Diffractive Orbits in Quantum Billiards

Nicolas Pavloff and Charles Schmit
Division de Physique Théorique, Institut de Physique Nucléaire, F-91406 Orsay Cedex, France
(Received 24 February 1995)

We study diffractive effects in two-dimensional polygonal billiards. We derive an analytical trace formula accounting for the role of the nonclassical diffractive orbits in the quantum spectrum. As an illustration, the method is applied to a triangular billiard.

PACS numbers: 05.45.+b, 03.65.Sq

During the last decade several methods based on periodic orbit (PO) theory have been successfully employed to study quantum systems whose classical equivalent is chaotic (see, e.g., [1]). PO theory applies also when the system is not fully hyperbolic (when some orbits appear in families [2]) or integrable [3]. More recently it has been refined to include complex orbits [4] and diffractive effects [5,6]. In this line we aim at studying the problem of wedge diffraction as an extension of the standard PO theory. This is one of the oldest and simplest examples of diffraction (see, e.g., [7]), and it is also the case where the diffractive corrections to semiclassics are the more important.

In this Letter we calculate for the first time the role of nonclassical diffractive orbits in the spectrum of two-dimensional polygonal billiards. We derive a trace formula embodying the contribution of diffractive PO's to the level density [Eq. (9)]. This contribution is of order $\sqrt{\hbar}$ smaller than the contribution of isolated PO's and is the next order term in the trace formula. As an example, the formalism is applied to a triangular billiard with angles $(\pi/4, \pi/6, 7\pi/12)$, and one sees that it provides a very accurate description of the Fourier transform of the spectrum.

We consider a quantum particle enclosed in a polygonal billiard $\mathcal{B}$, and we impose Dirichlet boundary conditions on the frontier $\partial\mathcal{B}$. Hence the associated Green function is the solution of the following equation:

$$\begin{aligned}(\Delta_B + k^2)G(\mathbf{q}_B,\mathbf{q}_A,k) &= \delta(\mathbf{q}_B - \mathbf{q}_A) \quad \text{inside } \mathcal{B},\\ G(\mathbf{q}_B,\mathbf{q}_A,k) &= 0 \quad \text{on } \partial\mathcal{B}, \end{aligned}\tag{1}$$

where $\mathbf{q}$ is a coordinate in configuration space.

The semiclassical approximation for G reads (see, e.g., [8])

$$G_0(\mathbf{q}_B,\mathbf{q}_A,k) = \sum_{\mathbf{q}_A\to\mathbf{q}_B} \frac{e^{i(kL-\mu\pi/2)}}{i\sqrt{8i\pi kL}}, \tag{2}$$

where the sum is taken over all classical trajectories going from $\mathbf{q}_A$ to $\mathbf{q}_B$. In (2) L is the length of the trajectory and μ is the associated Maslov index [8]. In polygonal enclosures the boundary has no focusing components, there are no caustics, and μ is simply twice the number of bounces of the trajectory on $\partial\mathcal{B}$.

In polygonal billiards the Hamiltonian flow is discontinuous on the vertices [9] and when the angle at a vertex is not of the form π/n ($n \in \mathbb{N}^*$) this causes diffraction (see, e.g., [10]). Then, following Keller's geometrical theory of diffraction [11], one is led to consider nonclassical contributions to the Green function which are "diffractive orbits" starting at $\mathbf{q}_A$, going to a vertex $\mathbf{q}_1$ and then to $\mathbf{q}_B$. These orbits are nonclassical because at $\mathbf{q}_1$ the reflection is not specular. Far from the region of discontinuity of the Hamiltonian flow, the corresponding Green function may be taken to be

$$G_1(\mathbf{q}_B,\mathbf{q}_A,k) = G_0(\mathbf{q}_1,\mathbf{q}_A,k)\mathcal{D}_1(\theta,\theta')G_0(\mathbf{q}_B,\mathbf{q}_1,k), \tag{3}$$

