Trace formula for counting nodal domains on the boundaries of chaotic 2D billiards

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Given a Dirichlet eigenfunction of a 2D quantum billiard, the boundary domain count is the number of intersections of the nodal lines with the boundary. We study the integer sequence defined by these numbers, sorted according to the energies of the eigenfunctions. Based on a variant of Berry’s random wave model, we derive a semi-classical trace formula for the sequence of boundary domain counts. The formula consists of a Weyl-like smooth part, and an oscillating part which depends on classical periodic orbits and their geometry. The predictions of this trace formula are supported by numerical data computed for the Africa billiard.

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Recently, the study of nodal patterns witnessed a remarkable renaissance, and attracted the active interest of scientists from very diverse fields—quantum chaos, acoustics, optics, spectral theory, percolation and more [1]. The number of nodal domains—connected components on which a real wave function has a constant sign, is an important feature, which has been used to characterize eigenfunctions of wave equations and even to resolve iso-spectral ambiguities [2]. For quantum billiards, the number $\nu_n$ of nodal domains of the $n$’th eigenfunction (sorted by increasing eigenvalues $E_n \leq E_{n+1}$) can never exceed $n$ [3]. The number of nodal domains can be computed explicitly for separable systems. However, in the non-separable cases, there exists no analytical tool which provides the number of nodal domains, and even the numerical counting problem is difficult due to the dependence on the detailed structure of the domains. In [4] it was shown that the asymptotic distribution of $\nu_n$ depends on the dynamics of the underlying classical system. In the separable case, the parameters of the classical phase space determine the nodal counts in the semi-classical limit. In the chaotic case, the distribution matches the predictions of a percolation model, which was proposed (but not rigorously justified) in [5].

The partition into nodal domains induces a partition of the boundary to “boundary domains”. They are defined as the nodal domains of a “boundary function”, which for Dirichlet billiards, is the normal derivative of the eigenfunction on the boundary. In 2D, the number $\eta_n$ of boundary domains equals the number of nodal points separating them—the boundary intersection (BI) points. This number is more accessible, both numerically and theoretically, than $\nu_n$. At the same time, it carries the fingerprints of the underlying classical dynamics of the billiard [4]. Also, the number of boundary domains provides information which is essential for estimating the total number of nodal domains [6]. It was recently shown [7] that $\eta_n = O(\sqrt{n})$. In [4], the asymptotic distribution of $\eta_n/\sqrt{n}$ was computed for a class of integrable billiards. For a chaotic billiard of area $\mathcal{A}$ and boundary length $\mathcal{L}$, a random wave model yields the estimate [4,8] $\eta_n \sim Lq/(2\pi)$, where $q = \sqrt{4\pi n/\mathcal{A}}$ is the leading asymptotic estimate for the $n$’th wave-number $k_n = \sqrt{E_n}$.

The purpose of the present paper is to go beyond the simple estimate $\eta_n \sim Lq/(2\pi)$, and provide a trace formula which approximates the mean value as well as the fluctuations in the sequence $\eta_n$, in terms of the periodic orbits of the classical billiard. Such formulæ were proposed in the past for the counting of nodal domains in separable billiards [9]. Here is the first time that a counting trace formula is written down for the chaotic case.

The counting of boundary intersections is performed by computing the density $d_\eta(n) = \sum_{m \in \mathbb{N}} \delta(n - m)\eta_m$. For a chaotic Dirichlet billiard with a smooth boundary, we derive in the sequel the following asymptotic expression:

$$d_\eta(n) \approx \frac{\mathcal{L}}{2\pi q} + \frac{\mathcal{L}^2}{4\pi \mathcal{A}} - \frac{6\pi \mathcal{A}}{4\pi \mathcal{A}} + \frac{1}{\pi} \sum_{p,r} \frac{\Phi_p}{\sqrt{|\text{Tr}[M_p^{-1}]|}} \cos(r(\tilde{q}L_p - \nu_p \frac{\pi}{2})), \quad (1)$$

