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Mathematical Scattering Theory in Quantum Waveguides

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Abstract—A waveguide occupies a domain G with several cylindrical ends. The waveguide is described by a nonstationary equation of the form $i\partial_t f = \mathcal{A}f$, where $\mathcal{A}$ is a selfadjoint second order elliptic operator with variable coefficients (in particular, for $\mathcal{A} = -\Delta$, where Δ stands for the Laplace operator, the equation coincides with the Schrödinger equation). For the corresponding stationary problem with spectral parameter, we define continuous spectrum eigenfunctions and a scattering matrix. The limiting absorption principle provides expansion in the continuous spectrum eigenfunctions. We also calculate wave operators and prove their completeness. Then we define a scattering operator and describe its connections with the scattering matrix.

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1. WAVEGUIDE AND OPERATORS

Let G be a domain in $\mathbb{R}^d$ coinciding outside a large ball with the union of finitely many mutually disjoint semicylinders $\Pi_+^q = \{(y,z) : y \in \Omega^q, z \in \mathbb{R}_+\}$, $q = 1, 2, \ldots, \mathcal{T}$; the boundary ∂G is smooth. We consider initial boundary value problem

$$i\partial_t \Psi(x,t) = \mathcal{A}(x, D_x)\Psi(x,t), \quad x \in G,$$
$$\Psi(x,t) = 0, \quad x \in \partial G, \quad \Psi(x,0) = \Psi_0(x), \quad x \in G,$$

where $\mathcal{A}(x, D_x) = \sum_{j,l=1}^{d} D_j a_{j,l}(x) D_l + a_0(x)$, and $D_j = -i\partial/\partial x_j$. We assume that the matrix $a(\cdot)$ with entries $a_{j,l}(\cdot) \in C^1(\overline{G})$ is positive definite, that is $\langle a(x)\xi, \xi\rangle \geq c\langle \xi, \xi\rangle$ for $\xi \in \mathbb{C}^d$, where $c > 0$, and $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{C}^d$; $a_0(\cdot) \in C^1(\overline{G})$ is a real function. Moreover, for a certain $\delta > 0$ in every cylindrical end $G \cap \Pi_+^q$ there are fulfilled the stabilisation conditions

$$|a_{j,l}(y,z) - a_{j,l}^q(y)| + |\nabla(a_{j,l}(y,z) - a_{j,l}^q(y))| = O(e^{-\delta z}), \quad z \to +\infty; \tag{1}$$
$$|a_0(y,z) - a_0^q(y)| + |\nabla(a_0(y,z) - a_0^q(y))| = O(e^{-\delta z}),$$

here (y, z) are local coordinates in $G \cap \Pi_+^q$. The operator A in $L_2(G)$, given by the differential expression $\mathcal{A}(x, D_x)$ on the domain $\mathcal{D}(A) = H^2(G) \cap H_0^1(G)$, is selfadjoint, where, as it usually is, $H^2(G)$ and $H_0^1(G)$ are Sobolev spaces.

2. POINT AND CONTINUOUS SPECTRA

A number μ is called an eigenvalue (belongs to the point spectrum $\sigma_p(A)$), if there exists a solution $u \in \mathcal{D}(A)$ of the equation $Au = \mu u$; such a solution is called an eigenfunction. The eigenvalues of the operator A are of finite multiplicities and can not accumulate at finite distance.

A number μ is said to be in the continuous spectrum $\sigma_c(A)$, if the image of operator $A - \mu$ is nonclosed in $L_2(G)$. This is the case if and only if there exists a solution $u \notin L_2(G)$ of the problem

$$\mathcal{A}(x, D_x)u(x) - \mu u(x) = 0, \quad x \in G,$$
$$u(x) = 0, \quad x \in \partial G, \tag{2}$$

with $|u(x)| \leq C(|x|+1)^N$, $N < \infty$ (see [1]). Such a solution is called a continuous spectrum eigenfunction. For all μ, except a set of isolated values, the continuous spectrum eigenfunctions are bounded. These isolated values are called thresholds and accumulate at $+\infty$ only. The semiaxis $[\tau_1, +\infty)$ coincides with the continuous spectrum of A; here $\tau_1 > 0$ is the minimal threshold. Denote by $\mathcal{E}_c(\mu)$ the linear hull of the continuous spectrum eigenfunctions corresponding to μ; $\dim \mathcal{E}_c(\mu) < \infty$ for all μ. If a number μ is not an eigen-

