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LETTER TO THE EDITOR

Semiclassical wavefunctions in chaotic scattering systems

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Abstract
We have computed quantum wavefunctions in the high-energy (semiclassical) regime in a system—the stadium billiard with leads allowing particles to enter and escape—exemplifying chaotic scattering. The results exhibit a structure associated with classical paths that is dramatically more pronounced than the scars due to periodic orbits seen in bound systems. Moreover, this structure is seen at all energies. Our results differ significantly from those previously conjectured on the basis of computations in the low-energy regime. The dominant role played by short classical paths is explained by a semiclassical theory based on the analytic structure of the Green function. This is verified by a direct semiclassical computation of wavefunctions using classical scattering trajectories.

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One of the central problems in the field of quantum chaos is to elucidate the semiclassical structure of quantum wavefunctions in systems having a chaotic classical limit. In bound systems, when the classical dynamics is ergodic Shnirelman's theorem [1] asserts that, on scales that are large compared to a de Broglie wavelength, typical eigenfunctions are equidistributed on the corresponding surface of constant energy in phase space in the limit as $\hbar \to 0$. This is consistent with the general expectation that eigenfunctions should be semiclassically related to invariant sets in phase space. On the wavelength scale, fluctuations around this average value are believed to be universal, and to be described by Berry's random wave model [2]. For example, this model is believed to describe statistical properties of individual eigenfunctions, such as spatial correlations defined with respect to averages over position.

In 1984 Heller [3] observed that even in strongly chaotic systems some eigenfunctions are noticeably scarred by (unstable) short periodic orbits; that is, the probability density is enhanced in the vicinity of such orbits. Periodic orbits also represent classical invariant sets, and so this is consistent with the general semiclassical expectation outlined above. Shnirelman's theorem implies that scarred states are rare, in the sense that sequences of states which do not converge to the equidistributed limit have zero density. Recently scarring has been proved to occur in two model systems [4, 5], but not to occur in a third [6]. However, these systems are all atypical and the status of scarring in generic examples remains open.

The basic general semiclassical theories of scarring that have been developed apply to averages of eigenstates over energy ranges in which the number of levels increases as $\hbar \to 0$ [3, 7–10]. This is often referred to as *weak scarring*. In these theories, the energy-averaged eigenfunctions are related to sums over classical periodic orbits which diverge in the limit as the energy averaging range tends to zero. The fine structure of individual eigenfunctions is therefore governed by properties of semiclassically long orbits. Consistency with Shnirelman's theorem is guaranteed by the fact that, when weighted appropriately, these long orbits are themselves equidistributed on the corresponding surface of constant energy in phase space [11].

We focus our attention here on the wavefunctions of chaotic *open* (i.e. scattering) systems [12, 13]. The quantum and semiclassical properties of such systems have been the subject of extensive study [14–16]. Our aim is to demonstrate that for all energies the wavefunctions exhibit structures in the semiclassical regime that are predominantly supported (i.e. dominated) by short classical trajectories. They are therefore far from being equidistributed and far from being universal. We do this by computing high-energy wavefunctions in a system exemplifying chaotic scattering. The results of these computations are explained in terms of a general semiclassical theory. Crucially, this does not rely on energy averaging—the structures we here draw attention to seem to occur at any given energy. Finally, as a test, the theory is used to make direct semiclassical computations of wavefunctions using classical trajectories.

The main conclusion therefore is that semiclassical wavefunctions in chaotic scattering systems are qualitatively different from those in bound systems in that classical trajectories generate the dominant structures, rather than occasionally appearing as decorations. The complexity of these trajectories manifests itself as complexity in the wavefunctions, which have a dramatically richer texture than those in bound systems, where large scale uniformity is the main characteristic. This difference arises because the relevant trajectories in scattering systems are themselves non-uniform, a consequence of the fact that they can escape.

