Boundary integral method applied in chaotic quantum billiards

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Abstract. The boundary integral method (BIM) is a formulation of Helmholtz equation in the form of an integral equation suitable for numerical discretization to solve the quantum billiard. This paper is an extensive numerical survey of BIM in a variety of quantum billiards, integrable (circle, rectangle), KAM systems (Robnik billiard) and fully chaotic (ergodic, such as stadium, Sinai billiard and cardioid billiard). On the theoretical side we point out some serious flaws in the derivation of BIM in the literature and show how the final formula (which nevertheless was correct) should be derived in a sound way and we also argue that a simple minded application of BIM in nonconvex geometries presents serious difficulties or even fails. On the numerical side we have analyzed the scaling of the averaged absolute value of the systematic error $\Delta E$ of the eigenenergy in units of mean level spacing with the density of discretization ($b =$ number of numerical nodes on the boundary within one de Broglie wavelength), and we find that in all cases the error obeys a power law $< |\Delta E| > = Ab^{-\alpha}$, where $\alpha$ (and also $A$) varies from case to case (it is not universal), and is affected strongly by the existence of exterior chords in nonconvex geometries, whereas the degree of the classical chaos seems to be practically irrelevant. We comment on the semiclassical limit of BIM and make suggestions about a proper formulation with correct semiclassical limit in nonconvex geometries.

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1 Introduction

In the studies of quantum chaos (Gutzwiller 1990, Giannoni et al 1989) good numerical methods are not only indispensable but quite essential. We need them in order to illustrate and verify the theoretical developments. Also, new numerical experiments provide valuable material as evidence and inspiration for new theories. Quantum billiards are certainly very useful model systems since dynamically they are generic and - depending on the design - they can cover all regimes of classical motion between integrability and full chaos (ergodicity). Their classical dynamics can be easily followed for very long time periods because no integration is necessary but only searching for zeros of certain functions at collision points. Quantumly they have the advantage of having a compact configuration space admitting application of various numerical methods such as the Boundary Integral Method (BIM) (Banerjee 1994, Berry and Wilkinson 1984, henceforth referred to as BW, and the references therein), the Plane Wave Decomposition Method (PWDM) employed by Heller (1984), conformal mapping diagonalization technique introduced by Robnik (1984) and further developed by Berry and Robnik (1986) and recently by Prosen and Robnik (1993, 1994), also by (Bohigas et al 1993), and a number of other methods, which, however, might be adapted to some special systems. Among the general methods BIM is probably most widely used, even in quite practical engineering problems. The main task of the present paper is to point out some logical flaws in deriving this method in the context of the existing literature, to analyze its limitations in cases of nonconvex geometries with suggestions for improvements and generalizations, and to perform an extensive numerical investigation of its accuracy in relation to geometrical properties and classical dynamics.

In order to clearly expose the difficulties and the errors in the derivation of BIM offered in the literature, e.g. in BW, we present our regularized derivation, by which we mean that we construct and use a Green function which automatically (by construction) satisfies the Dirichlet boundary condition (vanishes on the boundary $\partial B$ of the billiard domain $B$), which is achieved by employing the method of images (see e.g. Balian and Bloch (1974) and the references therein). This will enable us to avoid committing two errors, which, however, luckily compensated each other: Firstly, in taking the normal derivatives on the two sides of equation (6) in BW, on the rhs
we must use the value of $\psi(r)$ which is the interior solution inside $B$ rather than $\frac{1}{2}\psi(r)$ which is the value exactly on the boundary, simply because in taking the derivatives we must evaluate the function at two infinitesimally separated points normal to the boundary; Secondly, this error of taking the unjustified factor $1/2$ is then exactly compensated by another error in arriving at the equation (8) in BW, namely by interchanging the integration along the boundary $\partial B$ and the normal differentiation, because due to singularities on the boundary these two operations do not commute.