where $p$ enumerates classical periodic orbits, $r \in \mathbb{N}^*$ counts repetitions of the orbit, $L_p$ is the length of the orbit, $M_p$ the monodromy matrix, $\nu_p$ the Maslov index, and $\tilde{q} = q + \mathcal{L}^2/(2\mathcal{A})$. $\Phi_p$ is a trigonometrical factor depending on the $n_p$ bounce angles of the orbit $p$:

$$\Phi_p = \sum_{i=1}^{n_p} (4\cos^2 \psi_i^{(p)} - 1)2\sin \psi_i^{(p)}. \quad (2)$$

Before sketching the derivation of the trace formula, we shall demonstrate its application. We computed the lowest 20,000 eigenfunctions ($0 < k_n < 260$) of the Africa billiard [10], the corresponding BI count sequence $\eta_n$, and the density $d_\eta^0(q) = \sum_p \rho(q - \sqrt{4\pi n/\mathcal{A}})\eta_n$ (where here and in what follows $\rho(x)$ is a narrow Gaussian approximating the Dirac $\delta$). $\rho$ is defined as a density, so $\rho(q - q_0) = \rho(n - n_0) \cdot A(q_0)/(2\pi)$. Subtracting the predicted smooth part $d_\rho^0(q)$ and scaling, we computed $f(q) = (d_\eta(q) - d_\rho(q))/q \cdot W(q)$, where $W$ is a Gaussian “window function” of width $\sigma = 50$ and center $q_0 = 130$, which was used for softening the sharp cutoff due to the finiteness
of the computed spectrum. The length spectrum, which is the Fourier transform of \( f(x) \) of \( f(q) \) was compared with \( f_{sc}(x) \), the theoretical prediction based on the oscillating part of \( f \). The latter was computed using 70 classical periodic orbits (with up-to 7 bounce points) and 15 complex periodic orbits whose lengths had a very small imaginary part (however, the complex orbits did not have a significant effect).

FIG. 1(a) displays several peaks centered at lengths of periodic orbits which match quite well with the theoretical predictions. A more detailed comparison is presented in FIG. 1(b). Due to \( \delta \), orbits whose angles are close to 60° are inhibited. Indeed, the triangular periodic orbits of the billiard, whose lengths are in the range 5.07–6.05, cannot be seen above the background level. The structure around \( x = 6.5 \) is due to several periodic orbits that pass very close to the boundary at the region of its highest concavity. This phenomenon will be discussed below.

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The derivation of the trace formula (1) starts by expressing \( \eta_n \) as \( \eta_n = \oint \hat{b}_n(s) ds \), where \( 0 < s < L \) is the boundary arc length and the BI density \( b_n(s) \) is given by

\[
\hat{b}_n(s) = \sum_{i=1}^{\eta_n} \delta(s_i^{(n)} - s) = \delta(u_n(s)) \left| \hat{u}_n(s) \right|.
\] (3)

Here, \( u_n(s) = n(s) \cdot \nabla \psi_n(r(s))/k_n \) is the scaled normal derivative of the \( n \)th eigenfunction \( \psi_n \), taken at the boundary point \( r(s) \), \( \hat{u}_n(s) = \frac{du_n(s)}{ds} \), and \( s_i^{(n)} \) are the BI points (zeros of \( u_n \)).

The trace formula will be derived for a smoothed version \( \rho_X^{(y)}(y) = \int \rho_{\eta}(m)\rho(n-m)dm = \sum_{n \in \mathbb{N}^+} \rho(n-m)m \). (The smoothing kernel \( \rho \) was defined above.) In the sequel we shall consistently use the notation \( \rho_X^{(y)}(y) \) to denote the \( \rho \) smoothed density of the quantity \( X \) in the variable \( y \).