These conclusions differ markedly from conjectures put forward by Akis *et al* [17], who suggested that quantum wavefunctions in classically chaotic scattering systems should be semiclassically scarred by short periodic orbits. We did not find this in our computations. In our case the dominant structures are associated with scattering trajectories rather than periodic orbits. Moreover, these orbits provide the support for the wavefunctions, rather than scarring a quantum-ergodic background. We believe that the difference is due to the fact that the computations reported in [17] relate to relatively low energies and so are not representative of the semiclassical limit.

The system for which we calculate wavefunctions is an open two-dimensional hard-wall Bunimovich stadium with area A coupled to a pair of leads of width d. The stadium is characterized by the radius a of the semicircles and the half-length l of the straight sections. We choose $a = l$ and $d/\sqrt{A} = 0.0935$; the billiard is then maximally chaotic and weakly (but perfectly) open. In the leads, the wavefunctions are quantized in the transverse direction. The maximum number of quantized transmittable modes increases as the energy grows (i.e. as one approaches the semiclassical regime). As an initial condition, a wave in a given propagation mode n enters the cavity. To find the scattered wavefunction ψ for particles entering and leaving the cavity via the leads we solve the time-independent Schrödinger equation with Dirichlet boundary conditions using the plane-wave-expansion method [18]. This method involves discretization of angles for propagation of the base functions, giving rise to a matrix equation that has to be solved numerically. We then apply the singular value decomposition to avoid numerical instability in the solution, obtaining reflection and transmission amplitudes

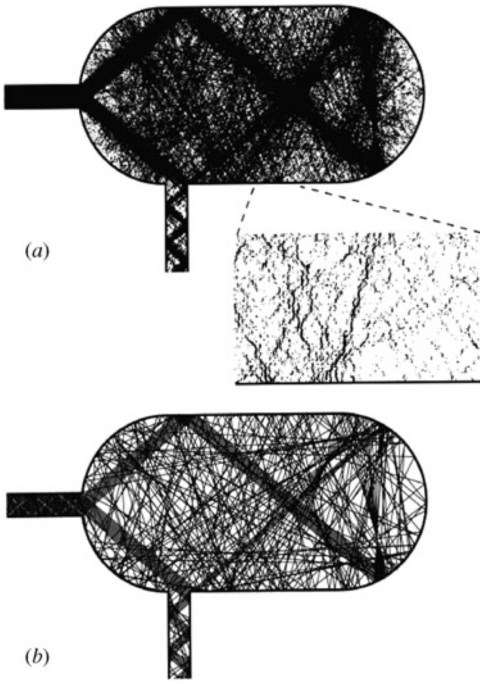

Figure 1. (*a*) The wavefunction probability density and its partial magnification (inset) for $k\sqrt{A} = 2672.3758$ ($kd/\pi = 79.577\,472$). An initial wave in a mode corresponding to $n = 51$ comes through the left lead into the cavity. The density plot shows about 95% of the largest wavefunction probability density. (*b*) Corresponding classical trajectories. Eleven equidistant injection positions with injection angles $\pm\theta_{51} = \pm 0.695\,650\,47$ at the entrance are chosen. The injection angle (both positive and negative) into the cavity is chosen to coincide with the quantization condition in the lead for the initial wave in (*a*). Each trajectory is plotted until it escapes from one of the leads.

and ψ for a given wave number $k = \sqrt{E}$, where E is the energy. This method—principally the introduction of the singular value decomposition—has led to a very significant improvement in our ability to compute the scattered wavefunction in the high-energy regime; for example, we have computed wavefunctions when the ratio of the system dimension to the wavelength is of the order of 1000 (see figures 1 and 2).

