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Bound-State Eigenfunctions of Classically Chaotic Hamiltonian Systems: Scars of Periodic Orbits

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Certain unstable periodic orbits are shown to permanently scar some quantum eigenfunctions as $\hbar \rightarrow 0$, in the sense that extra density surrounds the region of the periodic orbit.

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Periodic orbits have played a large role in the theory of semiclassical quantization of bound states. Applications have involved the Green's-function coordinate-space trace formula, which squarely places the burden of quantization on a sum over classically periodic orbits, in the asymptotic (stationary phase) limit. In particular, Gutzwiller,¹ Berry and Tabor,² and Balian and Bloch³ have made much progress with level densities and eigenvalues of nonintegrable systems using periodic-orbit theory. In the mathematical literature, the related Selberg trace formula gives exact eigenvalues for the Laplacian in certain cases as sums over all periodic orbits (see Hejhal⁴).

These earlier studies have been concerned with eigenvalues. Here, I outline a proof of an important effect of short-term, unstable periodic orbits on the *eigenfunctions* of classical chaotic systems: They induce "scars" of larger than expected density in at least some of the wave functions. The scars coalesce around the unstable periodic orbit ever more closely as $\hbar \rightarrow 0$. These are new implications of periodic-orbit theory for *eigenfunctions* of chaotic systems.

In the pioneering studies by McDonald⁵ (see also McDonald and Kaufman⁶), what are here called "scars" were noticed for the stadium billiard system, but their connection with the periodic orbit ("rays") was termed "unknown," and "an enigma." My own work on smooth potentials⁷ showed similar scarring effects.

In the irregular (chaotic) classical regime, phase space may be dense with strictly periodic orbits, but their measure is zero.⁸ All the periodic orbits are unstable, but the stability parameter governing the exponential separation varies from orbit to orbit. We focus on that small subset of periodic orbits with the shortest periods and the smallest separation rates. It is assumed that orbits of similar periods and stabilities are isolated.

The classical equations governing stability of orbits are expressed in terms of small deviations δp_t in momentum and δx_t in position from the reference trajectory. They are (mass = 1)

$$\frac{d}{dt} \begin{pmatrix} \delta p_t \\ \delta x_t \end{pmatrix} = \begin{pmatrix} 0 & -V'' \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \delta p_t \\ \delta x_t \end{pmatrix}, \quad (1)$$

where V'' is the $N \times N$ matrix of second derivatives of $V(x)$ at x_t , 1 is the $N \times N$ unit matrix, 0 the $N \times N$ null matrix, and δp_t , δx_t are $N \times 2N$ matrices corresponding to the $2N$ linearly independent deviations about the reference trajectory. The deviations δp_t and δx_t may be expressed in terms of the initial deviations δp_0 and δx_0 as

$$\begin{pmatrix} \delta p_t \\ \delta x_t \end{pmatrix} = M \begin{pmatrix} \delta p_0 \\ \delta x_0 \end{pmatrix}, \quad (2)$$

where M is the so-called monodromy matrix.⁸

Equations (1) and (2), together with the trajectory (x_t, p_t) and the action integral $\phi_t = \int p_t \cdot dx_t - Et$ are sufficient to propagate Gaussian wave packets semiclassically.⁹ They take the form

$$g(x, t) = \exp \{ (i/\hbar) [(x - x_t) \cdot A_t \cdot (x - x_t) + p_t \cdot (x - x_t) + \gamma_t] \}, \quad (3a)$$

where

$$A_t = \frac{1}{2} \delta p_t \cdot (\delta x_t)^{-1}, \quad (3b)$$

and

$$\gamma_t = \phi_t + \frac{1}{2} i\hbar \text{Tr}[\ln \delta x_t \cdot (\delta x_0)^{-1}] + \gamma_0. \quad (3c)$$

For our present purposes, (x_t, p_t) will be the periodic orbit.

Hepp¹⁰ and Hagedorn¹¹ showed that such semiclassical Gaussian wave packet dynamics are *arbitrarily accurate* for any finite time t , as $\hbar \rightarrow 0$. Choosing our $g(x, 0)$ to be centered on a periodic orbit can make precise statements about the time evolution $g(x, t)$, and thus the partially resolved spectrum

$$\epsilon_T(\omega) = (1/2\pi) \int_{-T}^T \exp(i\omega t) \langle g | g(t) \rangle dt \quad (4a)$$

$$= (1/\pi) \sum_n \{ [\sin(E_n/\hbar - \omega) T] / (E_n/\hbar - \omega) \} |\langle g | \psi_n \rangle|^2. \quad (4b)$$

In Eq. 4(b) we see that $\epsilon_T(\omega)$ is a smoothed version of the fully resolved spectrum, $\epsilon_\infty(\omega)$.