So, let us offer our regularized derivation. We are searching for the solution $\psi(r)$ with eigenenergy $E = k^2$ obeying the Helmholtz equation

$$\nabla^2 \psi(r) + k^2 \psi(r) = 0, \quad (1)$$

with the Dirichlet boundary condition $\psi(r) = 0$ on the boundary $r \in \partial B$. We will transform this Schrödinger equation for our quantum billiard $B$ into an integral equation by means of the regularized Green function $G(r, r')$, which solves the following defining equation

$$\nabla^2 G(r, r') + k^2 G(r, r') = \delta(r - r') - \delta(r - r'_{R}), \quad (2)$$

where $r$ and $r'$ are in $B \cup \partial B$, and $r'_{R}$ is the mirror image of $r'$ with respect to the tangent at the closest lying point on the boundary, and thus if $r'$ is sufficiently close to the boundary then $r'_{R}$ is outside the billiard $B$. The solution can easily be found in terms of the free propagator (the free particle Green function on the full Euclidean plane)

$$G_0(r, r') = -\frac{1}{4i}H_0^{(1)}(k|r - r'|), \quad (3)$$

where $H_0^{(1)}$ is the zero order Hankel function of the first kind (Abramowitz and Stegun 1972), namely

$$G(r, r') = G_0(r, r') - G_0(r, r'_{R}), \quad (4)$$

such that now $G(r, r')$ is zero by construction for any $r'$ on the boundary $\partial B$, in contradistinction to the Green function defined and used in equation (5) in BW. Multiplication of the equation (2) by $\psi(r)$ and the Helmholtz
equation (1) by $G(r, r')$, subtraction, integration over the area inside $B$ and using Green’s theorem, yields

$$
\oint ds (\psi(r) n \cdot \nabla_r G(r, r') - G(r, r') n \cdot \nabla_r \psi(r)) = \psi(r'),
$$

where $s$ is the arclength on the boundary $\partial B$ oriented anticlockwise, $n$ is the unit normal vector to $\partial B$ at $r$ oriented outward, and this equation is now valid for all $r'$ inside and on the boundary of $B$. Since in this equation everything is regular we can take the normal partial derivatives on both sides. Following the usual notation in BW we define the normal derivative of $\psi$ at the point $s$ as

$$
u(s) = n \cdot \nabla_r \psi(r(s)),
$$

and thus using the boundary condition $\psi(r) = 0$ we arrive at

$$u(s) = -2 \oint ds' u(s') n \cdot \nabla_r G_0(r, r'),
$$

In this way we have correctly derived the main integral equation of the boundary integral method which is correctly given as equation (8) in BW (where the two errors exactly compensate), so that all the further steps in working out the geometry of equation (5) and the numerical discretization are exactly the same as in BW. As shown in figure 1 we define the length of the chord between two points on the boundary $r(s)$ and $r(s')$ as

$$\rho(s, s') = |r(s) - r(s')|
$$

and the angle $\theta(s', s)$ is the angle between the chord and the tangent to $\partial B$ at $s'$. Of course $\theta(s, s') \neq \theta(s', s)$. Thus following the notation of BW we can write

$$n' \cdot \frac{\partial G_0(r, r')}{\partial r'} = \sin \theta(s', s) \frac{\partial G_0}{\partial \rho}
$$

and we obtain finally

$$u(s) = -\frac{1}{2} ik \oint ds' u(s') \sin \theta(s, s') H_1^{(1)}\{k \rho(s, s')\}.
$$

In numerically solving this integral equation we have used precisely the same primative discretization procedure as BW, which turned out to be better than
some other more sophisticated versions. So we simply divide the perimeter \( \mathcal{L} \) into \( N \) equally long segments and thus define

\[
s_m = m\mathcal{L}/N, \quad \rho(s_l, s_m) = \rho_{lm}, \quad \theta(s_l, s_m) = \theta_{lm}, \quad l \leq l, m \leq N, \quad (11)
\]

Therefore numerically we are searching for the zero of the determinant \( \Delta_N(E) = \text{det}(M_{lm}) \) where \( M_{lm} \) are the matrix elements of the \( N \times N \) matrix,

\[
M_{lm} = \delta_{lm} + \frac{ik\mathcal{L}}{2N} \sin \theta_{lm} H_1^{(1)}(kr_{lm}), \quad (12)
\]

where \( E = k^2 \). Due to the asymmetry \( \theta_{lm} \neq \theta_{ml} \) this matrix is a general complex non-Hermitian matrix.

