

Interior Dirichlet eigenvalue problem, exterior Neumann scattering problem, and boundary element method for quantum billiards

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(Received 9 December 1996)

An explicit expression for the Fredholm determinant $D(E)$ appearing in the boundary element method for two-dimensional quantum billiards is derived in terms of the interior Dirichlet eigenenergies and exterior Neumann scattering phase shifts. Not only in the semiclassical regime but also in all order of \hbar , $D(E)$ admits the factorization into the interior and exterior contributions, where the former has zeros at interior Dirichlet eigenenergies and the latter at resonances of the Neumann scattering. A new aspect of the Kac's inverse problem is also discussed. [S1063-651X(97)50507-1]

PACS number(s): 05.45.+b, 02.60.Lj, 03.65.Sq

The billiard problem is one of the simplest but nontrivial models to see the manifestation of classical chaos in quantum mechanics [1]. The eigenvalue problem of quantum billiards, i.e., the Helmholtz equation on a certain bounded domain, cannot be solved analytically in general. The boundary element method (BEM) [2,3] is a powerful numerical approach in that it does not require any special conditions on the billiard shape but merely solves an integral equation approximately by discretizing the boundary. Also, the BEM provides an idea for the novel semiclassical quantization rule using the transfer operator [4]. Direct connection in the semiclassical regime can be made between the determinant of the kernel appearing in the BEM and the semiclassical zeta function of the Gutzwiller-Voros type [5]. Recently, Georgeot and Prange have shown that the BEM can be characterized by the Fredholm theory and obtained a resummation formula of the periodic orbit sum [6]. Furthermore, based on his study on the nonconvex billiard system, Hesse conjectured that the Fredholm determinant is factorized into two parts, one related to the interior Dirichlet problem and the other to the exterior Neumann problem, and that the complex zeros of the determinant are resonances of the exterior problem [7]. Not only in the semiclassical regime, but as fully quantum problem, this inside-outside duality of quantum billiards, especially with Dirichlet boundary conditions for both interior and exterior problems, is drawing a lot of attention [7-12]. Some rigorous relations between the interior and exterior problems are proved by Eckmann and Pillet [11,12].

Here we present a natural extension of our previous work [5] and some rigorous and explicit relations among the determinant appearing in the BEM, eigenenergies of the interior Dirichlet problem, and the scattering phase shifts of the exterior Neumann problem. Our results positively solve Hesse's conjecture to all orders of \hbar and reproduce one of the relations found by Eckmann and Pillet [12]. In the light of our results, we finally argue a new aspect of the Kac's famous inverse problem [13].

First let us briefly formulate the BEM. Consider B , a two-dimensional bounded domain with a boundary ∂B . The eigenenergy E of a particle with mass m moving in B is the eigenenergy of the interior Dirichlet problem for the Helmholtz equation:

$$\nabla^2 \psi(\mathbf{r}) + \frac{2mE}{\hbar^2} \psi(\mathbf{r}) = 0 \quad (\mathbf{r} \text{ in } B), \quad (1)$$

where the wave function vanishes on the boundary ∂B . With the aid of the free Green's function for the Helmholtz equation $G_0(\mathbf{r}, \mathbf{r}'; E) = -\frac{1}{4} i H_0^{(1)}[(\sqrt{2mE}/\hbar)|\mathbf{r} - \mathbf{r}'|]$ with $H_0^{(1)}$ the zero-order Hankel function of the first kind [14], this problem can be rewritten as a Fredholm integral equation of the second kind:

$$\frac{\partial \psi(\mathbf{r}(t))}{\partial n_t} - \oint_{\partial B} ds K(t, s) \frac{\partial \psi(\mathbf{r}(s))}{\partial n_s} = 0, \quad (2)$$

$$K(t, s) \equiv -2 \frac{\partial G_0(\mathbf{r}(t), \mathbf{r}(s); E)}{\partial n_t}.$$

