# Exact and Quasiclassical Fredholm Solutions of Quantum Billiards

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Quantum billiards are much studied as perhaps the simplest case which presents the central difficulty that the quasiclassical approximation is expressed as a divergent series. We find here, using the Fredholm method, an exact Green's function for billiards expressed as a ratio of absolutely convergent series. We make the quasiclassical approximation to this ratio. The method provides a convergence argument for previous results and an extension of results obtained for the spectrum to the full Green's function.

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It has been more than twenty years [1] since physicists realized that there is much we have failed to understand in the simplest quantum problems which are not exactly solvable. Among the questions studied are correlations between energy levels and the degree of pseudorandomness of the levels. Similar questions can be asked of wave functions, matrix elements, and scattering amplitudes. Attempts are made to classify the quantum problems, in particular, by the nature of the classical limit, e.g., whether the classical limit is chaotic [2].

Of these problems, doubtless the most thoroughly studied is that of the wave mechanics of a real time independent nonseparable two-dimensional potential. Two further specializations are also commonly made: First (in spite of much evidence that the wave functions are very interesting [3]), the study is restricted to the spectrum, and second, attention is confined to billiards, that is, systems for which the motion is free in the interior, and for which the essential problem is posed by the imposition of conditions on the boundary. Some celebrated billiards are the Sinai billiard, the Bunimovich stadium billiard, and billiards on spaces of negative curvature. Billiards gain mathematical and numerical conveniences, and it is hoped that not much generality is lost. Indeed, there is a vast literature on boundary integral methods (BIM) which are basically restricted to billiards. As a rule, BIM are used to obtain numerical solutions, and this is advantageous since it is only necessary to discretize the boundary and not the interior area. (See Boasman [4] for further references.) We discuss here one of the less frequently used BIM, which requires solution of a Fredholm integral equation of the second kind.

Our point is that this exact Fredholm solution is closely related to the approximate solutions obtained by making a quasiclassical (short wavelength) approximation (QCA). The QCA is very natural and is much studied in the physics literature, since the conceptual difficulties are with higher energy levels where the wavelength becomes short compared with the length scale of the billiard. The straightforward QCA yields *divergent* series in the generic case that the classical limit is chaotic. Because of this difficulty, up to now most work has concentrated on the *spectrum*, and then for the case of *hard chaos* where all orbits are unstable, because these cases are simpler.

This *divergence problem* due to the *exponential proliferation of classical orbits* is a central problem of the subject of *quantum chaos* [2]. It has been more or less solved for the hard chaos spectral problem by several authors [5–7]. These authors make the QCA at the outset, however, and so it is difficult to make rigorous arguments. By making the QCA only at the end, we clarify the issues and we find a formulation of the QCA in terms of *absolutely convergent* series. A by-product is that our formulation is simpler than previous ones, and, more importantly, it can be extended to cases such as finding *wave functions* or finding *scattering amplitudes* in open systems. It also is *not* restricted to hard chaos, or to any chaos at all, for that matter.

We want to find a convenient expression for the Green's function $G(\mathbf{r}, \mathbf{r}', E)$ at fixed energy $E$ which satisfies Helmholtz's equation

$$\left(\tfrac{1}{2}\hbar^2\nabla^2 + E\right)G(\mathbf{r}, \mathbf{r}', E) = \delta^2(\mathbf{r} - \mathbf{r}') \qquad (1)$$

in the interior $B$ of the billiard, and which satisfies the conditions $G(\mathbf{r}, \mathbf{r}', E) = 0$, for $\mathbf{r}$ or $\mathbf{r}'$ on the boundary $\partial B$. We know $G(\mathbf{r}, \mathbf{r}', E) = \sum_\alpha \Psi_\alpha(\mathbf{r})\bar{\Psi}_\alpha(\mathbf{r}')/(E - E_\alpha)$, where $\Psi_\alpha(\mathbf{r})$, vanishing on $\partial B$, is the $\alpha$th eigenstate and $E_\alpha$ is its energy.