Consider the spectral density of \( b(s) \) at wavenumber \( k \), \( \rho_{\eta}(s; k) = \sum_{n=1}^{\eta_n} \delta(k_n - k) b_n(s) \). It is approximated by \( \rho_{\eta}(s; k) = \frac{d\rho_X^{(y)}(y)}{dy}(s)_, \) where \( d\rho_X^{(y)}(y)/dy(s) \) is the smoothed spectral density and \( \rho(s) = \sum_{n} b_n(s) \cdot \rho(k_n - k)/d\rho_X^{(y)}(s) \) is the spectral average of \( b_n(s) \) around \( k \). If we choose the width of \( \rho \) to be of order \( k^{-1/2} \), then as \( k \to \infty \), the discrete ensemble of boundary functions in the corresponding spectral window around \( k \) approaches a continuous distribution. To proceed, we introduce the conjecture that for chaotic billiards this limiting distribution is Gaussian. This conjecture, may be seen as a variant of Berry’s random wave model [12], adjusted to the boundary as in [13] and [14]. While the validity of the conjecture is expected to improve in the semiclassical limit, numerical tests within the range of \( k \) values used here reveal a residual Kurtosis which might explain the background observed in the length spectrum. Adopting the random waves conjecture enables us to express the mean of the density \( b(s) \) in terms of the variances of the field \( u(s) \) and its derivative \( \hat{u}(s) \):

\[
\langle b(s) \rangle = \frac{1}{\pi} \sqrt{\frac{\langle \hat{u}^2(s) \rangle}{\langle u^2(s) \rangle}} = \frac{1}{\pi} \sqrt{\frac{d^2\rho_X^{(y)}(s)}{dy^2}(k)}.
\] (4)

To compute the required densities, we write

\[
d_{u^2}(s) = \sum_n \delta(k_n - k) u_n^2(s) = \frac{2k}{\pi} \text{Im} g(s; s; k)
\] (5)

where \( g(s; s'; k) = \sum_n u_n(s)u_n(s')/(k_n^2 - k^2) \) is the boundary Green function. As shown in [16], \( g \) can be expanded as \( g = \sum_{n=0}^{\infty} \hat{h}^n g_0 \), where \( \hat{h} \) is the integral operator with kernel function \( h \). The functions \( g_0 \) and \( h \) are given by

\[
h(s, s'; k) = 2n(s) \cdot \nabla \psi_n(r(s)) G_0(r(s), r(s'); k)
\]

\[
g_0(s, s'; k) = \frac{2}{k^2} \sum_{i,j} n_i n_j' \frac{\partial^2 G_0(r(s), r(s'); k)}{\partial r_i \partial r_j'}
\]

and \( G_0 = \frac{i}{2} H_0^+(k|r - r'|) \) is the free Green function in 2D. To handle the singularities involved in this expansion and make it more amenable to semi-classical treatment, we choose a large cutoff \( 1 \ll x_C \ll kL \), and split \( g_0 \) into a “far” (off diagonal) part and a “near” (close to the diagonal) part:

\[
g_0^{(N)}(s) = g_0(s, s') H(x_C/k | s - s'|) + g_0^{(F)}(s, s') H(|s - s'| - x_C/k)
\]

(6)

where \( H \) is the Heaviside step function. It can be shown that for large \( k \)

\[
\hat{h} g_0^{(N)}(s) = \int_0^L h(s, s_1) g_0^{(N)}(s_1, s') ds_1 \sim g_0^{(F)} + g_1^{(N)}
\]

Substituting this result in (5), we get a similar expansion for \( d_{u^2}(s, s') \). The first two terms, which were explicitly computed in [16] for \( s' \to s \), yield the “smooth part” \((k - \kappa(s))/(2\pi)\), where \( \kappa \) is the curvature (note that this can also be derived by applying the methods of [8] on the curved boundary corrections to Berry’s random wave model, which are described in [14]). The third term is interpreted as a summation over possible paths from \( s' \to s \), where the \( n \)th summand includes integration over \( n \) intermediate bounce points. Approximating the integrals by the stationary phase method (closely following [18]), we get a
sum over classical paths (allowing only specular bounces). The oscillating part for $d_{uu'}$ is given by

$$
\left( \frac{2}{\pi} \right)^{\frac{3}{2}} \sum_{t} \sqrt{\sin \psi \sin \psi'} \cos (kL_{t} + \frac{3}{2} \pi - \frac{\pi}{2} \nu_{t}),
$$