The Fredholm theory tells us that the eigenenergies are zeros of the Fredholm determinant $D(E)$:

$$D(E) \equiv 1 + \sum_{n=1}^{\infty} D_n(E), \quad (3)$$

where

$$D_n(E) = \frac{(-1)^n}{n!} \oint_{\partial B} ds_1 \cdots \times \oint_{\partial B} ds_n \begin{vmatrix} K(s_1, s_1) & \cdots & K(s_1, s_n) \\ \vdots & \ddots & \vdots \\ K(s_n, s_1) & \cdots & K(s_n, s_n) \end{vmatrix}. \quad (4)$$

The BEM is the numerical method that gives approximate eigenenergies as the minima of the absolute value of the determinant calculated by discretizing the boundary integral in Eq. (4).

By similar arguments to those of [5], one can show Hesse's conjecture of the factorization of the Fredholm determinant for strongly chaotic billiards in the semiclassical regime:

$$D^{\text{sc}}(E) = e^{\oint_{\partial B} (1/2\pi)\kappa(s)ds} \widetilde{d}_{\text{int}}^{\text{sc}}(E) \widetilde{d}_{\text{ext}}^{\text{sc}}(E), \quad (5)$$

where

$$\begin{aligned} \widetilde{d}_{\text{int}}^{\text{sc}}(E) = & \prod_{p:\text{interior}} \prod_{k=0}^{\infty} \left\{ 1 - \exp \left[i \frac{\sqrt{2mE}}{\hbar} l_p - \frac{\sigma_p}{2} \pi i \right. \right. \\ & \left. \left. + N_p \pi i - \left(k + \frac{1}{2} \right) \lambda_p l_p + k_p \pi i \right] \right\}, \end{aligned} \quad (6)$$

$$\begin{aligned} \widetilde{d}_{\text{ext}}^{\text{sc}}(E) = & \prod_{p:\text{exterior}} \prod_{k=0}^{\infty} \left\{ 1 - \exp \left[i \frac{\sqrt{2mE}}{\hbar} l_p - \frac{\sigma_p}{2} \pi i \right. \right. \\ & \left. \left. - \left(k + \frac{1}{2} \right) \lambda_p l_p + k_p \pi i \right] \right\}, \end{aligned} \quad (7)$$

In the above the products $\prod_{p:\text{interior}}$ and $\prod_{p:\text{exterior}}$ run over all primitive periodic orbits inside B and outside B , respectively. l_p , σ_p , N_p , λ_p , and k_p represent length, number of conjugate points, number of bounces at the boundary, stability index and index specifying the type of primitive periodic orbit p , respectively. And $\kappa(s)$ is the curvature of the boundary at the point $\mathbf{r}(s)$.

As already discussed in [5], zeros of the interior part $\widetilde{d}_{\text{int}}^{\text{sc}}(E)$ can give the eigenenergies of the interior Dirichlet problem because it is equal to the Gutzwiller-Voros zeta function $\zeta(E)$. On the other hand, following the discussion by Gaspard and Rice [15], the exterior part $\widetilde{d}_{\text{ext}}^{\text{sc}}(E)$ is found to be related to the S matrix of the Neumann scattering problem:

$$\frac{1}{2\pi i} \text{tr} \left(\hat{S}_N^\dagger(E) \frac{d\hat{S}_N(E)}{dE} \right) \cong -\frac{1}{\pi} \text{Im} \frac{\partial}{\partial E} \ln \widetilde{d}_{\text{ext}}^{\text{sc}}(E) - \frac{mA}{2\pi\hbar^2}, \quad (8)$$

where A is the area of the billiard domain and $\hat{S}_N(E)$ is the on-shell S matrix with energy E for the Neumann scattering:

