Poincaré's Recurrence Theorem and the Unitarity of the S-Matrix

by

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Abstract

A scattering process can be described by suitably closing the system and considering the first return map from the entrance onto itself. This scattering map may be singular and discontinuous, but it will be measure preserving as a consequence of the recurrence theorem applied to any region of a simpler map. In the case of a billiard this is the Birkhoff map. The semiclassical quantization of the Birkhoff map can be subdivided into an entrance and a repeller. The construction of a scattering operator then follows in exact analogy to the classical process. Unitarity of the Birkhoff map implies that this scattering operator is itself unitary, as a consequence of a quantized version of the recurrence theorem.

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For a classical conservative system, whether discrete or continuous in time, Poincaré's celebrated theorem can be reduced to the general statement that the probability for an orbit to return to any given region is unity if the motion is bounded. There is no restriction on the time this recurrence will take, which may vary widely among orbits starting in different subregions. In any case, by waiting a sufficiently long time, the first return of each trajectory defines a measure preserving map of the region onto itself.

The essential boundedness of the system in no way hinders its application to classical scattering problems, because we can always choose the appointed region to coincide with the opening of the scattering system to the outside world. Since we are only interested in the first return of the orbits to the chosen region, it makes no difference that the system is not really closed. In other words, we can still apply the theorem if the union of the scatterer and the opening combine to form a bounded measure preserving map.

As a first example consider the simple scattering system composed of a circular billiard opening onto a straight tube, as shown in Fig. 1. In this case, the closure of the dynamical system can be reduced to the Birkhoff map (or bounce map) for specular collisions of the straight trajectories with the circular boundary. The phase space is defined by the boundary coordinate s (or the angle θ , in the case of unit radius) and p_s , the tangential momentum (proportional to $\cos \alpha$, where α is the angle of incidence).

The closed dynamics is very simple in this case: p_s is constant (integrable motion) and $\Delta \theta = 2\alpha$. Nonetheless, the scattering map of the orbits returning to the opening is discontinuous. Indeed it is composed of an infinite sequence of diminishing subregions, of which the first few are shown in Fig. 2. Therefore a maximally simple closed dynamics induces a relatively complex (resonant) scattering map. It is only in the (non resonant) limit where the size of the opening approaches the diameter of the circle that the scattering map is also simple.

Consider now the less obvious example of the specular scattering from three disks, that has become the paradigm of chaotic classical scattering [1]. It may appear that our choice of closing surface in Fig. 3 amounts to an overkill, since we are not interested in orbits such as **a** in Fig. 3. However this integrable motion described in the previous example does not mix with the scattering orbits such as **b**, so we can substract it from the phase space of our system. This is then composed of the Birkhoff coordinates of the external circuit, restricted to small p_s added to the full Birkhoff coordinates of the three scattering circles, as shown in Fig. 4. Evidently, we obtain the useful asymptotic scattering picture by making the radius of the outer circle arbitrarily large, so that we can identify the exit direction of an orbit with the point where it collides with the outer circle. Even so, the useful area for the outer circle in the phase space of Fig. 4 will be smaller than that of the three disks combined.

The dynamics for the first return of the closed map is indicated by the different regions in Fig. 4. This is less trivial than in the previous example, but it is nowhere singular. The first return map between the four circles is hyperbolic and discontinuous similarly to the baker's transformation [2], but the full complexity of the motion only arises through the multiple iterations needed to compose the scattering map of first returns to the outer circle. This map exhibits a fractal structure of singularities generated by motion that nearly enters on the stable manifold of periodic orbits within the scatterer [3].

An evident conceptual advantage is achieved by understanding the structure of scattering maps on the basis of multiple iterations of their closure, even though it may be necessary to reverse this procedure in experimental situations. Our purpose is now to show that we can transfer to semiclassical scattering a construction of open and closed systems corresponding to the one which we have been employing in the classical theory.