One important aspect of this formalism is the semiclassical limiting form which has been extensively studied by Boasman (1994) and which is the subject of our current investigation (Li and Robnik 1995a). At this point we just want to make the following comment. In cases of nonconvex geometries we will have exterior chords connecting two points on the boundary such that they lie entirely, or at least partially, outside \( \mathcal{B} \). While formally the method and the procedure in such cases is perfectly right, in reality it fails completely, and this can be seen by considering the semiclassical limit. The formal leading order in the asymptotic expansion of the Hankel function \( H_1^{(1)} \) (Debye approximation) does not match the actually correct semiclassical leading approximation which would be spanned by the shortest classical orbit connecting the two points via at least one or many collision points. Therefore we understand and expect that the method must fail or at least must meet severe difficulties in cases of nonconvex geometry. This has been completely confirmed in our present work as we will show in the next section, whilst the analytical work to reformulate the method including the multiple collision expansions is in progress (Li and Robnik 1995b) and is expected to deal satisfactorily with nonconvex geometries.

In the next section we shall analyze the numerical accuracy of BIM as a function of the density of discretization

\[
b = \frac{2\pi N}{k\mathcal{L}}, \quad (13)
\]
in a variety of quantum billiards with integrable, KAM-type or ergodic classical dynamics, including such with nonconvex geometry. The main result is that there is always a power law so that the error of eigenenergy in units of mean level spacing, after taking average of the absolute value over a suitable ensemble of eigenstates, obeys \( \langle |\Delta E| \rangle = Ab^{-\alpha} \), but the exponent \( \alpha \) is nonuniversal and typically becomes almost zero if there are nonconvex segments on the boundary.

2 Numerical results

The numerical procedure we have used to solve the variety of quantum billiards is exactly as described in the introduction and therefore it is precisely the same as in BW. Our main task in this work is to analyze in detail the behavior of BIM as a function of the density of discretization \( b \), especially in relation to the geometrical properties of \( B \) (nonconvexities) and in relation to classical dynamics, whose chaotic behaviour is expected to imply interesting methodological and algorithmical manifestation of quantum chaos.

This to end we have to measure the numerical error of the eigenenergies in some natural units, which obviously is the mean level spacing. In plane billiards this is well defined and determined by the leading term of the Weyl formula, namely in our units it is equal to \( 4\pi/\mathcal{A} \), where \( \mathcal{A} \) is the area of the billiard \( B \). Since the error \( \Delta E \) of the eigenenergies thus defined still fluctuates widely from state to state we have to perform some kind of averaging over a suitable ensemble of consecutive states. But this will make sense only if such a local average of the error is stationary (constant) over a suitable energy interval. This condition has been confirmed to be satisfied in almost all cases which we checked. In case of the circle billiard and in case of half circle billiard (which embodies all the odd states of the full circle billiard) this stationarity of the locally averaged error is shown in figures 2(a-b), respectively.

Having established that we have always taken the average of the absolute value of the error (in units of the mean level spacing) over a suitable ensemble
of eigenstates, for which we have chosen the lowest one hundred eigenstates in all cases. This quantity will be henceforth denoted by $\langle |\Delta E| \rangle$.

In figure 3(a-f) we show the error $\langle |\Delta E| \rangle$ versus $b$ for three shapes of the Robnik billiard with the shape parameter $\lambda = 0, 1/4, 1/2$. (The billiard shape is defined by the quadratic conformal map of the unit disk $|z| \leq 1$ onto to the $w$-plane, namely $w(z) = z + \lambda z^2$.) We show the normal plot of the averaged absolute value of the error versus $b$ in the figures 3(a,c,e) and the log-log plot in figures 3(b,d,f). The best fitting power law curve is described by