The trace of $G$, $\int d\mathbf{r}\, G(\mathbf{r}, \mathbf{r}, E) = \sum (E - E_\alpha)^{-1}$, gives the spectrum. In QCA this leads to the Gutzwiller trace formula [1]. This formal expression is singular, both because $E \to E_\alpha$ is divergent and because the sum is divergent. These difficulties were avoided by studying instead the *spectral determinant* [5] (S$\Delta$), or equivalently the *dynamical* (or Gutzwiller-Voros, or Selberg) *zeta function* [8,9] (D$\zeta$), an analog of Riemann's zeta function [5].

Here we provide a rigorous formulation giving an expression for the full Green's function itself in which a well-defined version of the D$\zeta$ quite naturally appears and all series are convergent, all functions are analytic. This formulation is based on the well-known theory of Fredholm integral equations. The QCA can be left to the end, recovering the earlier results, as well as providing some new ones. There is one work [4] which arrives at our expression for the D$\zeta$ by means of a BIM. This work is concerned with numerical issues and the accuracy of the QCA.

We now obtain an integral equation characterizing $G$. To do this, we utilize a free space Green's function $G_0(\mathbf{r},\mathbf{r}',E)$ which satisfies the differential equation (1), but does *not* satisfy the boundary conditions. It is at this stage we have specialized to billiards, since, in more general potentials, there is no obvious choice of $G_0$. [We will eventually choose outgoing wave conditions on $G_0$ and thus take $G_0(\mathbf{r},\mathbf{r}',E) = H_0^{(1)}(k|\mathbf{r}-\mathbf{r}'|)/2i\hbar^2$, where $H_0^{(1)}(x)$ is the Hankel function of the first kind, and $k \equiv p/\hbar \equiv +\sqrt{2E}/\hbar$.] Applying Green's theorem yields

$$G(\mathbf{r},\mathbf{r}',E) = G_0(\mathbf{r},\mathbf{r}',E) - \frac{1}{2}\hbar^2 \int_{\partial B} dq'\, G_0(\mathbf{r},q',E)\mu(q'), \tag{2}$$

where $\mu(q) = \partial G(\mathbf{r}(q),\mathbf{r}',E)/\partial n$ is the outward normal derivative of $G$ with respect to its first argument. The arguments $\mathbf{r}'$ and $E$ are regarded as parameters in $\mu$. Distance along the boundary is given by $q$, $\mathbf{r}(q)$ is the position vector at the boundary point $q$, and we shorten the notation to write $q$ where we sometimes mean $\mathbf{r}(q)$. A knowledge of $\mu$ therefore reduces the problem to quadratures.

We find an equation for $\mu$ by taking the normal derivative of Eq. (2) and letting the argument $\mathbf{r}$ approach a boundary point $q$. This yields

$$\mu(q) = V_+(q) + \int_{\partial B} dq'\, \mathbf{K}(q,q')\mu(q'), \tag{3}$$

Here $\mathbf{K}(q,q') = -\hbar^2 \partial G_0(\mathbf{r}(q),\mathbf{r}(q'),E)/\partial n$ and $V_+(q) = 2\partial G_0(\mathbf{r}(q),\mathbf{r}',E)/\partial n$. In $\mathbf{K}$, $\mathbf{r}(q)$ is evaluated directly on the boundary *not* as a limit from inside. Equation (3) was found by Balian and Bloch [10] in their seminal paper on the distribution of eigenvalues of billiards. The homogeneous version of Eq. (3) was studied in Ref. [4]. The operator $\mathbf{K}(q,q')$ is well behaved for all values of its arguments including $q = q'$, if the billiard boundary is smooth. (Special account must be made of kinks on the boundary, and, indeed, there are diffraction effects coming from such features.)