The results of our computations show clearly that in all wavefunctions (i.e. at all energies) the dominant structures are associated with classical trajectories that scatter from the incoming lead to the outgoing lead. This is illustrated in figures 1 and 2, where both wavefunctions and trajectories are plotted. Because of the quantization in the transverse direction in the entrance lead, all waves enter the cavity with the fixed angle $\theta_n = \sin^{-1}(n\pi/(kd))$ (with the same probability for $\pm\theta_n$). The trajectories shown also enter with this angle. The quantum wavefunctions are clearly far from uniform in the stadium—instead they inherit the complex hyperbolic structure of the classical orbits, as well as caustics, right down to the finest scales. This structure can be perceived even for orbits that make many bounces on the boundaries of the cavity (it even continues into the exit lead). It is apparent that it is nonuniversal. We emphasize that the pictures represent wavefunctions associated with particular energies, rather than energy averages, and that they represent typical rather than special behaviour. We also

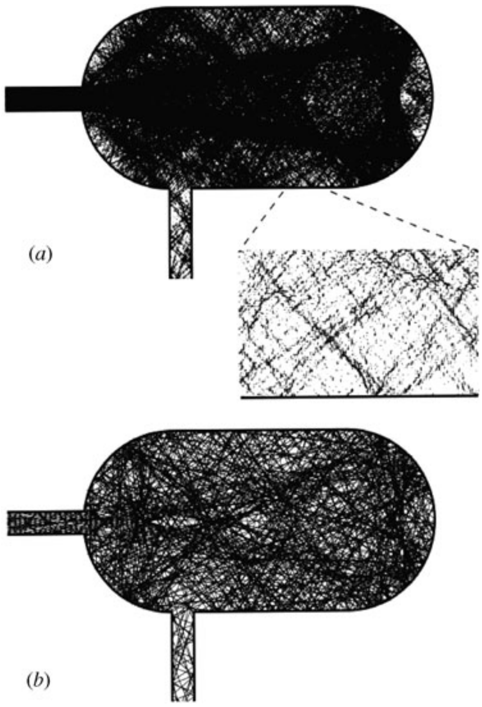

Figure 2. (a) The wavefunction probability density and its partial magnification (inset) for $k\sqrt{A} = 3046.8419$ ($kd/\pi = 90.728\,249$). An initial wave in a mode corresponding to $n = 16$ comes through the left lead into the cavity. The density plot shows about 95% of the largest wavefunction probability density. (b) Corresponding classical trajectories. Eleven equidistant injection positions with injection angles $\pm\theta_{16} = \pm 0.177\,277\,92$ at the entrance are chosen. The injection angle (both positive and negative) into the cavity is chosen to coincide with the quantization condition in the lead for the initial wave in (a). Each trajectory is plotted until it escapes from one of the leads.

point out that diffraction effects due to the opening corners are relatively small at these high energies.

In order to understand the classical structures apparent in figures 1 and 2 we develop a simple semiclassical theory. This generalizes straightforwardly to quantum scattering in all chaotic systems. We begin with the wave number dependent (or energy-dependent, i.e. time-independent) Green function for open (unbounded) systems with partial boundary conditions. This may be expressed as

$$G(\mathbf{q}', \mathbf{q}; k) = \int \frac{\psi_\gamma^*(\mathbf{q}')\psi_\gamma(\mathbf{q})}{k^2 - k_\gamma^2} d\gamma \tag{1}$$

where the wavefunctions ψ_γ corresponding to the wave numbers k_γ form a complete orthonormal set and individually satisfy the boundary conditions. The Green function for open systems can also be expressed as a sum over resonances in the complex plane:

$$G(\mathbf{q}', \mathbf{q}; k) = \sum_r \frac{\phi_r(\mathbf{q}', \mathbf{q})}{k^2 - \alpha_r^2} \tag{2}$$

where α_r and $\phi_r(\mathbf{q}', \mathbf{q})$ are, respectively (complex) resonance poles and strengths, $\mathrm{Re}\,\alpha_r > 0$, and $\mathrm{Im}\,\alpha_r < 0$.