As discussed before,¹² the main qualitative features of $|\langle g | g(t) \rangle|$ are (1) a rapid decay to zero, and (2) recurrences of decreasing strength at multiples of the period of the orbit, τ . The strengths are determined by the monodromy matrix M , and the matrices A_0 and A_t . Since the motion is unstable in the chaotic regime, M will have at least one real, positive characteristic exponent (RPCE). The decay of $|\langle g | g(t) \rangle|$ at multiples of the period can be shown to go approximately as $\exp[-n\tau\lambda/2]$, where λ is the sum of the RPCE's. For small \hbar , the series of recurrences is long over before the overlap reactivates. The decay of the series of recurrences is due to spreading of the Gaussian wave packet.

The consequence of (1) and (2) for $\epsilon_T(\omega)$, where T is taken to be some time after the recurrences have exhausted themselves, is a structured spectrum with an overall width $\propto \hbar^{1/2}$. The structure takes the form of broadened bands (regions of larger spectral density) spaced by $\delta E = \hbar\omega = h/\tau$, with a bandwidth $\hbar\lambda$. The ratio of the width to the spacing is λ/ω , independent of \hbar .

Berry's conjecture¹³ states that "each semiclassical eigenstate has a Wigner (phase space) function concentrated on the region explored by a typical orbit over *infinite times*" (italics added). This was taken further in the case of irregular motion to imply *uniform* concentration, as embodied in the microcanonical density (see also Voros¹⁴)

$$\rho_m(p, x) = \delta[E - H(p, x)]/D(E), \quad (5)$$

where $D(E)$ is the density of states and H is the Hamiltonian. From this we easily estimate the *a priori* spectral intensity

$$I_n = |\langle g | \psi_n \rangle|^2 = \text{Tr}(\rho_g \rho_\psi) \\ \simeq \text{Tr}(\rho_g \rho_m) = S_g(E_n)/D(E_n), \quad (6)$$

where $S_g(E)$ is the normalized energy probability distribution for $g(x, 0)$. $S_g(E)$ is also the low-resolution version of the spectrum, i.e., $\epsilon_T(\omega)$ for

T sometime after the first decay but before the first recurrence.

The existence of the bands imposes new requirements on the intensities I_n . A band near $E \approx E_b$ will have a strength (total intensity) $S_g(E_b)/D_b$, where D_b is the density of bands. Since $\hbar\omega$ is the spacing of these bands, $D_b = (\hbar\omega)^{-1}$. The bandwidth of $\hbar\lambda$ implies there are $\hbar\lambda D(E)$ states under the band. These must collectively have the band strength $S_g(E_b)/D_b$, so if they share this burden equally they must have a higher intensity

$$I_n^b = [S_g(E_b)/D_b]/[\hbar\lambda D(E_b)] \\ = (\omega/\lambda) I_n > I_n. \quad (7)$$

If the burden is not shared equally, then some eigenstates must have even higher intensities. Thus, for large ω/λ , the square of the overlap $|\langle g | \psi_n \rangle|^2$ for some subset of the ψ_n must be large compared to the statistical estimate, Eq. (6).

Moreover, since

$$|\langle g | \psi_n \rangle|^2 = |\langle g(t) | \psi_n \rangle|^2, \quad (8)$$

a ψ_n with large overlap with $|g\rangle$ has large overlap with $|g(t)\rangle$, which is localized periodic orbit for the first period for large ω/λ . Thus, ψ_n has large probability all along the periodic orbit.

If $g(x, 0)$ is launched just off the periodic orbit, then as $\hbar \rightarrow 0$ there will be no recurrences; the spectrum will be unstructured, and no extra localization to that off-periodic orbit region is implied.

The scars are expected to be most prominent around periodic orbits with large ω/λ . The factor ω/λ controls the local density enhancement of the scar and is \hbar independent. As $\hbar \rightarrow 0$, the scar narrows around the periodic orbit, while maintaining a constant density along the orbit. In this way, the scar "heals" as $\hbar \rightarrow 0$.

We have shown the scars manifest themselves as enhanced probability in phase space, as measured by overlap with coherent states placed on the periodic orbits. This translates also into enhanced

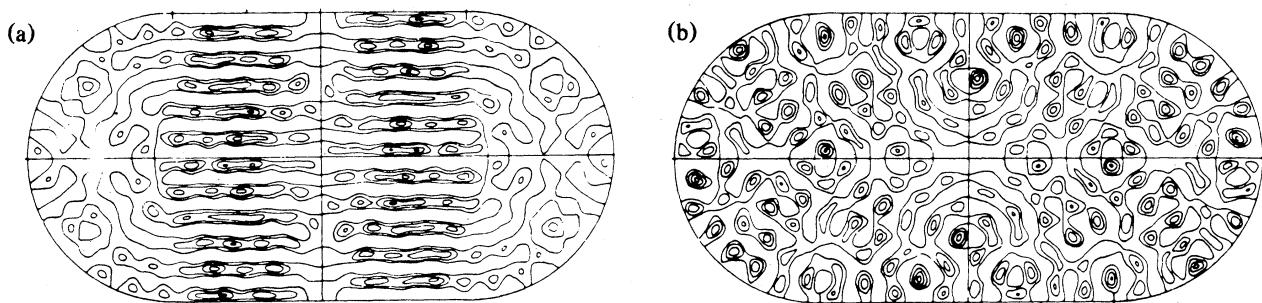


FIG. 1. (a) Localized and (b) chaotic states of the stadium potential; only the negative contours are shown. From Ref. 15, with permission.

