Boundary element method and isospectrality in quantum billiards

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Abstract. An application of Fredholm theory to the boundary element method and its association to the Kac's inverse question "can one hear the shape of a drum?" are reviewed.

Dedicated to the memory of Professor Shuichi Tasaki

This article is devoted to presenting a brief summary of a series of our collaborations with Professor Shuichi Tasaki about an application of Fredholm theory to quantum billiard problems. We have published 6 joint papers since 1997, and learned so much from Professor Tasaki through collaborations. Since Professor Tasaki's contributions to this subject were crucial and exhaustive, we deeply regret that we could not publish detailed calculations and proofs for the main result presented below before his untimely death.

Our scientific communication with Professor Tasaki has started since he kindly put a brief remark on our review paper [1], which was published in Bussei Kenkyu in 1993 [2]. Our review paper was based on the Ph.D thesis of one of the present authors (T.H.), in which we discussed the Gutzwiller's trace formula for strongly chaotic billiards, especially its rederivation starting from the boundary element method [3]. It was surprising since Professor Tasaki's comment was so pertinent although the topics discussed there were not close to his own field. After such a communication, Professor Tasaki suggested us to employ Fredholm theory to understand the integral equation appearing in the boundary element method.

1. Boundary element method and Fredholm theory

The boundary element method is well known as a standard numerical technique and frequently used to solve the eigenvalue problem for the Helmholz equation:

$$(\Delta + E)\psi(\boldsymbol{r}) = 0 \qquad\qquad (\boldsymbol{r} \text{ in } \Omega). \tag{1}$$

Here Ω denotes a 2-dimensional closed domain, and the Dirichlet boundary condition, $\psi(\boldsymbol{r}) = 0$, is imposed on $\partial\Omega$. Using the free Green's function $G_0(\boldsymbol{r}, \boldsymbol{r}'; E)$, which is given as a fundamental solution of $(\Delta + E)G_0(\boldsymbol{r}, \boldsymbol{r}'; E) = \delta(\boldsymbol{r} - \boldsymbol{r}')$ for $\boldsymbol{r} \in \mathbb{R}^2$, the Helmholtz equation for the closed region Ω is cast into an integral form as

$$u(t) - (\hat{K}u)(t) = 0, \tag{2}$$

where

$$(\hat{K}u)(t) = \int_{\partial\Omega} ds\, K(t,s,E)\, u(s), \tag{3}$$

and

$$u(t) \equiv n_t \cdot \nabla_r \psi(\boldsymbol{r})\Big|_{\boldsymbol{r}=\boldsymbol{r}(t)}, \tag{4}$$

$$K(t,s,E) \equiv -2n_t \cdot \nabla_r G_0(\boldsymbol{r}(t), \boldsymbol{r}(s); E)\Big|_{\boldsymbol{r}=\boldsymbol{r}(t)}. \tag{5}$$

For numerical calculations, one discretizes the boundary $\partial\Omega$ to convert the integral equation (2) to a set of simultaneous equations

$$u(t_i) - \sum_{j=1}^{N} K(t_i, s_j, E) u(s_j) = 0, \tag{6}$$

where N denotes the number of discretized points along the boundary $\partial\Omega$. This linear system has a non-trivial solutions if

$$\Delta^{(N)}(E) \equiv \det\left[\delta_{ij} - K(t_i, s_j, E)\right] = 0. \tag{7}$$

One may easily notice that the integral equation (2) has a form of the Fredholm integral equation (of the 2nd kind) if it is expressed in such a concise manner. However, we have not noticed that it is so until Professor Tasaki pointed out to us after his remark on our review paper.

Fredholm theory guarantees that

(i) $D(E) \; = \; {}^{\exists}\lim_{N\to\infty} \Delta_N(E)$

(ii) E_n is an eigenvalue of the Helmholz equation (1) with the Dirichlet boundary condition iff $D(E_n) = 0$

hold for the domain Ω with C^2 boundary. $D(E)$ is called the Fredholm determinant.

The idea to apply Fredholm theory to analyze the semiclassical determinant and the associated zeta function has been published prior to us [4], but we have independently started our discussion after some correspondences.

