Fine structure of the wave functions of quantum systems

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The wave functions of quantum systems which are ergodic in the classical limit, $\hbar \to 0$, have an elevated density near unstable periodic paths. The mean square value of the wave function near a periodic orbit is expressed in terms of the monodromy matrix of the orbit. The results are compared with numerical calculations of the wave functions for a stadium billiard system.

1. Let us examine the structure of the semiclassical wave functions for nonintegrable quantum systems, i.e., systems for which some of the classical orbits of the given problem do not lie on invariant tori. In this case the ordinary semiclassical-quantization rules, of the Bohr-Sommerfeld type, are not applicable,[1] and the proper-

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ties of the wave functions and the energy levels in the limit $\hbar \to 0$ have not been studied adequately.

In this letter we show that the wave functions of such systems have an elevated density near unstable periodic orbits of the corresponding classical problem. The mean square value of the wave functions near a given periodic orbit is expressed in terms of the elements of the monodromy matrix of this orbit. Speaking a bit freely, we might say that the quantum stochastic nature reveals latent ordered structures of the classical motion. In classical mechanics, these structures have a zero measure and can be observed only if the initial conditions are chosen directly on the periodic orbits (and on their incoming separatrices).

2. We denote by $G(q'',q',E)$ the Green's function of the Schrödinger equation in the energy representation. We can then write

$$\langle |\psi(q)|^2 \rangle \equiv \frac{1}{N} \sum_{\{n\}} |\psi_n(q)|^2 = \frac{\langle \operatorname{Im} G(q, q, E) \rangle}{\int \langle \operatorname{Im} G(q, q, E) \rangle dq}, \tag{1}$$

where the angle brackets mean an average over the region $E_0 - \Delta E/2 < E < E_0 + \Delta E/2$, the sum is over all the eigenfunctions with energies in the given interval, and N is the number of such functions.

In the limit $\Delta E \to 0$ and $E_0 \to E_n$, this relation has different meanings for systems which are and are not integrable. For multidimensional integrable problems, a degeneracy of highly excited levels is unavoidable, and the sum in (1) includes a large number of degenerate states. For nonintegrable systems of general position, only an accidental degeneracy is possible, and the right side of this formula becomes the square modulus of the individual wave function.

3. The calculations below are based on the standard expression for the semiclassical limit of the Green's function as a sum over all classical orbits connecting two points (see, e.g., Refs. 2 and 3 and the bibliographies there). In $2D$ space we would have

$$\begin{aligned} G(q, q, E) &= \tilde{G}(q, E) + G^{osc}(q, E), \\ \tilde{G}(q, E) &= -\pi i \delta(E - H(p, q)) \frac{d^2p}{(2\pi\hbar)^2}, \\ G^{osc}(q, E) &= \frac{1}{i\hbar(2\pi i\hbar)^{1/2}} \sum |\Delta|^{1/2} \exp\left(\frac{i}{\hbar} S(q, q, E) - i\nu\frac{\pi}{2}\right), \end{aligned} \tag{2}$$

where $\tilde{G}(q,E)$ is the contribution of orbits of zero length, which correspond to the Thomas-Fermi approximation, $G^{osc}(q,E)$ is the contribution of classical orbits with a finite action $S(q,q,E)$, Δ is a determinant of the second derivatives of the action, and ν is the phase, equal to the number of conjugate points on an orbit. For billiard systems, under the condition that the wave function vanishes at the boundary, we would have to add to ν twice the number of reflections from the boundary. Assuming $G^{osc} \ll \tilde{G}$ and $H(p,q) = \frac{1}{2}p^2 + U(q)$, we find

$$\langle |\psi(q)|^2 \rangle = \frac{1}{V}\left(1 - 2\hbar^2\left(\langle \operatorname{Im} G^{osc} \rangle - \frac{1}{V}\int \langle \operatorname{Im} G^{osc} \rangle \, dq\right)\right), \tag{3}$$

where V is the area of the allowed region in q space [outside this region, the first term in (3) vanishes].

4. Formally, the sum in $G^{osc}(q,E)$ includes all classical orbits with a fixed energy which begin and end at point q. The time of the motion along the orbit can be arbitrarily long. There are an infinite number of such orbits, and for nonintegrable problems a summation over them is essentially impossible (incidentally, see Ref. 4), or at any rate it would not be simpler than to solve the Schrödinger equations directly. Since the adjacent energy levels and the small-scale fluctuations of the wave functions can reasonably be described by a statistical approach,[1,5] an exact calculation of the Green's function would apparently be pointless. We smooth the wave functions over both the energy and the coordinates. After taking an average over the interval ΔE, we find that (2) is dominated by classical orbits along which the time of motion, $T = \partial S/\partial E$, is bounded: $T \lesssim 2\pi\hbar/\Delta E$. Analogously, after an average is taken over a small interval Δq, a significant contribution is made to the sum by orbits for which the momentum change $\Delta p = \partial S/\partial q'' + \partial S/\partial q'$ is small: $\Delta p \lesssim \hbar/\Delta q$. If, under the condition $\Delta p \neq 0$, the matrix of second derivatives is not degenerate, then near the given orbit there will be a periodic orbit on which the relation $\partial S/\partial q'' + \partial S/\partial q' = 0$ holds with $q'' = q'$. This result means that after these averages are taken, the semiclassical Green's function receives contributions from only those orbits which lie in a small neighborhood of short-period paths. Here it is being assumed implicitly that these periodic orbits are isolated (and hyperbolic). For ergodic systems, no other cases are possible (except families of neutral orbits).

