuing these goals.

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