where $\mathcal{D}_1(\theta,\theta')$ is a diffraction coefficient evaluated in the solvable case of two semi-infinite straight lines meeting with an angle γ equal to the interior angle of the polygon at $\mathbf{q}_1$. θ (θ') is the angle of the incoming (outcoming) trajectory at q_1 with the boundary. $\mathcal{D}_1(\theta,\theta')$ reads [10–12]

$$\mathcal{D}_1(\theta,\theta') = -\frac{4}{N}\,\frac{\sin(\pi/N)\sin(\theta/N)\sin(\theta'/N)}{(\cos(\pi/N) - \cos[(\theta+\theta')])(\cos(\pi/N) - \cos[(\theta-\theta')])}, \tag{4}$$

where $N = \gamma/\pi$ is not assumed to be an integer.

As stated above, one sees in expression (4) that when γ is of the form π/n, $\mathcal{D}_1$ is zero and there is no diffraction. Indeed, in this case a trajectory passing by $\mathbf{q}_1$ is the limit of a trajectory bouncing specularly n times near the vertex, and a contribution of type (2) accounts for the effect of the wedge. This is to be related to the fact that, in this case there exists a nth iterate of the flow which is continuous [9]. Note also that $\mathcal{D}_1$ is zero if θ or θ' is equal to 0 or γ (i.e., in the case of a diffractive trajectory having a segment lying on a face).

For an orbit with several diffractive reflections at points $\mathbf{q}_1, \dots, \mathbf{q}_\nu$, formula (3) becomes

$$\begin{aligned} G_\nu(\mathbf{q}_B, \mathbf{q}_A, k) = {} & G_0(\mathbf{q}_1, \mathbf{q}_A, k) \\ & \times \left\{ \prod_{j=1}^{\nu-1} \mathcal{D}_j G_0(\mathbf{q}_{j+1}, \mathbf{q}_j, k) \right\} \mathcal{D}_\nu \\ & \times G_0(\mathbf{q}_B, \mathbf{q}_\nu, k)\,, \end{aligned} \qquad (5)$$

where $\mathcal{D}_j$ is the diffraction coefficient at point $\mathbf{q}_j$ as given by (4).

In (2), (3), and (5) the indices 0, 1, or ν of the Green function recall that diffractive effects are subdominant (by a factor of order $k^{-\nu/2}$). There might be less severe nonanalyticities on the boundary leading to higher-order diffractive corrections. Note also that we are using here a simple approximation for the Green function which is not valid when the angles θ and θ' at an edge are such that the diffractive orbit is close to being real; in this case the coefficient $\mathcal{D}_1(\theta, \theta')$ diverges. This occurs in the vicinity of the line of discontinuity of the Hamiltonian flow. In order to have a formula valid in all regions of space, one should use a uniform approximation such as first provided by Pauli [12] and whose general form is given in [10] (see also [13]).

The level density $\rho(k)$ is then obtained from the Green function by the usual formula:

$$\rho(k) = -\frac{2k}{\pi} \operatorname{Im} \int_{\mathcal{B}} d^2q\, G(\mathbf{q}, \mathbf{q}, k)\,. \qquad (6)$$

$\rho(k)$ can be separated in a smooth function of k, $\overline{\rho}(k)$ plus an oscillating part $\tilde{\rho}(k)$. The zero-length trajectories in (6) contribute to $\overline{\rho}$ and will not be considered in detail here (see [14]). When G is replaced by its semiclassical approximation (2), a stationary phase evaluation of (6) corresponds in considering only the contribution of classical PO's to $\tilde{\rho}$. When diffractive orbits such as (5) are taken into account, one is led to consider also "diffractive PO's," [5] which are PO's with one or several diffractive reflections (examples of such orbits are given in Fig. 1).