Equation (3) is a Fredholm integral equation of the second kind. Since this theory is well known [11], we simply write down the result, in operator (continuous matrix) notation,

$$G(\mathbf{r},\mathbf{r}',E) = G_0(\mathbf{r},\mathbf{r}',E) + V_-(\mathbf{r},E)\left(\frac{1}{\mathbf{1}-\mathbf{K}(E)}\right)V_+(\mathbf{r}',E). \tag{4}$$

We have defined $V_-(\mathbf{r},E,q) = -\frac{1}{2}\hbar^2 G_0(\mathbf{r},\mathbf{r}(q),E)$. The operator $\mathbf{K}$ acts on the Hilbert space of functions on $\partial B$; $V_\pm$ are vectors in this space, depending parametrically on $\mathbf{r},\mathbf{r}'$, as shown. They, and $\mathbf{K}$, depend parametrically on the energy $E$, as well. The operator inverse is formal, but for sufficiently nice operators $\mathbf{K}$ (as generally occur for billiards), Fredholm theory rigorously gives the inverse. Introducing the bookkeeping parameter $\lambda$ the result is $(\mathbf{1}-\lambda\mathbf{K})^{-1} = \mathbf{N}(\lambda)/D(\lambda)$, where the operator $\mathbf{N}$ and the *Fredholm determinant* $D$ are expressed as *absolutely convergent* series for *any* $\lambda$, $\mathbf{N}(\lambda) = \sum_{n=0}^{\infty}\mathbf{N}_n\lambda^n$, $D(\lambda) = \sum D_n\lambda^n$. The result for $D_n$ is

$$D_n = \frac{(-1)^n}{n!}\int\int_{\partial B} dq_1\cdots dq_n \det\begin{vmatrix} K(q_1q_1)\cdots K(q_1q_n) \\ \vdots\cdot\cdot\vdots \\ K(q_nq_1)\cdots K(q_nq_n)\end{vmatrix} \tag{5}$$

and $D_0 = 1$. Since $\mathbf{K}$ and $\partial B$ are finite, a standard application of Hadamard's inequality [11] establishes that $D$ is an *entire* function of $\lambda$ (and $\mathbf{N}$ an entire operator valued function). $\mathbf{N}$ is related to $D$ by $\mathbf{N}_n = \sum_{r=0}^{n}\mathbf{K}^{n-r}D_r = \mathbf{1}D_n + \mathbf{K}\mathbf{N}_{n-1}$.

We now obtain the analyticity properties for the exact solution which were used in the QCA [5]. Since $\mathbf{K}$ and $\partial B$ are finite, if $D \neq 0$ there is a unique solution $\mu$ of Eq. (3) [11]. It follows that $\mu$ is indeed the normal derivative of the wanted Green's function, for $E \neq E_\alpha$. Thus $\mu$ is *independent* of the choice of $G_0$ which is so far determined only up to an arbitrary symmetrical solution of the homogeneous Helmholtz equation. However, $\mathbf{K}$ and $V_+$ *do* depend on the choice of $G_0$.

Regarding $D$ as a function of energy, for $\lambda = 1$, it is clear that the eigenvalues $E_\alpha$ are zeros of $D$ for which $\mu$ has poles. If $G_0$ is not carefully chosen, however, there can be *spurious* zeros $z_s$ of $D$, which may be real or complex, and these are a nuisance. It turns out that for two cases, outgoing or incoming boundary conditions on $G_0$ (Hankel functions of the first or second kind), there are no spurious zeros [4], so we make this choice.

The kernel $\mathbf{K}$ is an analytic function of complex momentum $p$, except for a branch cut which can be taken from $(-\infty,0)$. For $\mathrm{Im}\,p \to +\infty$, $\mathbf{K} \to 0$ and $D \to 1$. It is a property of Hankel functions that $H_0^{(1)}(e^{i\pi}x) = -H_0^{(2)}(x)$. Thus, $p \to e^{i\pi}p$ replaces the outgoing wave Green's function by the one for incoming waves. For real $p$, this gives therefore $D(e^{i\pi}p) = \bar{D}(p)$. Since $\mathbf{K}$ is analytic in $p$, so is $D_n$, and thus $D$, as an absolutely convergent sum of analytic functions, *is* itself analytic. Considering $D$ now as a function of complex energy $z = p^2/2$, we see that $D(z)$ is analytic except for a branch cut along the positive real $E$ axis. Then $D(E - i\eta) = \bar{D}(E + i\eta)$. We introduce $\hat{G}(z) = [D(z)]^{-1}dD(z)/dz$. Like $D$, $\hat{G}$ is an analytic function of $z$, except for poles and a cut along the positive real axis, where it has a pure imaginary discontinuity, for $E \neq E_\alpha$, $\hat{G}(E + i\eta) - \hat{G}(E - i\eta) = 2i\,\mathrm{Im}\,\hat{G}(E + i\eta) \equiv 2\pi i\rho(E)$. Since $\hat{G}(z) \to 0$ for $z \to \infty$ there is a representation for $z$ not real and positive,