The starting point is to note that we can always define a finite Hilbert space that will correspond semiclassically to a finite phase space [8]. Indeed, the dimension of the Hilbert space corresponding to a two dimensional classical phase space of area A will be $N = A/2\pi\hbar$, where \hbar is Planck's constant. The prescription given by Miller [7] for the approximately unitary quantum map U, is given in the coordinate representation as

$$U(q,q') \simeq \frac{1}{\sqrt{2\pi\hbar}} \sum_{j} \left| \frac{\partial^2 \sigma_j}{\partial q \partial q'} \right|^{1/2} e^{i\sigma(q,q')/\hbar + i\mu_j} , \qquad (1)$$

where μ_j is the Maslov phase and $\sigma_j(q, q')$ stands for the generating function of the classical

map, given implicitly by

$$p' = \frac{\partial \sigma_j}{\partial q'}, \quad p = -\frac{\partial \sigma_j}{\partial q},$$
 (2)

the index j indicating that there may be more than one orbit for a given pair of points (q',q). Of course, we should worry about the discretization of coordinates, due to the finite dimension (N) of the Hilbert space, but the approximations will hold when N is large. Furthermore, the semiclassical approximation (1) will leave out evanescent modes [4] and diffraction effects (*e.g.* in the three disks problem), but again these will give relatively small contributions in the large N limit.

We can check the approximate unitarity of (1) by noting that, for each continuous region of area A_j

$$N_j = \operatorname{Tr} U_j U_j^{\dagger} \simeq \int \frac{dq \, dq'}{2\pi\hbar} \left| \frac{\partial^2 \sigma_j}{\partial q \partial q'} \right| = \frac{A_j}{2\pi\hbar} \,. \tag{3}$$

Thus, we are quantizing separately each subregion in a way that increases border effects for discontinuous maps with many subdivisions. We have shown that this is typical of scattering maps. If they are sufficiently resonant as in our examples, we obtain $N_j \stackrel{<}{\sim} 1$ for many subregions, which are hence beyond the range of validity of the Miller prescription.

The way out is to rely on the construction of the scattering map from the multiple iterations of the simpler closed unitary map. We thus need the following result, which may be considered as the quantization of the recurrence thorem:

Given a finite Hilbert space H_N subdivided into two orthogonal subspaces $H_{N_0} = P_0 H_N$ and $H_{N_1} = P_1 H_N$ (such that the projection operators $P_0 + P_1 = 1_N$) and given an unitary operator U_N defined on H_N , then the operator

$$S_{N_0} = P_0 U_N \left[1 - P_1 U_N \right]^{-1} P_0 = P_0 U_N \sum_{m=0}^{\infty} \left(P_1 U_N \right)^m P_0 \tag{4}$$

is unitary on H_{N_0} .

To outline the proof we define the rectangular blocks of the operator U_N , namely $U_{ij} = P_i U P_j$, and their hermitian conjugates $U_{ij}^{\dagger} = P_j U^{\dagger} P_i$. The unitarity of U_N implies

$$U_{00}U_{00}^{\dagger} + U_{01}U_{10}^{\dagger} = 1_{N_0} \tag{5}$$

$$U_{00}U_{01}^{\dagger} + U_{01}U_{11}^{\dagger} = 0 \tag{6}$$

$$U_{10}U_{01}^{\dagger} + U_{11}U_{11}^{\dagger} = 1_{N_1} , \qquad (7)$$

where 1_{N_j} coincides with the nonsingular block of P_j . In this notation Eq. (4) reads $S_{N_0} = U_{00} + U_{01}[1_{N_1} - U_{11}]^{-1}U_{10}$. Then it is straightforward, though a little lengthy, to verify that $S_{N_0}S_{N_0}^{\dagger} = S_{N_0}^{\dagger}S_{N_0} = 1_{N_0}$ is a consequence of Eqs. (5–7).

Our formula for S_{N_0} strongly resembles Feshbach's construction of nuclear scattering theory [5], but at this stage we have only a prescription for generating an unitary operator. It is important to note that the map P_1U that is iterated an infinite number of times is not itself unitary. It corresponds to the classical scatterer that looses orbits at each iteration. The phase space area of orbits that remain thus diminishes, that is, the classical map is dissipative. Maps of this kind have been quantized by Saraceno and Vallejos [6]. Generically their eigenvalues lie inside the unitary circle. This prevents the ocurrence of poles in S_{N_0} as a parameter is varied, and ensures the convergence of the expansion of S_{N_0} in powers of P_1U as given in (4).