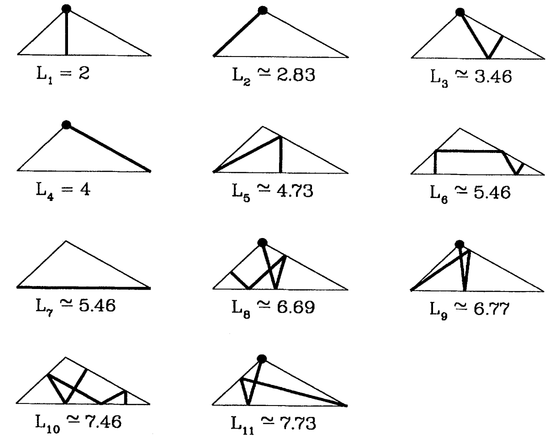

FIG. 1. The shortest classical and diffractive PO's in the triangle $(\pi/4, \pi/6, 7\pi/12)$. All these orbits are self-retracing. For diffractive PO's the diffraction point is marked with a black spot. Orbits 6 and 10 form families, 5 and 7 are isolated. The lengths are given in units of the height of the triangle.

Let us consider first the contribution of classical PO's. In a polygonal enclosure there is a drastic difference between PO's with even and odd number of bounces. The latter ones do not remain periodic when a point of reflection is translated along a face (they period double into a PO with twice as many bounces). This can be understood by remembering that, for the phase-space coordinates transverse to the direction of an orbit, a bounce on a straight segment leads to an inversion. On the other hand, PO's with an even number of bounces form families which correspond to local translation parallel to the faces of the polygon. They are neutral (or direct parabolic; see [8]) PO's to which the usual trace formula does not apply; we use a generalization of Gutzwiller's theory which is valid for the case of degenerate PO's [2]. We quote here the result and leave detailed discussion for the future [13]. A family of orbits contributes to $\tilde{\rho}(k)$ as

$$\tilde{\rho}(k) \longleftarrow \sqrt{\frac{kL}{2r\pi^3}}\, d_\perp \cos(krL - \pi/4)\,. \qquad (7)$$

Equation (7) is written for the general case of the rth iterate of a primitive orbit of length L ($r \in \mathbb{N}^*$). $d_\perp$ is the length occupied by the family perpendicular to the orbit's direction. It is equal to $d \cos\phi$, where d is the length occupied by the family on a face and ϕ is the angle between the direction of the orbit and the normal to this face.

For an isolated PO with an odd number of bounces, one has the following contribution:

$$\tilde{\rho}(k) \longleftarrow -\frac{L}{2\pi} \cos(krL)\,. \qquad (8)$$

Formula (8) holds when the number of repetitions is odd. When r is even, the rth iterate of an isolated orbit leads to a family, and formula (7) applies.

The derivation of the contribution of a diffractive PO is patterned on what is done in Gutzwiller's trace formula for an isolated PO. The length of a closed diffractive orbit in the vicinity of the diffractive PO is expanded up to second order, and the trace of the Green function is evaluated by a stationary phase approximation. The final contribution of a generic diffractive PO with ν diffractive reflections to the oscillating part of the level density reads:

$$\tilde{\rho}(k) \longleftarrow \frac{L}{\pi} \left\{ \prod_{j=1}^{\nu} \frac{\mathcal{D}_j}{\sqrt{8\pi k L_j}} \right\} \cos(kL - \mu\pi/2 - 3\nu\pi/4)\,. \qquad (9)$$

In (9) $L_1, \ldots, L_\nu$ are the lengths along the orbit between two diffractive reflections. $L_1 + \cdots + L_\nu = L$ is the total length of the diffractive PO. μ is the Maslov index which is here twice the number of specular reflections. Formula (9) is the most important result of this paper. Note that different diffractive orbits may combine if they have diffraction points in common. Hence, repetitions of a primitive diffractive orbit appear as a special case of (9); in this case, however, in the first factor L/π of the right hand side of (9), L should be understood as the primitive length of the orbit. The above formulas show that the contribution of a family of orbits is of order $\mathcal{O}(k^{1/2})$, for an isolated orbit it is $\mathcal{O}(1)$ and for a diffractive PO it is $\mathcal{O}(k^{-\nu/2})$. Nevertheless, we will see in the following that diffractive orbits have a very noticeable contribution to the level density.