$$\langle |\Delta E| \rangle = A b^{-\alpha}, \quad (14)$$

and is seen to provide a very significant fit in all three cases. One should be reminded that at $\lambda = 0$ we have integrable classical dynamics in the circle billiard, at $\lambda = 1/4$ we have almost ergodic but nevertheless KAM-type dynamics with very tiny islands of stability (see e.g. Li and Robnik (1994,1995c); it should be emphasized that at $\lambda = 1/4$ we have zero curvature point at $z = -1$, and for all $\lambda > 1/4$ the shape is nonconvex), whilst at $\lambda = 1/2$ we have rigorous ergodicity (Markarian 1993) and also nonconvex geometry. So one can observe that increasing chaos from integrability (circle) to almost ergodicity ($\lambda = 1/4$) has almost no effect on $\alpha$, whereas the nonconvexities at $\lambda > 1/4$ seem to imply a complete ”collapse” of $\alpha$: As it will be shown in figure 5(a) $\alpha$ drops to zero almost discontinuously at $\lambda = 1/4$ and then increases up to 0.4 at $\lambda$ close to 1/2. This is because, perhaps, close to $\lambda = 1/2$ where we have the cusp singularity at $z = -1$, the role of the nonconvexities is smaller. In all cases we have calculated all states by applying BIM but then for technical reasons compared only the odd states with their exact value, which are supplied by the conformal mapping diagonalization technique (see e.g. Robnik 1984, Prosen and Robnik 1993).

It is then interesting to look at the similar plots for BIM as applied to half billiard by which we mean the upper part of the Robnik billiard defined for $\Im(z) \geq 0$, implying also $\Im(w) \geq 0$, still with the Dirichlet boundary conditions everywhere on the boundary. This embodies all the odd states of the full billiard. The classical dynamics in the two billiards is of course exactly the same and yet in figures 5(a-f) for the half billiard we see that $\alpha$ is now notably different, showing that there is no universality in the value of $\alpha$ so
that \( \alpha \) is certainly not uniquely determined by the classical dynamics of the underlying quantum billiard. On the other hand we can also see the effect of nonconvexities of the boundary \( \partial B \): Namely for the half (cardioid) billiard at \( \lambda = 1/2 \) we have no nonconvexities and this probably is precisely the reason for large increase of \( \alpha \) from 0.4 in figure 3(e-f) to 2.4 in figure 4(e-f).

Having established the validity of the power law (14) it is now most interesting and also immensely CPU-time consuming (it took almost one month of CPU-time on Convex C3860 to produce figure 5(a,c) and a little bit less for figure 5(b,d)) to look at the variation of \( \alpha \) with the billiard shape parameter \( \lambda \). For the full Robnik billiard this is shown in figure 5(a) and for the half billiard in figure 5(b). In both cases there is a flat region of almost constant \( \alpha \) within \( 0 \leq \lambda \leq 1/4 \): In the former case it fluctuates slightly around 3.5 and in the latter case it is surprisingly stable around 2.9. At \( \lambda > 1/4 \) the nonconvexities of boundary appear and this implies - as explained qualitatively in the introduction - strong drop of \( \alpha \) which is much sharper (almost discontinuous) in case of the full billiard because obviously the nonconvexities are more pronounced there than in the half billiard. So in the former case \( \alpha \) drops almost to zero, whereas in the half billiard it decreases rather smoothly to about 0.16 at \( \lambda = 0.36 \), and then increases again reaching the value of 2.4 at \( \lambda = 1/2 \).

Apart from \( \alpha \) in (14) we would also like to know the value of the constant \( A \) (the pre-factor) in each case. This is given by fixing \( b = 12 \) and plotting the mean absolute value of the error (averaged over the lowest one hundred odd states) versus \( \lambda \) logarithmically. Here we see that in both cases the mean error \( \langle |\Delta E| \rangle \) is almost constant up to \( \lambda \leq 1/4 \) and is about \( 5 \times 10^{-6} \) for the full billiard whilst for the half billiard it is about \( 7 \times 10^{-5} \). This discrepancy by almost an order of magnitude is not completely understood. At \( \lambda \geq 1/4 \) please observe the dramatic increasing of \( \langle |\Delta E| \rangle \). For the full billiard it increases almost discontinuously up to \( 2 \times 10^{-2} \) whereas in the half billiard it reaches the minimum of \( 4 \times 10^{-3} \) at about \( \lambda = 0.36 \) and decreases then again to \( 2 \times 10^{-4} \) at \( \lambda = 1/2 \). This difference again is qualitatively explained by the role of nonconvexities.