$$\hat{G}(z) = \lim_{E_1\to\infty}\int_0^{E_1} dE\,\frac{A(E)}{z - E}. \tag{6}$$

Since $D(z)$ has zeros at $z = E_\alpha$, $\hat{G}$ has poles there, so $A$ is of the form $A(E) = \sum_\alpha \delta(E - E_\alpha) - \rho(E)$. Thus $\rho(E)$ is such that the limit in Eq. (6) converges. Clearly, $\rho$ is a smoothed density of states, presumably nearly that given by the QCA. Now integrate $\hat{G}$ using Eq. (6) to find

$$D(z) = \lim_{E_1 \to \infty} \exp[\mathcal{F}(z, E_1)] \prod_{E_\alpha < E_1} \left(1 - \frac{z}{E_\alpha}\right), \quad (7)$$

where $\mathcal{F}(z, E_1) = -\int_0^{E_1} dE\, \rho(E) \ln(1 - z/E)$. The logarithm is cut on $(-\infty, 0)$ so the exponential has the phase $e^{\pm i\pi \mathcal{N}(E)}$ for $z \to E \pm i\eta$, where $\mathcal{N}(E) = \int_0^E d\bar{E}\, \rho(\bar{E})$. Let $\Delta(z) \equiv D(z) \exp[\mathcal{F}_1(z)]$, where $\mathcal{F}_1(z) = \lim_{E_1 \to \infty}[z \sum_{E_\alpha < E_1} E_\alpha^{-1} - \mathcal{F}(z, E_1)]$. The discontinuity on the real axis due to $\mathcal{F}_1$ exactly cancels that coming from $\mathcal{F}$. Therefore, $\Delta(z)$ is an *entire* function of $z$, manifestly real on the real axis, with zeros on the spectrum.

As a function of $p$, therefore, $\Delta(p)$ is entire, real for real $p$, and $\Delta(p) = \Delta(-p)$. This is precisely the analyticity and functional relation needed in a celebrated paper [5] (BK), for the S$\Delta$, constructed by manipulating the quasiclassical series over periodic orbits, as discussed below. Our $\Delta(p)$, which is exactly defined, formally reduces to the spectral determinant S$\Delta$ in the quasiclassical limit. (The next steps of BK can be formally made also, but we need the QCA to interpret them as a resurgence phenomenon.)

So far, everything is exact. There is no restriction to hard chaos or indeed to any particular classical limit. Previous work has treated just the QCA, and then only $D$, expressed as a product, the D$\zeta$, or $\Delta$, the real spectral determinant. A similar treatment of the numerator $\mathbf{N}(\lambda)$ makes its first appearance in this paper. We make three levels of QCA, A1, A2, and A3.

The first level is to approximate $\mathbf{K}(q, q')$ from the asymptotic form of the Hankel function for $k|\mathbf{r}(q, q')| \gg 1$, where $\mathbf{r}(q, q') = \mathbf{r}(q) - \mathbf{r}(q')$. It is expressed [4] in terms of Bogomolny's [6] operator $\mathbf{T}$, $\mathbf{K}(q, q') = \mathbf{T}(q, q')(|\hat{n} \cdot \hat{\mathbf{p}}|/|\hat{n}' \cdot \hat{\mathbf{p}}|)^{1/2}$, where

$$\mathbf{T}(q, q') = -(2\pi i \hbar)^{-1/2}[\partial^2 S(q, q')/\partial q \partial q']^{1/2} e^{iS(q,q')/\hbar} \quad (8)$$

and $S = p|\mathbf{r}(q, q')|$. Here $\hat{\mathbf{p}} = \mathbf{r}(q, q')$ and $\hat{n}, \hat{n}'$ are the unit normals at $q, q'$. This expression for $\mathbf{K}$ is valid only if the $\hat{n} \cdot \hat{\mathbf{p}}$ do not vanish. Such a case can occur if a classical orbit is tangent to the boundary, as can happen for nonconvex billiards. This again is expected to exhibit diffraction effects not accounted for in the simplest QCA. Leaving this aside, we recall that Bogomolny [6] obtains a QCA expression whose zeros are an approximation to the spectrum: $\det[1 - \mathbf{T}(E)] = 0$. It has been found that a discretization and numerical evaluation yields excellent results in the cases considered [12].