$$\begin{aligned} \hat{S}_N(E)f(\theta) = & f(\theta) - \frac{1}{2\pi} \oint_{\partial B} ds e^{-i\kappa\mathbf{v}_\theta \cdot \mathbf{r}(s)} \\ & \times \int_0^{2\pi} d\theta' k \mathbf{v}_{\theta'} \cdot \mathbf{n}_s e^{ik\mathbf{v}_{\theta'} \cdot \mathbf{r}(s)} f(\theta') \\ & - \frac{1}{2\pi} \oint_{\partial B} ds \oint_{\partial B} dt e^{-i\kappa\mathbf{v}_\theta \cdot \mathbf{r}(s)} \frac{N(s,t;E)}{D(E)} \\ & \times \int_0^{2\pi} d\theta' k \mathbf{v}_{\theta'} \cdot \mathbf{n}_t e^{ik\mathbf{v}_{\theta'} \cdot \mathbf{r}(t)} f(\theta'). \end{aligned} \quad (9)$$

In the above, $f(\theta)$ is a function of the scattering angle θ ($0 \leq \theta < 2\pi$), $k = \sqrt{2mE}/\hbar$, $\mathbf{v}_\theta = (\cos \theta, \sin \theta)$, $\mathbf{r}(s)$ stands for a

position on the boundary ∂B and \mathbf{n}_s for the outer normal vector to ∂B at $\mathbf{r}(s)$, and $N(s,t;E)$ is the Fredholm first minor:

$$N(s,t;E) \equiv K(s,t) + \sum_{n=1}^{\infty} N_n(s,t;E), \quad (10)$$

where $N_n(s,t;E)$'s are the kernels of the operators \mathbf{N}_n defined via the recursion relation $\mathbf{N}_n = D_n(E)\mathbf{K} + \mathbf{K}\mathbf{N}_{n-1}$, with $D_n(E)$ of Eq. (4), $\mathbf{N}_0 = \mathbf{K}$, and \mathbf{K} the operator corresponding to $K(s,t;E)$ [6,16].

Actually, the factorization [5] holds to all order of \hbar and thus fully quantum mechanically.

Proposition 1. Suppose that B is a bounded domain in \mathbb{R}^2 with piecewise C^2 boundary ∂B and \mathbb{R}^2/B is connected (i.e., the standard domain of Eckmann and Pillet [11,12]). Then (1) $D(E)$ admits the decomposition

$$D(E) = D(0) d_{\text{int}}(E) d_{\text{ext}}(E), \quad (11)$$

$$\begin{aligned} d_{\text{int}}(E) = & \exp \left\{ \frac{2m}{\hbar^2} \int_0^E dE' \right. \\ & \left. \times \int_B d^2\mathbf{r} [G_D(\mathbf{r}, \mathbf{r}'; E) - G_0(\mathbf{r}, \mathbf{r}'; E')] \Big|_{\mathbf{r}'=\mathbf{r}} \right\}, \end{aligned} \quad (12)$$

$$\begin{aligned} d_{\text{ext}}(E) = & \exp \left\{ \frac{2m}{\hbar^2} \int_0^E dE' \lim_{R \rightarrow \infty} \right. \\ & \left. \times \int_{C_R \setminus B} d^2\mathbf{r} [G_N(\mathbf{r}, \mathbf{r}'; E) - G_0(\mathbf{r}, \mathbf{r}'; E')] \Big|_{\mathbf{r}'=\mathbf{r}} \right\}, \end{aligned} \quad (13)$$

where G_D and G_N are, respectively, the Green's functions for the interior Dirichlet and exterior Neumann problems, C_R the disk of radius R containing B , and the value $D(0)$ of $D(E)$ at $E=0$ is real. (2) The interior part $d_{\text{int}}(E)$ admits the Hadamard factorization:

$$\begin{aligned} d_{\text{int}}(E) = & e^{i(mA/2\hbar^2)E} \left(\frac{m\ell^2 E}{2\hbar^2} \right)^{-(mA/2\pi\hbar^2)E} \\ & \times e^{-(mA/\pi\hbar^2)\gamma'E} \prod_{n=1}^{\infty} \left(1 - \frac{E}{E_n} \right) e^{E/E_n}, \end{aligned} \quad (14)$$