As one of our outcomes based on Fredholm theory [5], we could extend our previous work [3] and develop a more precise semiclassical formulation for strongly chaotic systems, for which several proposals have been presented regarding the convergency of the trace formula or the zeta function. The reason why Fredholm theory enjoys a especially privileged position is that the expansion for the Fredholm determinant

$$D(E) = 1 + \sum_{n=1}^{\infty} D_n(E), \tag{8}$$

which is obtained by discretizing the billiard boundary $\partial\Omega$, and

$$D_n(E) \equiv \frac{(-1)^n}{n!} \oint_{\partial\Omega} ds_1 \cdots ds_n \begin{vmatrix} K(s_1,s_2,E) & K(s_1,s_2,E) & \ldots & K(s_1,s_n,E) \\ K(s_2,s_1,E) & K(s_2,s_2,E) & \ldots & K(s_2,s_n,E) \\ \vdots & \vdots \ddots & \vdots & \\ K(s_n,s_1,E) & K(s_n,s_1,E) & \ldots & K(s_n,s_n,E) \end{vmatrix}$$

converges as long as the integral kernel satisfies a certain mild condition. This is just as a consequence of general arguments in Fredholm theory. In [5], we derived an semiclassical expression for $D_n(E)$ in terms of unstable periodic orbits (more precisely for $D_n(E) = e^{-\oint_{\partial\Omega}\frac{1}{2\pi}\kappa(s)ds}$ where $\kappa(s)$ is the curvature of the boundary) to give

$$D_n^{\rm sc}(E) = \sum_{\gamma, n_\gamma = n} C_\gamma e^{\frac{i}{\hbar}L_\gamma}, \tag{9}$$

where γ denotes the so-called peudo-orbit with the bounce number n_γ. Thus, the convergency of the original Fredholm determinant turns out to be automatically linked to the convergence of the semiclassical sum in terms of periodic orbits. In this way, Professor Tasaki's idea has brought our naive semiclassical arguments [3] to quite a self-consistent and general stage.

2. Interior and exterior problems in quantum billiards

Professor Tasaki's wide-range knowledge about applied mathematics allows us to go further. Using the potential theory for the Green function [6], it was shown in [7] that $D(E)$ admits the decomposition

$$D(E) = D(0)D_{\rm int}(E)D_{\rm ext}(E), \tag{10}$$

where

$$D_{\rm int}(E) = \exp\left[\int_0^\infty dE' \int_\Omega d^2\boldsymbol{r}\Big(G_D(\boldsymbol{r},\boldsymbol{r}',E) - G_0(\boldsymbol{r},\boldsymbol{r}',E')\Big)_{\boldsymbol{r}'=\boldsymbol{r}}\right], \tag{11}$$

$$D_{\rm ext}(E) = \exp\left[\int_0^\infty dE' \lim_{R\to\infty}\int_{C_R\setminus\Omega} d^2\boldsymbol{r}\Big(G_N(\boldsymbol{r},\boldsymbol{r}',E) - G_0(\boldsymbol{r},\boldsymbol{r}',E')\Big)_{\boldsymbol{r}'=\boldsymbol{r}}\right]. \tag{12}$$

Here G_D and G_N are the Green functions for the interior Dirichlet and exterior Neumann problems, respectively, and C_R the disk of the radius R containing out billiard domain Ω. Moreover, we could obtain explicit expressions for $D_{\rm int}(E)$ and $D_{\rm ext}(E)$ as

$$D_{\rm int}(E) = \exp\left(i\frac{|\Omega|E}{4}\right)\left(\frac{|\partial\Omega|^2E}{4}\right)^{-\frac{|\Omega|E}{4\pi}}\exp\left(-\frac{|\Omega|\gamma'E}{4\pi}\right)\prod_{n=1}^\infty\left(1-\frac{E}{E_n}\right)\exp\left(\frac{E}{E_n}\right), \tag{13}$$

$$D_{\rm ext}(E) = \exp\left(\frac{E}{2\pi}\right)\int_0^\infty dE'\frac{1}{E-E'+0i}\left[\frac{|\Omega|}{2} - \frac{2}{E'}\sum_{m=1}^\infty \delta_m(E')\right], \tag{14}$$

where $\{E_n\}$ is the eigenvalues of the interior Dirichlet problem, $\{\delta_m(E)\}$ phase shifts of the exterior Neumann problem. $|\Omega|$ and $|\partial\Omega|$ denote the area and the length of the billiard boundary, and γ' is determined by more detailed geometry of the billiard boundary. Note that the interior part $D_{\rm int}(E)$ has zeros precisely at the eigenvalues of the interior Dirichlet problem. Concerning the exterior part, it was shown that $D_{\rm ext}(E)$ has no zeros on the first Riemann sheet: $\{E = |E|e^{i\theta} \mid 0 \le \theta < 2\pi\}$, but on the second Riemann sheet, we have

$$D_{\rm ext}^{\rm II}(E) = e^{-i\frac{|\Omega|E}{2}}\frac{D_{\rm ext}(E)}{\det S^{\rm II}(E)}, \tag{15}$$

where $S^{\rm II}(E)$ is the analytic extension of the S-matrix $S(E)$ to the second Riemann sheet. Therefore, the exterior part $D_{\rm ext}(E)$ is specified by the poles of of the S-matrix, or resonances for the exterior Neumann scattering problem.