(7)

where $t$ enumerates classical orbits from $s'$ to $s$, $L_{t}$ is the length of the orbit, $\nu_{t}$ is the Maslov index (number of conjugate points plus twice the number of bounce points), $\psi$ and $\psi'$ are the angles between the orbit and the boundary at $s$ and $s'$ respectively, and $p' = k \cos(\psi')$ is the classical momentum at $s'$ (hence, the oscillating part of $d_{uu'}$ is $O(\sqrt{k})$). Taking derivatives of this expansion, we get an expression for $d_{uu'} \frac{\partial b}{\partial s}$, which has a similar form. Due to the rapid decay of the Fourier transformed convolution kernel $\hat{\rho}$, the expansions (taken at $s = s'$) of $d_{uu'}^\rho$ and $d_{uu'}^\rho$, converge, so the quotient required for substitution in (4) can be computed, and used to derive an expression for $\langle b(s) \rangle$. To compute $d_{n}^\rho(k)$, we multiply by $d^\rho(k)$ (for which we can use the Gutzwiller trace formula, again smoothed by $\rho$ to ensure convergence), and integrate over $s$. The stationary phase condition added by this extra integration ensures that $\psi = \psi'$, and the result includes summation over periodic classical orbits. Finally, we want to discard the spectral information and compute $\eta(n)$ rather than $\eta(k)$. Therefore, following the method described in [8], we substitute in the resulting expression for $d_{n}^\rho(k)$, an expansion for $k(n)$, achieved by formally inverting the Gutzwiller trace formula. This leads us to the trace formula for $d_{n}^\rho(n)$, presented in (1).

A stringent test of the theory above, is based on the following argument. A “partial” trace formula which counts BI located on a prescribed part $\Gamma \subset \partial \Omega$ of the boundary can be similarly derived by integrating the BI density over $\Gamma$ alone: $d_{\eta \Gamma}(k) = \int_{\Gamma} d_{\eta}(s; k) ds$. Since the formula for $d_{\eta}$, much like (7), involves summation over orbits starting and ending at $s$, we conclude that only periodic orbits that have a bounce point in $\Gamma$ will contribute to the sum in the resulting trace formula for $d_{\eta \Gamma}$. By choosing a $\Gamma$ which is bounded away from the bounce points of a specific orbit, we can effectively turn off the effect of that orbit. Similarly, we expect orbits that have some, but not all of their bounce points in the excluded regions $\partial \Omega \setminus \Gamma$, to have reduced amplitude in the length spectrum. This result is demonstrated in FIG. 2. In FIG. 2(b), $\Gamma$ is plotted with a wide line, while
FIG. 2. Restricting the BIC to $\Gamma \subset \partial \Omega$ reduces the amplitudes for orbits hitting the excluded region. Compare $\hat{f}$ to $\hat{f}_\Gamma$ for the 3 marked orbits.

the excluded part $\partial \Omega \setminus \Gamma$ is dotted. For demonstration purposes, the BI of $\psi_{150}$ are shown on the boundary (total $\eta_{150} = 24$), and the points to be excluded from $\eta_\Gamma$ are marked with empty circles ($\eta_{150} = 16$). Three orbits are shown, and the corresponding peaks in the length spectrum are also marked in FIG. 2(a). Orbit 1 has both its bounce points in the excluded regions, so it completely disappears from the length spectrum corresponding to the partial count $\eta_\Gamma$. Orbit 2, which has both of its bounce points in $\Gamma$ is not affected by the exclusion, and orbit 3, which has only 1 out of 4 bounce points in $\Gamma$, is significantly inhibited, and drops below the noise level for the numerical case. This test and the general agreement between the semi-classical and the numerical length spectra give credence to the validity of the proposed trace formula.

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