We can now apply the exact result (4) to semiclassical scattering by the identification of U_N with the approximate semiclassical map (1) for the closure of the scattering system. The resulting scattering matrix given by (4) is the on-shell S-matrix for fixed energy. In our examples, the energy dependence of the classical map is trivial and it can be scaled away, but the area of the phase space grows with energy, modifying the dimension of the corresponding Hilbert space. Another way to see this important energy dependence of the quantum mechanics is through the growth of the actions of the orbits, i.e. the generating functions σ_j in (1). In the case of smooth potentials, rather than billiards, even the energy dependence is nontrivial. These scattering systems can also be treated within our conceptual framework by introducing quantum Poincaré sections in the manner of Bogomolny [8] or Rouvinez and Smilansky [9].

There are two ways in which we can now obtain the scattering matrix S_{N_0} from the

unitary operator U_N . The first is to note that, contrary to the full expansion of standard quantum scattering theory (4), we can carry out the inversion of the finite matrix (1) in some chosen representation. This establishes a "semiquantal approximation" for scattering, in the nomenclature of Voros and Saraceno [11].

Of course, this becomes more difficult as the dimension of the matrix grows in the semiclassical limit. The alternative is to keep within the semiclassical representation (1) for the unitary matrix U and to compute $[1_{N_1} - U_{11}]^{-1}$ using "Fredholm theory". In fact, one can write $[1_{N_1} - U_{11}]^{-1} = Y/\Delta$ and calculate $Y = \sum_{m=0}^{N_1} Y_m$ (where $Y_0 = 1_{N_1}$), and the determinant $\Delta = 1 - \sum_{m=1}^{N_1} \frac{1}{m} \operatorname{Tr}[U_{11}Y_{m-1}]$, from the recursion relation $Y_m = U_{11}Y_{m-1} - \frac{1}{m}1_{N_1}\operatorname{Tr}[U_{11}Y_{m-1}]$ [10]. When the traces of U_{11}^k are evaluated in the stationary phase approximation, the scattering matrix can be expressed in terms of ressumed contributions of the periodic orbits of the scatterer which may be analized in terms of their symbolic representation [1]. This is exactly the procedure already followed by Georgeot and Prange in their important paper on semiclassical scattering [12]. We can now understand their results as originating in the quantized version of Poincaré's recurrence theorem.

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FIG. 2. The first-return map for the circular system of Fig. 1. Initial conditions having all possible momenta are launched from the entrance of the scattering system. In the Birkhoff plane $s-p_s$, this corresponds to the narrow rectangular region centered at $s = \pi$. We show the first two images of this region by the full internal map (strips bounded by the cosine curves). Also shown are the first returns after 2,3,...,6 bounces with the circular boundary, and the phase points that still stay inside the cavity after 6 bounces (dark strips ouside the initial rectangle). We have not plotted those points that return after one iteration as they do not correspond to the scattering process (for the system closed by a straight segment there would be no orbits leaving at the first return). The picture for $p_s < 0$ is obtained by reflection with respect to the point ($s = \pi, p_s = 0$).

FIG. 3. Scattering by three discs. An incident particle propagates trivially to the outer circle that closes the system. This defines an initial condition for the Birkhoff map of the closed problem, described by the full set of position coordinates $\{s, s_1, s_2, s_3\}$ together with the tangent momenta. After colliding with the discs a certain number of times, the particle returns to the outer circle, *i.e.* it escapes.

FIG. 4. The return map for the three-discs system. Initial conditions are started at the outer circle of Fig. 3, with momenta pointing inwards (upper rectangles). (a) The first iterate of the initial rectangle is shown in dark. Accordingly, white regions correspond to the first iterate of the phase space of the three discs. The dark region in the phase space of the outer circle is associated to scattering trajectories that do not hit the inner discs (indicated as **a** in Fig. 3). (b) After three iterations fractal structures begin to develop. Shown are those trajectories-stuck to the discs-that have not escaped after three bounces (like **b** in Fig. 3), and those which are escaping after two bounces (upper rectangle).



Fig. 1



Fig. 2







Fig. 4a



Fig. 4b

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