A similar but a bit different aspect of "inside-outside duality" for the billiard problem has been discussed in [8, 9, 10, 11]. The authors of [8, 9] discussed a close link between the inside Dirichlet and also outside Dirichlet problems, not like the present situation, and found that the spectrum of the interior problem is extracted from the scattering matrix of the exterior problem. It is therefore of particular interest to ask whether analogous inside-outside duality holds in case of interior Dirichlet and exterior Neumann problems.

3. Kac's question: revisited

The decomposition (10)-(15) tells us that analytic structure of $D(E)$ is completely specified by the eigenvalues for the inside Dirichlet problem and the resonances for the outside Neumann problem. This fact reminds us of a famous question posed by M.Kac: "can one hear the shape of a drum?" [12]. This inquires the existence of isospectral but non-congruent closed domains on $\mathbb{R}^2$. If the answer is yes, it turns out that the eigenvalues for the inside Dirichlet problem are sufficient to specify the shape of the billiard boundary, otherwise some information is missing to determine the shape. After Kac's question, several variants concerning isospectrality, not necessarily on $\mathbb{R}^2$ but on Riemannian manifolds for example, have been proposed, and recently isospectrality on the quantum graph attracts much attention [13]. The original question for the existence of isospectral pairs on $\mathbb{R}^2$ was finally solved by Gordon, Webb and Wolpert, who have concretely constructed a pair of non-congruent closed domains with identical eigenvalues [14].

In view of the decomposed form of the Fredholm determinant (10)-(15), it is not surprising that the inside eigvenvalue problem is not sufficient to specify the billiard shape since exterior resonances are necessary in addition to inside eigenvalues to fix the Fredholm determinant. Alternatively stated, one may distinguish isospectral billiards by the resonances of exterior Neumann scattering [7].

Such a question sounds reasonable and it looks straightforward to check it at least numerically. However, there is slight logical inconsistency between the speculation based on the decomposition (10)-(15) and the fact that all the counter examples of Kac's question found so far do not satisfy the condition for the class of boundaries Fredholm theory requires. Fredholm theory holds, as mentioned, as far as the boundary belongs to the C^2-class, while all the counter-example billiards discovered so far are constructed by glueing together a certain building block, so they necessarily have discontinuities of derivative, or at least second derivatives at their jointed points, thereby breaking the condition for Fredholm theory to be applied.

Not only invoking logical inconvenience, but also this causes a difficulty in actual numerical calculations. The is a bit technical issue, but any satisfactory solution has not been provided when we discussed this issue although a bunch of numerical calculations have been performed for the billiards whose boundaries have discontinuities or are not necessarily in C^2. The difficulty for the billiard table with discontinuities arises as follows: an explicit expression of the integral kernel is

$$K(t,s,E) = -\frac{i\sqrt{E}}{2}\frac{\tau(s,t)\cdot n_t}{|\tau(s,t)|}H_1^{(1)}\Big(\sqrt{E}|\tau(s,t)|\Big), \qquad (16)$$

where $\tau(s,t) = r(s) - r(t)$ and $H_1^{(1)}$ is the Hankel function of the first kind. Since the Hankel function behaves as $H_1^{(1)}(\sqrt{E}|\tau(s,t)|) \sim -2i/\pi\sqrt{E}|\tau(s,t)|$, $K(t,s,E)$ diverges as $\boldsymbol{r}(t) \to \boldsymbol{r}(s)$, so the integral kernel cannot be defined as it stands. For C^2 boundary cases, however, we can introduce the curvature $\kappa(t)$ at every point and it cancels the divergence as

$$\frac{\tau(s,t)\cdot n_t}{|\tau(s,t)|} \sim \frac{1}{2}\kappa(t)|\tau(s,t)|,$$

then one may introduce a finite kernel.