Although Bogomolny does not precisely define this infinite-dimensional determinant, we can treat it as a Fredholm determinant and compare it with $D(\lambda = 1)$. The expansion coefficients are obtained by use of the Smithies-Plemelj recursion relation [11], expressing $D_n$ in terms of the traces of $\mathbf{K}$ (or $\mathbf{T}$) by $D_n = -n^{-1} \sum_{r=1}^n \sigma_r D_{n-r}$ with $\sigma_r = \mathrm{Tr}\mathbf{K}^r = \int \int_{\partial B} dq_1 \cdots dq_r\, \mathbf{K}(q_1, q_2) \cdots \mathbf{K}(q_r, q_1)$. Now, using the QCA for $\mathbf{K}$, $\mathrm{Tr}\mathbf{K}^n = \mathrm{Tr}\mathbf{T}^n$, for $n > 1$ although $\mathrm{Tr}\mathbf{K} \neq 0$ while $\mathrm{Tr}\mathbf{T} = 0$. This, however, has no effect on the results, since, according to theory [11], $D_{[\mathbf{K}]} = e^{\lambda \sigma_1} D_{[\mathbf{T}]}$ and the two versions of $\mathbf{N}$ also differ by this nonvanishing factor. We remark that at level QCA1 the series for N and D are absolutely convergent.

Note that the expression for $D_n$ is *independent of representation.* Using the Fourier series representation on the boundary, it is found that only a finite number $N$ of Fourier components are finite when evaluated in stationary phase (S$\Phi$), where $N = k \int_{\partial B} dq/\pi$. In this context, S$\Phi$ and the QCA are equivalent. At this level, QCA2, we thus have $D_n = \mathbf{N}_{n-1} = 0$, for $n > N$, so the series is not only convergent, it is finite. Thus $\mathbf{T}$ is in QCA effectively an $N \times N$ unitary matrix $\mathbf{T}^\dagger = \mathbf{T}^{-1}$. Using this, Bogomolny [6] showed that the upper half of the series for $D$ is *"resurgent"* [5], i.e., it is the complex conjugate of the lower half, except for a phase. (More generally, resurgence is the idea that high order terms in a series contain information also contained in the low order terms.) Let $\lambda = \bar{\lambda}$, so with these assumptions $\overline{D(\lambda)} = \det(1 - \lambda \mathbf{T}^{-1}) = D(\lambda^{-1})\lambda^N e^{-i\Phi}$, where $e^{i\Phi} = \det(-\mathbf{T})$. This implies $D_n = \bar{D}_{N-n} e^{i\Phi}$, so (for $N$ odd) $D(\lambda = 1) = \sum_{n=0}^{(N-1)/2}(D_n + \bar{D}_n e^{i\Phi})$. This saves finding the most difficult half of the $D$'s, and allows the definition of a manifestly real function, $\Delta = e^{-i\Phi/2} D$. The phase is, of course, $\Phi = 2\pi \mathcal{N}$, in view of our earlier consideration.

The coefficients $\mathbf{N}_n$ are also resurgent in quite a novel way. Using $\mathbf{N}(\lambda) = D(\lambda)/(\mathbf{1} - \lambda \mathbf{T})$ gives $\mathbf{N}(\lambda)^\dagger = -\bar{D}(\lambda)(\lambda^{-1}\mathbf{T})/(\mathbf{1} - \lambda^{-1}\mathbf{T}) = -\lambda^{N-1} e^{-i\Phi} \mathbf{T}\mathbf{N}(\lambda^{-1})$. Equating coefficients of $\lambda^n$ gives

$$\mathbf{N}_n = -e^{i\Phi} \mathbf{T}^\dagger \mathbf{N}_{N-n-1}^\dagger . \quad (9)$$

In particular, $\mathbf{N}_{N-1} = -\mathbf{T}^\dagger e^{i\Phi}$. We have consequently succeeded in expressing *high powers* of $\mathbf{T}$ based on the outgoing Green's function, by *low powers* of $\mathbf{T}^\dagger$ based on the incoming Green's function.