5. Near the periodic orbit we introduce a coordinate system whose x axis runs along the orbit, and whose y axis runs perpendicular to it. After some simple calculations we find

$$\langle G^{osc}(q,E) \rangle = \frac{1}{i\hbar(2\pi i\hbar)^{1/2}} \sum_{\substack{\text{per.}\\ \text{path}}} \frac{D(x)^{1/2}}{|\dot{q}(x)|} \exp\left(\frac{i}{\hbar}\left(\bar{S} + \frac{w(x)}{2}y^2\right) - i\bar{\nu}\frac{\pi}{2}\right), \tag{4}$$

where $|\dot{q}(x)|$ is the modulus of the velocity along the periodic orbit,

$$D(x) = 1/M_{12}(x), \qquad w(x) = (M_{11}(x) + M_{22}(x) - 2)D(x),$$

and $M_{ij}(x)$ are elements of the monodromy matrix in the variables $y, \dot{y}$ at the point x over a period:

$$\begin{pmatrix} y(T) \\ \dot{y}(T) \end{pmatrix} = \begin{pmatrix} M_{11}(x) & M_{12}(x) \\ M_{21}(x) & M_{22}(x) \end{pmatrix} \begin{pmatrix} y(0) \\ \dot{y}(0) \end{pmatrix}. \tag{5}$$

The summation in (4), in contrast with that in (2), is over a finite number of periodic orbits with a period $T \lesssim 2\pi\hbar/\Delta E$, where ΔE is the interval of the averaging over the energy (the sum also includes repeated traversals of a single orbit).

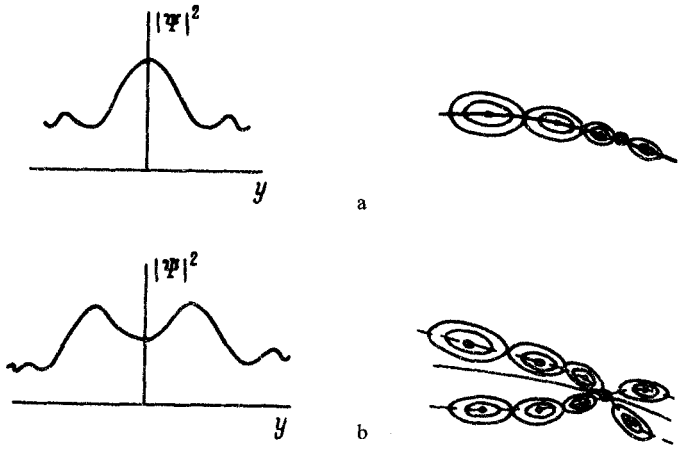

FIG. 1. Illustrative behavior of the mean square value of the wave function near an unstable periodic orbit. Shown at the left is a section across the orbit; shown at the right is the relief of the wave function along the orbit.

Expressions (3) and (4) relate the mean square wave function near the periodic orbit to classical quantities characterizing this orbit. The contribution of each periodic orbit is proportional to $\sqrt{\hbar|D|}/|\dot{q}|$ and is significant in a narrow band of width $\sqrt{2\pi\hbar/|w|}$ near it. Depending on the values of the parameters, the wave function may reach its maximum either on the periodic orbit itself (Fig. 1a) or at some distance. proportional to $1/\sqrt{|w|}$, from it (Fig. 1b). A significant increase in $\langle|\psi(q)|^2\rangle$ will be observed near points at which we have $D\to\infty$. These points (which are analogs of caustics) are self-focusing points, at which the outgoings rays come back together after a period. Near these points, the simple semiclassical approximation in (2) is not applicable. The corresponding equations are given in Ref. 6, among other places. An increase in the density will also occur near sharp changes in the direction of an orbit.

6. Let us consider a model quantum-mechanical problem: that of determining the eigenfunctions of the Laplacian with homogeneous boundary conditions in a "stadium" region, i.e., a square of side $2R$ flanked by two semicircles of radius R. Heller[7] asserted that in this problem a significant fraction of the highly excited wave functions have an elevated density near periodic orbits. When calculations are carried out on the basis of (4), the short-period orbits which are required and their monodromy matrices are not difficult to find numerically. For simple orbits, the calculations can be carried out analytically. Let us look at some results of calculations which have been carried out (Fig. 2). For hyperbolic orbits without reflections, the wave functions has the form shown in Fig. 1b. A double-humped structure structure of this sort can be seen quite well in the figures in Ref. 7. The periodic orbit shown in Fig. 2b has an interesting feature. The square modulus of the wave function is ordinarily symmetric with respect to a periodic orbit, but this is not the case for this particular orbit, because it is reflected for singular points of the boundary, where the second derivative is discontinuous. As a result, there is not just one monodromy matrix (5) corresponding to it, but

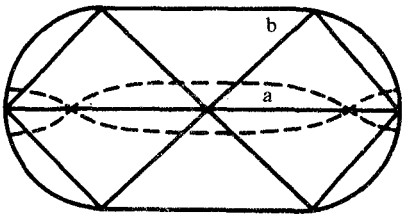

FIG. 2. Some periodic orbits for a stadium billiard system. a—Simplest periodic orbit; dashed line—position of the maxima of the wave function near the orbit; b—singular periodic orbit.

four, corresponding to the different signs of y and $\dot{y}$. As a result, the wave function is significantly larger on one side of a periodic orbit. This is precisely the behavior which Heller observed in Ref. 7. It is not possible to make a quantitative comparison with the results of Heller's paper, since it did not report the values of the energy corresponding to the figures showing the relief of the wave functions.

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