To secure this situation, we split the integral kernel as $\hat{K} = \hat{K}_R + \hat{K}_S$ such that $\hat{K}_R$ is bounded and continuous on each $\partial\Omega \times \Gamma_i$ where the boundary $\partial\Omega$ is supposed to consist of a finite number of C^2 arcs $\{\Gamma_1, \Gamma_2, \cdots, \Gamma_m\}$, and $\hat{K}_S$ is a bounded on $C^0(\partial\Omega)$ with $\|\hat{K}_S\| < 1$ [15]. Then we could prove that the original integral equation (2) is converted into

$$u - (1-\hat{K}_S)^{-1}\hat{K}_R u = 0, \tag{17}$$

and the resulting kernel $\hat{\mathcal{K}}(t,s,E) = [(1-\hat{K}_S)^{-1}\hat{K}_R(\cdot,s,\sqrt{E})](t)$ is bounded and continuous on each $\partial\Omega \times \Gamma_i$ [15]. Hence we may apply Fredholm theory. Since the analytic structure preserves after modifying the integral kernel, the decomposition (10)-(15) holds for the new Fredholm determinant as well. So it indeed makes sense to ask "can one distinguish isospectral billiards by the resonances of exterior Neumann scattering?"

We have numerically computed the location of zeros of the Fredholm determinant for several types of isospectral billiard [16]. As an example we show in Fig.1 that complex zeros of the Fredholm determinant are different from each other between isospectral billiard tables whereas zeros on the real axis are completely the same as predicted. All other examples studied in [16] led the same conclusion, which therefore invokes us the conjecture that isospectral pair can be distinguished by measuring the poles of S-matrix or the cross section of exterior Neumann scattering.

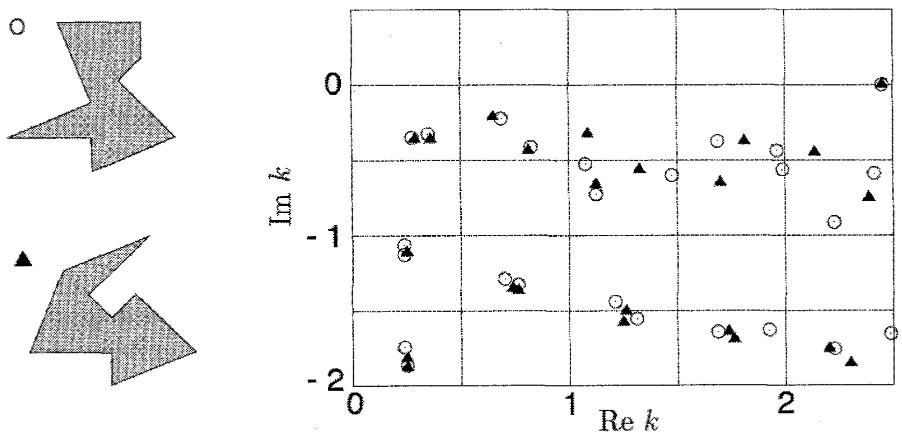

Figure 1. A pair of Isospectral billiards and the distribution of zeros of the Fredholm determinant $D(E)$ on the $k(=\sqrt{E})$ plane.

For quantum graphs, however, it was recently shown that this conjecture is not necessarily true [17]; isospectral quantum graphs constructed using generalized Sunada's theorem [18] can be "isoscattering" if conversion of a given quantum graph into a scattering system preserves a certain symmetry reflecting the symmetry used to construct the isospectral pair. It should be at the same time noted that not every way of converting a graph into a scattering system leads to the isospectral graphs would make them isoscattering. The scattering system should be designed in such a way that it reflects the underlying symmetry that was used for the construction of the isospectral pair. Our numerical result shown above suggests that the outside scattering problem of the isospectral billiards breaks the symmetry that was used in the isospectral drum construction. The question of what type of symmetry is required to have isoscattering systems is still open.

4. Concluding remarks

As explained above, it would be natural and was actually fruitful to apply Fredholm theory to the integral equation appearing the boundary element method. A careful observation made by Professor Tasaki leads a comprehensive understanding of analytical structure of the Fredholm determinant thus obtained. It is truly regrettable that rigorous proofs for the decomposition theorem (10)-(15) have not been published yet, but what is more sad is that we lost further opportunities to talk and discuss with Professor Tasaki not only on the present issue but also on other fundamental questions in physics Professor Tasaki must have kept in his mind. Professor Tasaki always encouraged young researchers and we are really benefitted from his exhaustive knowledge on physics, mathematics and so on. Professor Tasaki's gentle personality and sincere attitude not only to science but to every aspects were truly respectable.

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