We will now illustrate our approach by studying a specific example. Let us consider a triangle with angles $(\pi/4, \pi/6, 7\pi/12)$. As explained above, diffraction occurs only at the vertex with angle $7\pi/12$. The scale of lengths and wave vectors is fixed by the value h of the height going from this vertex to the opposite face. We take $h = 1$ in the following: The shortest classical and diffractive PO's in this triangle are shown in Fig. 1. Diffractive reflections are indicated with a black spot. Note that the first orbits are diffractive; classical orbits (isolated or in families) occur at greater lengths. The spectrum was computed numerically by expanding the wave function around the vertices with angles $\pi/4$ and $\pi/6$ in "partial waves," which are Bessel functions with a sinusoidal dependence on the angle defined near the considered vertex. More precisely, if r_n and φ_n are polar coordinates defined near the vertex π/n ($n = 4$ or 6), the partial waves in this region are of the form $J_{nm}(kr_n)\sin(nm\varphi_n)$ with $m \in \mathbb{N}^*$. One then imposes matching the wave function and its first derivative along the height h (see details in [13]). We determined the first 957 levels, up to $k_{\max} \simeq 96$. The accuracy of the computation was tested by varying the number of matching points and partial waves. We evaluate the typical error on an eigenvalue as being of the order of a hundredth of the mean-level spacing.

In order to visualize the importance of classical and diffractive PO's of successive lengths in the spectrum, we study the regularized Fourier transform of the level density:

$$F(L) = \int_0^{k_{\max}} k e^{ikL-\alpha k^2} \rho(k)\, dk\,. \qquad (10)$$

If $k_{\max} \longrightarrow +\infty$ and if the regularizing coefficient α is set to zero in (10), $F(L)$ is just a series of delta peaks centered on the lengths of the classical and diffractive PO's. The multiplicative factor k in (10) is meant to cancel the singularity $k^{-\nu/2}$ of the contribution of a diffractive PO of type (9) with up to $\nu = 2$ diffractive reflections. We take here $\alpha = 9/k_{\max}^2$ and plot $|F(L)|$ in Fig. 2. The numerical result is represented by a thin line; and the semiclassical approach (7,8), corrected by diffractive PO's (9), is represented by a thick line. We also included the contribution of $\overline{\rho}(k)$ in order to reproduce the initial peak at $L = 0$. We see that the agreement is excellent. Note that the existence of diffractive PO's is of great importance for reproducing all the peaks in $|F(L)|$. This is illustrated in the figure where their contribution (9) has been shaded.

Here, several comments are in order. Note first that the diffractive PO's labeled 2 and 4 in Fig. 1 have not been included because their diffraction coefficient is zero. Also, the orbit labeled 7 in Fig. 1 has a nonstandard contribution; it is an isolated orbit, which accounts for boundary effects on the family with the same length (labeled 6 in Fig. 1). In addition to the orbits of this family, it has an extra reflection on the bottom face (the same type of orbit was considered in Refs. [15,16]). The weight of PO number 7 is reduced by a factor of 1/2 compared to (8) since one integrates only over closed orbits on one side of this limiting PO. Also, we included repetitions of diffractive PO's, numbers 1 and 3, and they can be seen to still have a noticeable contribution. We did not include the diffractive PO composed by the sum of orbit 1 and 3, although it can be considered as a small diffractive correction to the contribution of family 6. Indeed, the orbit "1 + 3" lies just on the region separating real orbits from diffractive ones; and, as mentioned above, it cannot be accounted for by a simple diffraction coefficient such as (4). This type of correction will be treated in a forthcoming publication [13].

To summarize, let us emphasize the important role of nonclassical orbits in the spectrum of quantum billiards.