Resurgence is a property of the QCA. Evaluated in S$\Phi$, the somewhat surprising result, $\mathbf{T}^\dagger V_+ = V_-^\dagger$ is obtained. Further, the expression $V_-(\mathbf{r}) V_-^\dagger(\mathbf{r}')$ is a contribution of a *direct* orbit (not bouncing from the boundary) from $\mathbf{r}$ to $\mathbf{r}'$. Thus the contribution of $\mathbf{N}_{N-1}$ can be directly related to the contribution of $G_0$ in Eq. (4). The exploitation of resurgence, that the high terms of certain series contains essential information of the same type found in the low terms, is becoming popular in mathematics. We have used this technique to obtain the result of Agam and Fishman [13] for scars and the Wigner function by a simpler and more rigorous method [14].

So far, we have used the QCA to find expressions for **K** or **T**. A third level QCA3 can be obtained by doing the trace integrals $\sigma_n$ by S$\Phi$ for $n > 1$, with the result $\sigma_n = \sum_{rn_p=n} n_p e^{irS_p(E)/\hbar}/|\det(M_p^r - 1)|^{1/2}$, where $p$ labels the primitive periodic orbits with $n_p$ bounces from the boundary, $r$ is the number of repetitions, $M_p^r$ is the $r$th power of the monodromy matrix for the primitive orbit, and the action $S_p = pL_p$ is the momentum times the length of the orbit. The D$\zeta$ is [8,15] $Z(E) = \prod_{pp0}\prod_m(1 - \Lambda_p^{-1/2-m}e^{i/S_p(E)/\hbar})$. (Such a simple expression for $Z$ is only possible if the eigenvalues of $M_p$ are $\Lambda_p$, $\Lambda_p^{-1}$, i.e., all orbits are hyperbolically unstable, the hard chaos case.) The product $\prod_{pp0}$ is *not* convergent [8], although the product over $m$ can be carried out by use of Euler's identity [5]. The result is given meaning by expanding into a series (which is not absolutely convergent) and grouping and ordering (and analytically continuing) the resulting terms into "composite" periodic orbits. Our $D$ is formally the same series and $D_n$ is a particular way of collecting terms into composite periodic orbits, that is, orbits the sum of whose periods, including repetitions measured in numbers of reflections from the boundary, add up to composite period $n$. (Such a collection is also called a pseudo-orbit [5], but we prefer Smilansky's more descriptive terminology.) Grouping terms according to $D_n$ *guarantees* absolute convergence unless the S$\Phi$ approximation to the exact integrals for $\sigma_n$ fails drastically *and* disagrees with QCA1 and QCA2. Whether the QCA ceases to be adequate at some large $n$ in this evaluation, however, is an interesting and open question.

In general, the improvement in convergence gained for $D$ is also gained for **N**. We remark that if a "curvature expansion" [9] effectively shortens the series for $D$, it likewise shortens the series for **N**. This is because all long orbits are close to periodic orbits and can thus be approximated by them. The Fredholm method provides a way to systematize this approximation.

To summarize, the Fredholm method applied to billiards provides a mathematically exact formulation whose QCA limit can be compared with various approximations obtained by making the QCA at an early stage. In particular, the Fredholm determinant is a rigorously defined version of the D$\zeta$.

The method goes beyond the study of the spectrum and in effect extends the methods used for studying the determinant to the entire Green's function. The Fredholm method is not restricted to billiards or exact formulations. If the QCA is made for Bogomolny's **T** at an early stage, the Fredholm method can be applied to a wide variety of cases (and a variety of surfaces of section), including scattering systems, mesoscopic systems, and correlation functions, whether or not these are chaotic in the classical limit. Many insights can be gained, some of which we report in a separate communication.

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