Finally in figure 6(a-f) we show the worst cases of applying BIM, namely the Robnik billiard at \( \lambda = 0.4 \) in figures 6(a,b), the half billiard in figures
6(c,d) with the same value of $\lambda = 0.4$ and the desymmetrized Sinai billiard (1/8 of the full billiard) with the unit side length and radius $R = 1/4$ of the circular obstacle. In all cases $\alpha$ is almost zero or even slightly negative which implies that there is practically no convergence of the numerical eigenvalues by increasing the density of discretization $b$. Clearly, this is due to the non-convex geometry of these billiards.

Most of our results are summarized in table 1 for three classes of billiard systems with different type of classical dynamics, namely integrable, KAM-type and ergodic systems. We show the calculated values of $\alpha$ and also the average absolute value of the error $< |\Delta E| >$ with fixed value of $b = 12$. The table clearly demonstrates that the power law (14) for BIM is universal but not the exponent $\alpha$ and the prefactor $A$. It also demonstrates that classical dynamics has little effect on $\alpha$ whereas the nonconvexities of the boundary are quite crucial: In all cases of pronounced nonconvex geometry $\alpha$ is typically close to zero or even slightly negative like in the Sinai billiard. In the table we include also the results on the integrable case of the rectangular equilateral triangle (half of the unit square) where $\alpha = 3.28$ is quite large, and the ergodic case of the 1/4 Heller’s stadium (2 × 2 square plus two semicircles with unit radius) in which case $\alpha = 3.0$ is also quite large. Both of these two cases have convex geometry and thus large $\alpha$ despite the completely different classical dynamics.

When thinking about improving the efficiency and the accuracy of BIM we have also tried a more sophisticated version of BIM, where we have explicitly used a Gaussian integration on the boundary when discretizing our main equation (7). However, this experience has been negative after many careful checks in various billiards, and therefore we decided to resort to the primitive discretization of BIM which is exactly the same approach as in BW.

3 Discussion and conclusions

The main purpose of this paper is to investigate the behaviour of the Boundary Integral Method (BIM) with respect to the density of discretization $b$ as defined in equation (13) ($b =$ the number of numerical nodes per de Broglie wavelength along the boundary). In all cases we discovered that there is a
power law behaviour described in (14): The average absolute value of the error measured in the units of mean level spacing is given by $< |\Delta E| > = Ab^{-\alpha}$. We wanted to verify whether there is any systematic effect of classical dynamics of quantum billiards on $\alpha$ and $A$. The answer is negative. On the other hand we found that the role of nonconvex geometry of the boundary is crucial: If there is a nonconvex part of the boundary $\alpha$ is typically close to zero or even slightly negative implying that there is practically no convergence of the eigenvalues with respect to the increasing $b$. This failure of BIM can be understood as explained in the introduction, and the easiest way to see that is to consider the semiclassical limiting approximation of BIM (Li and Robnik 1995a). After explaining two systematic errors in the literature where the integral BIM equation is derived and where luckily the two errors mutually compensate, we have given the correct (regularized) derivation and discussed the BIM formalism thus derived. We agree that even in nonconvex geometries it is formally right, but nevertheless practically fails which is most clearly demonstrated by the semiclassical limit mentioned above. Therefore we suggest a generalization of the BIM method by using multiple reflection (collision) expansion which is another subject of our current investigation (Li and Robnik 1995b), and is important not only for studies in quantum chaos but also in engineering problems (Banerjee 1994).

Most of our results are summarized in table 1, giving the evidence for the above conclusions. In another work (Li and Robnik 1995d) we have investigated the impact of classical chaos on another general numerical method for quantum billiards, namely the plane wave decomposition method employed by Heller (1984, 1991), where we have found that at fixed $b$ the average absolute value of the error $< |\Delta E| >$ does correlate with classical chaos and increases sharply with increasing classical chaos. In this method such a behaviour can be understood much more easily: In classically integrable cases the wavefunction in the semiclassical limit can be correctly described locally by a finite number of plane waves, whereas in classically fully chaotic (ergodic) systems we need locally infinite number of plane waves. Therefore at fixed $b$ the accuracy of Heller’s method strongly deteriorates as the system approaches ergodicity. More results on that will be published in a separate paper (Li and Robnik 1995d).