The connection with classical mechanics is achieved using the semiclassical approximation to the Green function. For systems with two degrees of freedom, this is [19]

$$G^{SC}(\mathbf{q}', \mathbf{q}; k) = \sum_{p(\mathbf{q}\to\mathbf{q}')} k^{-1/2} A_p \exp\left[\mathrm{i}\left(kl_p - \frac{\pi}{2}\nu_p\right)\right]. \tag{3}$$

Here l_p and ν_p denote, respectively, the length and the Maslov index of the path p, and $k^{-1/2}A_p \equiv (1/\sqrt{2\pi\mathrm{i}})\sqrt{\det(D_p(k))}$ where $D_p(k)$ denotes its weighting (deflection) factor. In the case of free motion, such as in billiard geometries, A_p does not depend on k. The semiclassical Green function $G^{SC}(\mathbf{q}', \mathbf{q}; k)$ describes the probability amplitude for propagation from $\mathbf{q}$ to $\mathbf{q}'$ at a fixed wave number k in terms of a sum over all classical paths (labelled p) connecting these two points.

Fourier transforming the Green functions in equations (2) and (3) gives [20]

$$-\frac{\mathrm{i}}{2}\sum_r \frac{\phi_r(\mathbf{q}', \mathbf{q})}{\sqrt{\alpha_r}} \exp(-\mathrm{i}\alpha_r|x|) \approx \sum_p A_p \exp\left(-\mathrm{i}\frac{\pi}{2}\nu_p\right)\delta(l_p - x). \tag{4}$$

After integrating each side of this equation from $x = X(>0)$ to ∞ we obtain

$$-\frac{1}{2}\sum_r \frac{\phi_r(\mathbf{q}', \mathbf{q})}{\alpha_r^{3/2}} \exp(-\mathrm{i}\alpha_r X) = \sum_{p(l_p>X)} A_p \exp\left(-\mathrm{i}\frac{\pi}{2}\nu_p\right). \tag{5}$$

This shows that (i) when most of the poles α_r are located very close to the real axis, the semiclassical contribution of paths with lengths larger than X is highly oscillatory, because of the oscillatory exponential factor on the left-hand side of equation (5); (ii) when most of the poles are located far from the real axis, the semiclassical contribution coming from paths with lengths larger than X vanishes exponentially, because of the exponential decay factor on the left-hand side of equation (5). If the system is almost (or completely) closed, (i) is the case and the semiclassical contribution of shorter paths to the semiclassical wavefunction is dominant only after averaging out the oscillatory contributions coming from the longer paths, as in the weak scarring theories of Heller [3], Bogomolny [7] and Berry [8] for bound systems. On the other hand, if the system is completely open, (ii) is the case and the semiclassical contribution of shorter paths dominates the wavefunctions without any need for averaging. The maximal length scale X for the semiclassical contribution to be important may be estimated in terms of the decay rate, the distance scale of the poles α closest to the real axis, to be $X = |\mathrm{Im}[\alpha]|^{-1}$. In the open billiard system we study here, X is roughly of the order of $10\sqrt{A}$ [21].

These results suggest that semiclassical approximations to quantum wavefunctions in scattering systems based on using only short paths should be much more accurate than in bound systems. They thus explain the dominant role played by classical paths in the quantum wavefunctions plotted in figures 1 and 2. They are in agreement with previous results concerning the spectral analysis of quantum fluctuating scattering amplitudes [22].

To make this connection more explicit we use the fact that the wavefunction $\psi(\mathbf{q})$ can be related directly to the semiclassical Green function. The initial wavefunction at the entrance may be written in the form

$$\psi_{\mathrm{in}} = \psi_n(\eta) \equiv \sqrt{2/d}\,\sin[(n\pi/d)(\eta + d/2)] \tag{6}$$

where η is a local coordinate in the transverse direction at the entrance. Then we have a general expression for the wavefunction in the cavity region in the form

$$\psi(\mathbf{q}') = \int G(\mathbf{q}', \mathbf{q}(\eta); k)\psi_n(\eta)\,\mathrm{d}\eta. \tag{7}$$