probability in *coordinate* space along the periodic orbits. The conjecture that the wave functions would be Gaussian random as $\hbar \rightarrow 0^{13}$ must now be modified to incorporate the presence of scars.

The wave functions shown in Fig. 1, computed by Taylor and Brumer¹⁵ using the algorithm of McDonald and Kaufman,⁵ illustrate the difference between the ergodiclike states [Fig. 1(b)] and the

states affected by periodic orbits [Fig. 1(a)]. The state of Fig. 1(a) reflects the existence of the *non-isolated* periodic orbits which bounce perpendicularly to the flat walls of the stadium, and it may be viewed as a “superscar,” resulting from the overlap of many scars. However, it does not fit the theory presented above because the orbits are not isolated.

The stadium potential, which is ergodic, also pro-

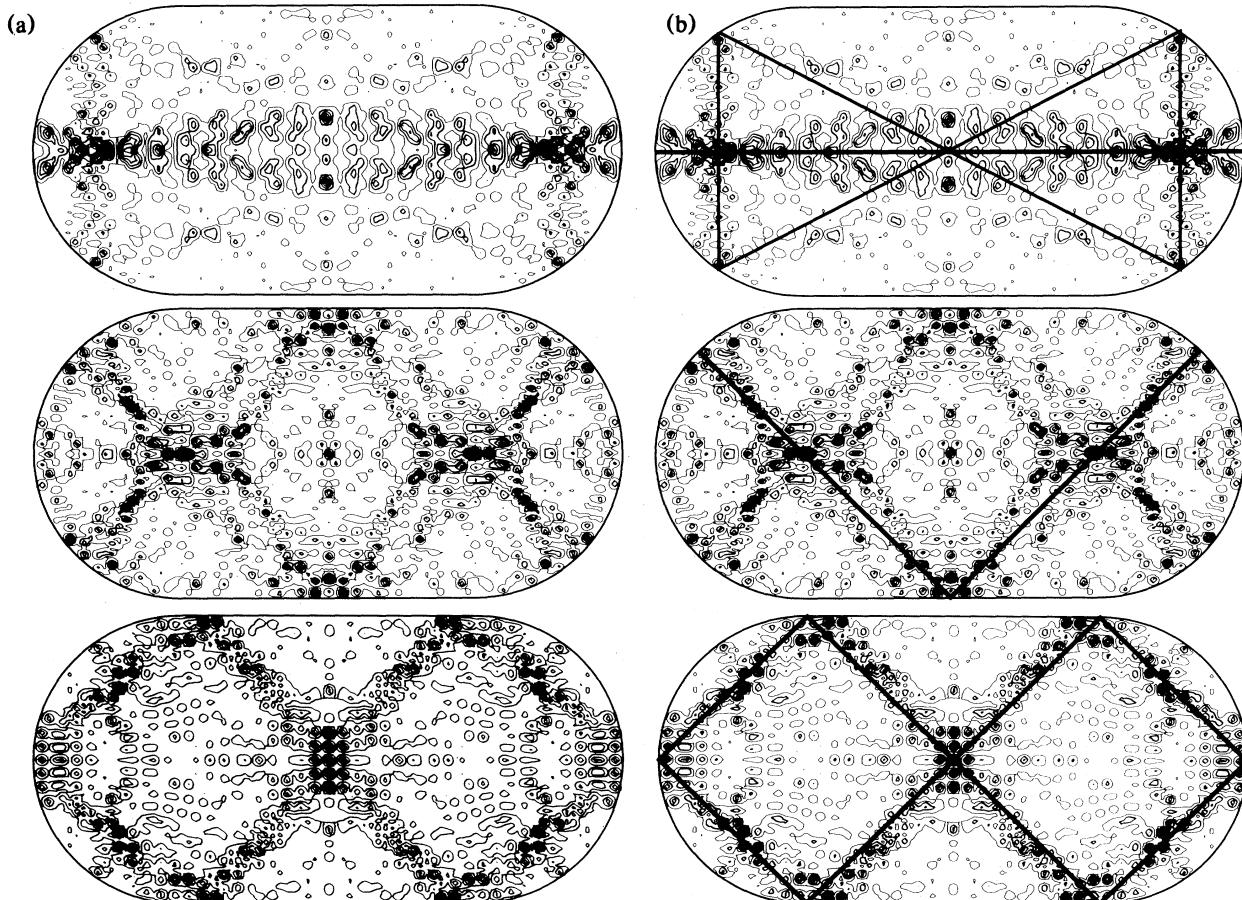


FIG. 2. Left column, three scarred states of the stadium; right column, the isolated, unstable periodic orbits corresponding to the scars.