It remains an interesting and important theoretical problem to study the
sensitivity of the eigenstates (eigenenergies and wavefunctions) on the boundary data of eigenfunctions, of which one aspect is also the dependence of the eigenstates on the billiard shape parameter. If such sensitivity correlates with classical chaotic dynamics and at the same time manifests itself in the accuracy of the purely quantal numerical methods then such a behaviour would be one important manifestation of quantum chaos. This interesting line of thoughts in the search of another face of quantum chaos will be further developed in another work (Li and Robnik 1995e) where we also present detailed studies of level curvature distribution and other measures of the sensitivity of the eigenstates.

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# Table

**Table 1.** The power law exponent $\alpha$ and the average absolute value of the error $<|\Delta E|>$ with $b = 12$ for different billiards. For details of the KAM-type see also figures 5(a,b).

| Type   | Quantum billiard       | $\alpha$   | $<|\Delta E|>_{b=12}$ |
|--------|------------------------|------------|------------------------|
| Integrable | Circle (half)        | 2.94 ± 0.17 | 6.74E−5               |
|        | Circle (full)          | 3.44 ± 0.18 | 5.97E−6               |
|        | Rectangle-triangle     | 3.28 ± 0.29 | 4.08E−5               |
| KAM    | Robnik (full) (0 < $\lambda$ < 1/4) | \(\approx 3.4\) | \(\approx 5.0E−6\)   |
|        | Robnik (half) (0 < $\lambda$ < 1/4) | \(\approx 2.9\) | \(\approx 7.0E−5\)   |
| Ergodic | Stadium (1/4)         | 3.00 ± 0.16 | 1.18E−4               |
|        | Cardioid (half)        | 2.42 ± 0.11 | 1.76E−4               |
|        | Cardioid (full)        | 0.42 ± 0.08 | 1.85E−2               |
|        | Sinai (1/8)            | −0.34 ± 0.11 | 3.63E−1               |
|        | Robnik (full) (0.3 < $\lambda$ < 1/2) | see figure 5a | see figure 5c         |
|        | Robnik (half) (0.3 < $\lambda$ < 1/2) | see figure 5b | see figure 5d         |
Figure captions

**Figure 1:** The notation of the angles and chords used in BIM.

**Figure 2:** The BIM error (measured in units of mean level spacing) of eigenstates versus energy. The error is difference between the BIM value and the exact value. The lowest 1000 odd states are shown. Plot (a) is for the full circle billiard and (b) for the half circle billiard. In both cases $b$ is fixed, $b = 6$.

**Figure 3:** The ensemble averaged (over 100 lowest odd eigenstates) absolute BIM error versus the density of boundary discretization $b$ and the best power law fit for the full Robnik billiard at different shape parameters $\lambda$. The $+$ represents the numerical data, the curve is the best power law fit whose $\alpha$ is given in (b,d,f). Figures (b,d,f) are log-log plots of the same quantities as in (a,c,e).

**Figure 4:** The same as in figure 3 but for the half Robnik billiard.

**Figure 5:** We show $\alpha$ versus $\lambda$ plot for Robnik billiard in (a) and for half Robnik billiard in (b). In (c) and (d) we plot $-\lg(\langle |\Delta E| \rangle)$ with fixed $b = 12$ versus $\lambda$ for the two billiards, respectively.

**Figure 6:** We show three examples of worst cases in applying BIM, Robnik billiard with $\lambda = 0.4$ in (a,b), half Robnik billiard with the same $\lambda$ in (c,d), and desymmetrized Sinai billiard ($1/8$) with unit side length and radius $R = 1/4$. In (a,c,e) we plot the averaged absolute value of the error versus $b$, and in (b,d,f) we plot log-log diagrams of the same quantities.