where E_n 's are the eigenenergies of the interior Dirichlet problem, A the area of the billiard domain B , ℓ the perimeter of the boundary ∂B , and γ' a real constant depending on the geometry of B . The product converges as a consequence of Weyl's relation between the cumulative density of states and energy E . (3) The exterior part is related to the scattering:

$$\begin{aligned} d_{\text{ext}}(E) = & \exp \left\{ E \int_0^{\infty} \frac{E'}{2\pi} \frac{1}{E - E' + i0} \right. \\ & \left. \times \left(\frac{mA}{\hbar^2} - \frac{2}{E'} \sum_{m=1}^{\infty} \delta_m(E') \right) \right\}, \end{aligned} \quad (15)$$

where $\delta_m(E)$ is the phase shift of the exterior Neumann scattering problem and $e^{-2i\delta_m(E)}$ is an eigenvalue of the on-shell S matrix $\hat{S}_N(E)$. The existence of the countable phase shifts and the convergence of the sum $\sum_{m=1}^{\infty} \delta_m(E)$ follow from the fact that $\hat{S}_N(E) - I$ is trace class. Note also that $\ln \det \hat{S}_N(E) = -2i \sum_{m=1}^{\infty} \delta_m(E)$.

In the following we show the outline of the derivation of Eqs. (11)–(15).

As is well known [17], by applying the potential theory, the Green function for the interior Dirichlet problem is given by

$$\begin{aligned} G_D(\mathbf{r}, \mathbf{r}'; E) &= G_0(\mathbf{r}, \mathbf{r}'; E) - 2 \oint_{\partial B} ds \left\{ G_0(\mathbf{r}, \mathbf{r}(s); E) \right. \\ &\quad \left. + \oint_{\partial B} dt G_0(\mathbf{r}', \mathbf{r}(t); E) \frac{N(t, s; E)}{D(E)} \right\} \frac{\partial G_0(\mathbf{r}(s), \mathbf{r}; E)}{\partial n_s} \end{aligned} \quad (16)$$

and that for the exterior Neumann problem by Eq. (16) with \mathbf{r} and \mathbf{r}' interchanged. Using this and after straightforward calculations we have

$$\begin{aligned} &\int_B d^2\mathbf{r} [G_D(\mathbf{r}, \mathbf{r}'; E) - G_0(\mathbf{r}, \mathbf{r}'; E)]_{\mathbf{r}'=\mathbf{r}} \\ &\quad + \lim_{R \rightarrow \infty} \int_{C_R \setminus B} d^2\mathbf{r} [G_N(\mathbf{r}, \mathbf{r}'; E) - G_0(\mathbf{r}, \mathbf{r}'; E)]_{\mathbf{r}'=\mathbf{r}} \\ &= -\frac{\hbar^2}{2m} \left[\oint_{\partial B} ds \oint_{\partial B} dt \frac{N(s, t; E)}{D(E)} \frac{\partial K(t, s)}{\partial E} \right. \\ &\quad \left. + \oint_{\partial B} ds \frac{\partial K(s, s)}{\partial E} \right] \\ &= \frac{\hbar^2}{2m} \frac{\partial}{\partial E} \ln D(E). \end{aligned} \quad (17)$$

Hence we get the desired factorization (11)–(13). As $[K(s, t)]_{E=0}$ is real, $D(0)$ is real.

Next we consider the interior part of Eq. (17), which is a sum of three terms. The first term is

$$\begin{aligned} &\int_B d^2\mathbf{r} [G_D(\mathbf{r}, \mathbf{r}'; E) - G_D(\mathbf{r}, \mathbf{r}'; 0)]_{\mathbf{r}'=\mathbf{r}} \\ &= \frac{\hbar^2}{2m} \sum_{n=1}^{\infty} \left(\frac{1}{E - E_n} + \frac{1}{E_n} \right), \end{aligned} \quad (18)$$

where E_n are the eigenenergies for the interior Dirichlet eigenvalue problem. The second term is