vides clear examples of scars due to *isolated* unstable orbits. Figure 2, shows three scarred eigenfunctions of the stadium, and the major contributing periodic orbit in each case. These are just a few of nearly a dozen types of scars found so far, using a simple algorithm written by the author.

These scars are considerably *denser* than the factor ω/λ , (at least by a factor of 10), which for the horizontal bounce case is only 1.8, and for the *V*-shaped orbit, only 1.5. The factor ω/λ is a *lower bound* to the scar density. First, we noted that ω/λ obtains when the states under the bands share the burden of the intensity of the band democratically. This need not be the case, which implies that some states are scarred to an extent greater than ω/λ .

Since these scarred states are so ubiquitous (about half the states have one or more recognizable scars), it seems unlikely that *any* eigenstate of the stadium is ergodic. It is true for example that the state in Fig. 1(b) looks ergodic, but one can easily be misled by looking only in coordinate space.

A theme of the investigations in Ref. 2 has been that periodic orbits say much about level densities. In particular, the periodic orbits of the type we have been considering induce fluctuations in the otherwise smooth background density of states. Clearly, an analogy exists between this and the density fluctuations (scars) we have shown must exist for the eigenfunctions.

Gutzwiller¹⁶ has emphasized extraction of eigenvalues of chaotic systems using periodic orbits. Extension of the analogy of the previous paragraph suggests that more detailed features of the eigenfunctions can be determined by the periodic orbits.

Very often the underlying classical mechanics is not so simple as an isolated, unstable periodic orbit. For example, complex regions of phase space, involving many similar periodic orbits and island structures may exist in small domains. Our theory does not strictly apply to such cases, but it seems evident that increasing the density of similar periodic orbits can only enhance the scarring effect.

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¹M. C. Gutzwiller, *J. Math. Phys.* **12**, 343 (1971), and references therein.

²M. V. Berry and M. Tabor, *Proc. Roy. Soc. London, Ser. A* **349**, 101 (1976), and *J. Phys. A* **10**, 371 (1977); M. V. Berry, *Ann. Phys. (N.Y.)* **131**, 217 (1981).

³R. Balian and C. Bloch, *Ann. Phys. (N.Y.)* **85**, 514 (1974), and references therein.

⁴D. A. Hejhal, *The Selberg Trace Formula for PSL(2, R), Parts 1 and 2*, Springer Lecture Notes in Mathematics, Vols. 548 and 1001 (Springer, Berlin, 1976 and 1983).

⁵S. W. McDonald, Lawrence Berkeley Laboratory Report No. LBL-14837, 1983 (unpublished).

⁶S. W. McDonald and A. N. Kaufman, *Phys. Rev. Lett.* **42**, 1189 (1979).

⁷E. J. Heller and R. L. Sundberg, "Proceedings of the NATO Conference on Quantum Chaos" (Plenum, New York, to be published); R. L. Sundberg and E. J. Heller, to be published; E. B. Stechel and R. L. Sundberg, to be published.

⁸V. I. Arnold and A. Avez, *Ergodic Problems of Classical Mechanics* (Benjamin, New York, 1968).

⁹E. J. Heller, *J. Chem. Phys.* **65**, 4979 (1976).

¹⁰K. Hepp, *Commun. Math. Phys.* **35**, 265 (1974).

¹¹G. A. Hagedorn, *Commun. Math. Phys.* **71**, 77 (1980).

¹²E. J. Heller, E. B. Stechel, and M. J. Davis, *J. Chem. Phys.* **73**, 4720 (1980); E. J. Heller, *J. Chem. Phys.* **72**, 1337 (1980).

¹³M. V. Berry, in *Chaotic Behavior of Deterministic Systems*, edited by G. Iooss, R. Hellman, and R. Stora, Les Houches Summer School Proceedings No. 36 (North-Holland, New York, 1981), Chap. 4.

¹⁴A. Voros, in *Stochastic Behavior in Classical and Quantum Hamiltonian Systems*, edited by G. Casati and J. Ford, Springer Lecture Notes in Physics, Vol. 93 (Springer, Berlin, 1979).

¹⁵R. D. Taylor and P. Brumer, *Faraday Discuss. Chem. Soc.* **75**, 170 (1983).

¹⁶M. C. Gutzwiller, *Physica (Utrecht)* **5D**, 183 (1982).