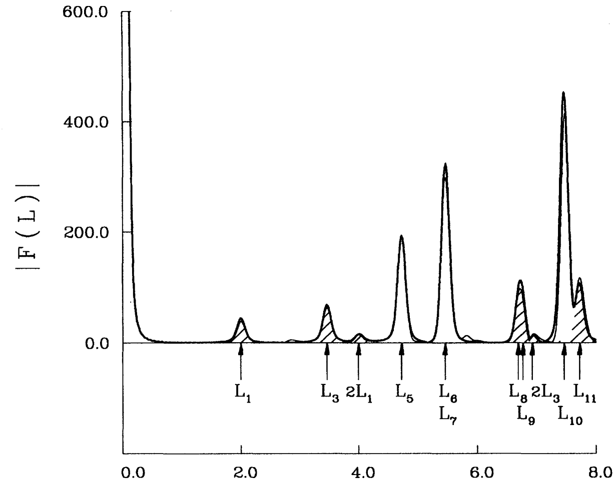

FIG. 2. $|F(L)|$ as a function of L. The thin line is the numerical result and the thick line the semiclassical approximation (7,8) with diffractive corrections (9). The two curves are hardly distinguishable. The contribution of the diffractive PO's has been shaded.

The existence of these orbits affects qualitatively the Fourier transform of the spectrum. The above example is only one among others where the discontinuity of the classical dynamics is linked to strong diffractive corrections to semiclassics. It was argued in [17] that the same type of corrections should be taken into account for the three-dimensional icosahedral billiard. We also expect diffractive effects—of the same order as those described here—in more general billiards with cusps (nonpolygonal or with an additional external field); in these cases a simple generalization of formula (9) accounts for the role of diffractive PO's. Finally, we note that the present work illustrates that semiclassical methods provide a very appealing tool which, when corrected with tunneling or diffractive effects, allows one to describe accurately the solution of partial differential equations using simple geometrical methods.

It is a pleasure to thank E. Bogomolny and D. Ullmo for fruitful discussions. Division de Physique Théorique is a Unité de Recherche des Universités de Paris XI et Paris VI associée au CNRS.

---

[1] For a review see *Chaos and Quantum Mechanics,* edited by M.J. Giannoni, A. Voros, and J. Zinn-Justin, les Houches Summer School Lectures LII (North-Holland, Amsterdam, 1989), and also Chaos **2**, 1–158 (1992).

[2] S.C. Creagh and R.G. Littlejohn, Phys. Rev. A **44**, 836 (1991); J. Phys. A **25**, 1643 (1992).

[3] M.V. Berry and M. Tabor, Proc. R. Soc. London, Sect. A **349**, 101 (1976); J. Phys. A **10**, 371 (1977).

[4] J.M. Robbins, S.C. Creagh, and R.G. Littlejohn, Phys. Rev. A **39**, 2838 (1989); M. Kuś, F. Haake, and D. Delande, Phys. Rev. Lett. **71**, 2167 (1993); P. Leboeuf and A. Mouchet, Phys. Rev. Lett. **73**, 1360 (1994).

[5] G. Vattay, A. Wirzba, and P.E. Rosenqvist, Phys. Rev. Lett. **73**, 2304 (1994).

[6] N.D. Whelan, Phys. Rev. E **51**, 3778 (1995).

[7] A. Sommerfeld, *Optics* (Academic, New York, 1954).

[8] M.C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, New York, 1990).

[9] T. Dagaeff and C. Rouvinez, Physica (Amsterdam) **67D**, 166 (1993).

[10] G.L. James, *Geometrical Theory of Diffraction for Electromagnetic Waves* (Peregrinus, Stevenage, 1976).

[11] J.B. Keller, J. Opt. Soc. Am. **52**, 116 (1962).

[12] W. Pauli, Phys. Rev. **54**, 924 (1938).

[13] N. Pavloff and C. Schmit (to be published).

[14] H. Baltes and E.R. Hilf, *Spectra of Finite Systems* (Bibliographisches Institute, Mannheim, 1976).

[15] B. Lauritzen, Phys. Rev. A **43**, 603 (1991).

[16] M. Sieber, U. Smilansky, S.C. Creagh, and R.G. Littlejohn, J. Phys. A **26**, 6217 (1993).

[17] N. Pavloff and S.C. Creagh, Phys. Rev. B **48**, 18164 (1993).