$$\begin{aligned} &-\int_B d^2\mathbf{r} \left[G_0(\mathbf{r}, \mathbf{r}'; E) - \frac{1}{2\pi} \ln \frac{|\mathbf{r} - \mathbf{r}'|}{\ell} \right]_{\mathbf{r}'=\mathbf{r}} \\ &= \frac{i}{4} A - \frac{A}{4\pi} \ln \left(\frac{m\ell^2}{2\hbar^2} E \right) - \frac{\gamma A}{2\pi}, \end{aligned} \quad (19)$$

where γ is the Euler constant. The third term defines a constant γ' as

$$\begin{aligned} &\int_B d^2\mathbf{r} \left[G_D(\mathbf{r}, \mathbf{r}'; 0) - \frac{1}{2\pi} \ln \frac{|\mathbf{r} - \mathbf{r}'|}{\ell} \right]_{\mathbf{r}'=\mathbf{r}} \\ &\equiv \frac{A}{2\pi} \left(\gamma - \frac{1}{2} - \gamma' \right), \end{aligned} \quad (20)$$

where γ is real since $G_D(\mathbf{r}, \mathbf{r}'; 0)$ is real. Combining Eqs. (12) and (18)–(20), we obtain Eq. (14).

Finally we discuss the exterior part. Since both G_N and G_0 are the Green functions for the outgoing boundary condition, we have

$$\begin{aligned} &\lim_{R \rightarrow \infty} \int_{C_R \setminus B} d^2\mathbf{r} [G_N(\mathbf{r}, \mathbf{r}'; E') - G_0(\mathbf{r}, \mathbf{r}'; E')]_{\mathbf{r}'=\mathbf{r}} \\ &= \int_0^{\infty} dE'' \frac{\rho(E'')}{E' - E'' + i0}, \end{aligned} \quad (21)$$

with the real density ρ :

$$\begin{aligned} \rho(E'') &= \frac{-1}{\pi} \operatorname{Im} \lim_{R \rightarrow \infty} \int_{C_R \setminus B} d^2\mathbf{r} [G_N(\mathbf{r}, \mathbf{r}'; E'') \\ &\quad - G_0(\mathbf{r}, \mathbf{r}'; E'')]_{\mathbf{r}'=\mathbf{r}}. \end{aligned}$$

Now, because of the Friedel relation [15,18,19]

$$\begin{aligned} &\lim_{R \rightarrow \infty} \left\{ \int_{C_R \setminus B} d^2\mathbf{r} [\operatorname{Im} G_N(\mathbf{r}, \mathbf{r}'; E)]_{\mathbf{r}'=\mathbf{r}} \right. \\ &\quad \left. - \int_{C_R} d^2\mathbf{r} [\operatorname{Im} G_0(\mathbf{r}, \mathbf{r}'; E)]_{\mathbf{r}'=\mathbf{r}} \right\} \\ &= -\frac{\hbar^2}{4mi} \operatorname{tr} \left[\hat{S}_N^\dagger(E) \frac{\partial \hat{S}_N(E)}{\partial E} \right], \end{aligned}$$

and $\int_B d^2\mathbf{r} [\operatorname{Im} G_0(\mathbf{r}, \mathbf{r}'; E)]_{\mathbf{r}'=\mathbf{r}} = -A/4$, we get

$$\rho(E) = \frac{1}{\pi} \frac{\partial}{\partial E} \left[\frac{AE}{4} + \frac{\hbar^2}{4mi} \ln \det \hat{S}_N(E) \right]. \quad (22)$$

Substituting Eq. (22) into Eq. (21), carrying out E' integration in Eq. (13), and using $\ln \det \hat{S}(E) = -2i \sum_{m=1}^{\infty} \delta_m(E)$, we obtain Eq. (15). Details of the proof of Proposition 1 will be shown elsewhere [20]. Proposition 1 also characterizes zeros of the interior and exterior parts.