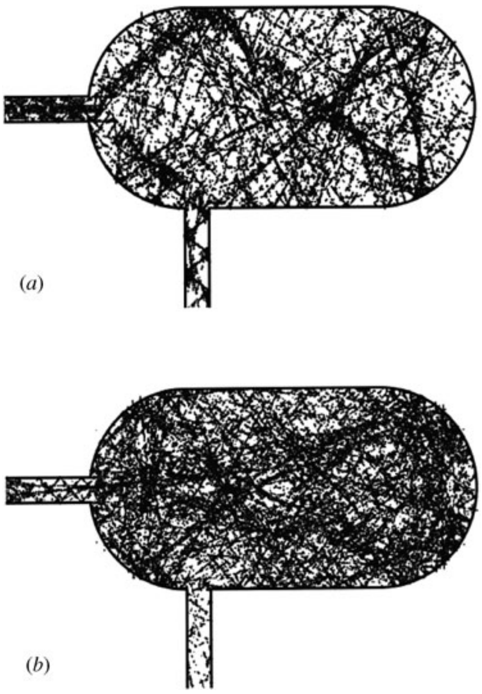

Figure 3. Semiclassical wavefunction probability densities for (a) $k\sqrt{A} = 2672.3758$ with $n = 51$ and (b) $k\sqrt{A} = 3046.8419$ with $n = 16$. An initial wave in a mode n comes through the left lead into the cavity. The density plot shows about 95% of the largest wave probability density. The classical trajectories shown in figures 1(b) and 2(b) are used for the semiclassical calculations in (a) and (b), respectively.

Applying the stationary phase approximation to the integral in equation (7) gives

$$\psi(\mathbf{q}') \approx \int G^{SC}(\mathbf{q}', \mathbf{q}(\eta); k)\psi_n(\eta)\,\mathrm{d}\eta$$
$$= \sqrt{\frac{2}{kd}} \sum_{p(\mathbf{q}(\pm\theta_n;\eta_p)\to\mathbf{q}')} A_p \exp\left[\mathrm{i}\left(kl_p - \frac{\pi}{2}\nu_p\right)\right] \sin\left[\frac{n\pi}{d}\left(\eta_p + \frac{d}{2}\right)\right]. \tag{8}$$

This expression allows for the direct calculation of the semiclassical approximation to wavefunctions using scattering paths. As we see in figure 3, this approximation agrees well with the exact quantum wavefunctions in the high-energy regime, plotted in figures 1(a) and 2(a). In particular, the structure associated with the classical paths is manifestly captured. As a crude test we computed the variance $\int |\psi(\mathbf{q}) - \psi^{SC}(\mathbf{q})|^2\,\mathrm{d}\mathbf{q}$ per unit area in the billiard and obtained significantly smaller values (1.04 for figures 1(a) and 3(a); 1.47 for figures 2(a) and 3(b)) for the same wavefunction compared to when the wavefunctions correspond to different states (2.27 for figures 2(a) and 3(a); 1.74 for figures 1(a) and 3(b)).

In conclusion, we have demonstrated that the wavefunctions in systems exhibiting chaotic scattering possess a rich and complex structure in the semiclassical regime associated with short classical scattering trajectories. Unlike in bound systems, they are therefore far from being equidistributed and far from being universal. This behaviour can be understood in terms of the decay properties of scattering systems.

Chaotic scattering systems are often used as models for transport through mesoscopic open devices. We note that the statistical properties of conductance fluctuations in such devices are universal. However, this emerges after averaging over energy, i.e. by sampling data at different energies. The nonuniversal features we draw attention to here relate to spatial correlations in wavefunctions at particular (fixed) energies. This distinction between spatial averaging and energy averaging is a key difference with respect to closed systems. It is also the case that we are considering systems in which the incoming and outgoing leads are semiclassically wide enough that the short-time dynamics dominates.

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