Proposition 2. (1) Interior part $d_{\text{int}}(E)$ has zeros precisely at the eigenenergies of the interior Dirichlet problem. (2) Exterior part $d_{\text{ext}}(E)$ has no zeros on the first Riemann sheet: $\{E = |E|e^{i\theta} | 0 \leq \theta < 2\pi\}$. Its analytic extension $d_{\text{ext}}^{\text{II}}(E)$ from the upper half plane of the first Riemann sheet to the lower half plane of the second Riemann sheet through the positive real axis is

$$d_{\text{ext}}^{\text{II}}(E) = e^{-i(mA/\hbar^2)E} \frac{d_{\text{ext}}(E)}{\det \hat{S}_N^{\text{II}}(E)}, \quad (23)$$

where \hat{S}_N^{II} is the analytic extension of \hat{S}_N to the second Riemann sheet. Equation (23) implies that zeros of $d_{\text{ext}}^{\text{II}}(E)$ are the poles of the S matrix, or the resonances.

The statement (1) is trivial from Proposition 1. Because of Eq. (15), we see that $\ln d_{\text{ext}}(E)$ is a boundary value of an analytic function to the positive real axis from above. Hence, $\ln d_{\text{ext}}(E)$ is analytic on the first Riemann sheet, and, thus, $d_{\text{ext}}(E)$ has no zeros there. From Eq. (15) for real $E(>0)$, we have

$$\frac{d_{\text{ext}}(E-i0)}{d_{\text{ext}}(E+i0)} = e^{i(mA/\hbar^2)E} \det \hat{S}_N(E). \quad (24)$$

By analytically continuing this with respect to E from the upper to the lower half plane, we obtain Eq. (23). This proves Proposition 2. Details will be discussed elsewhere [20].

Proposition 1 shows that Hesse's conjecture [7] on the factorization of the Fredholm determinant $D(E)$ into the interior and exterior parts holds in the semiclassical regime as well as to all order of \hbar . In particular an explicit closed form, including all regularization factors, of the Hadamard factorization is obtained for the factor related to the interior Dirichlet problem. Our results (11)–(15) also give one of the relations obtained by Eckmann and Pillet [12] for real $E(>0)$:

$$\pi \sum_{n=1}^{\infty} \theta(E-E_n) = \sum_{m=1}^{\infty} \delta_m(E) - \text{Im} \ln D(E+i0), \quad (25)$$

where $\theta(E)$ shows the Heaviside step function. This shows that the Fredholm determinant $D(E)$ and Eckmann-Pillet's function ζ_{DN} , which is related to the interior Dirichlet and exterior Neumann problem [12], differ by a real factor for

real $E(>0)$. Proposition 2 states that the zeros of the Fredholm determinant $D(E)$ are either the eigenenergies of the interior Dirichlet problem or the resonances of the exterior Neumann scattering problem. Hence, this fully characterizes zeros of $D(E)$. It is important that in the numerical calculation of the BEM not only the eigenenergies of the interior Dirichlet problem but also the resonance energies of the exterior Neumann scattering can give the minima of the absolute value of $D(E)$ when the poles of the S matrix are very near the real axis. This result implies the generality of Hesse's observation [7] on the zeros of the Fredholm determinant for nonconvex billiards.

Our result also gives an interesting insight into Kac's inverse problem: "Can one hear the shape of a drum?" [13]. To this problem, some nontrivial counterexamples of the two-dimensional planar billiards are known [21]. This fact can be reinterpreted from the present result. That is, even if two domains B and B' have the same eigenenergy spectra, they may have different scattering. This suggests that Kac's problem should be modified as "Can one determine the shape of a drum through the spectrum of the interior Dirichlet problem and the cross sections of the exterior Neumann scattering?"

We are grateful to Dr. N. Egami, Dr. P. Davis, Professor P. Gaspard, Professor K. S. Ikeda, and Professor Y. Takahashi for fruitful discussions and comments. S.T. thanks Professor K. Fukui for his encouragement and support. A.S. is very much grateful for warm hospitalities at Institute Henri Poincaré. The work was partially supported by a Grant-in-Aid for Scientific Research and a grant under the International Scientific Research Program both from Ministry of Education, Science and Culture of Japan as well as the Research for the Future of Japan Society of the Promotion of Science.

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