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value, then $\varkappa(\mu) := \dim \mathscr{E}_c(\mu)$ is called the continuous spectrum multiplicity at μ. If μ belongs to the continuous spectrum and is an eigenvalue, we set $\varkappa(\mu) := \dim(\mathscr{E}_c(\mu)/\mathscr{E}_p(\mu))$, where $\mathscr{E}_c(\mu)/\mathscr{E}_p(\mu)$ is a factor-space and $\mathscr{E}_p(\mu)$ stands for the subspace of eigenfunctions corresponding to μ. The function $\mu \mapsto \varkappa(\mu)$ remains constant between neighboring thresholds.

3. WAVES. CONTINUOUS SPECTRUM EIGENFUNCTIONS. SCATTERING MATRIX

In every cylinder $\Pi^q = \Omega^q \times \mathbb{R}$, $q = 1,\dots,\mathcal{T}$, we consider a problem (2) changing $a_{j,l}(y,z)$ for $a^q_{j,l}(y)$. For this model problem, we look for solutions of the form $(y,z) \mapsto \exp(i\lambda z)\varphi(y)$ with real λ. On the interval $\mu \in (\tau', \tau'')$ between neighbouring thresholds τ', τ'' there exist finitely many linearly independent solutions

$$u_j^{\pm}(y,z;\mu) = N_j^{\pm}(\mu)\exp(i\lambda_j^{\pm}(\mu)z)\varphi_j^{\pm}(y,\mu), \qquad (3)$$

where $y \in \Omega^q$, $z \in \mathbb{R}$, and $j = 1,\dots,\varkappa^q$. The functions $\mu \mapsto N_j^{\pm}(\mu), \lambda_j^{\pm}(\mu), \varphi_j^{\pm}(\cdot,\mu)$ are analytic on the interval $\mu \in (\tau', \tau'')$ and $\mp(\lambda_j^{\pm})'(\mu) > 0$ (see [7, Subsect. 2.5]). The energy flux of u_j^+ (u_j^-) through the cross-section Ω^q in the direction of z-axis is negative (positive). Therefore the wave u_j^+ (u_j^-) is called incoming from $+\infty$ (outgoing to $+\infty$). The coefficient $N_j^{\pm}(\mu)$ is chosen so that the density of flux is equal to unit for every wave.

Let us turn to problem (2) in the domain G. On the interval (τ', τ'') between neighbouring thresholds τ' and τ'' there exists the basis in the space of continuous spectrum eigenfunctions $\mathscr{E}_c(\mu)/\mathscr{E}_p(\mu)$ consisting of analytic functions $\mu \mapsto Y_j^+(\cdot,\mu)$, $j = 1,\dots,\varkappa$ with asymptotics

$$Y_j^+(x,\mu) = u_j^+(x,\mu) + \sum_{l=1}^{\varkappa} S_{jl}(\mu)u_l^-(x,\mu) + O(e^{-\alpha|x|}), \quad j = 1,\dots,\varkappa \qquad (4)$$

as $|x| \to \infty$. Here $\alpha = \alpha(\mu) > 0$ is a sufficiently small number, which is restricted by the rate of stabilization of coefficients ($\alpha < \delta$ in (1)) and the distance from μ to a threshold; for any interval $[\mu', \mu''] \subset (\tau', \tau'')$ one can chose α independent of μ. The u_j^+ and u_j^- denote the incoming and outgoing waves introduced in the cylinders $\Pi^1,\dots,\Pi^{\mathcal{T}}$ and numbered by a through index $j = 1, \dots, \varkappa$, $\varkappa = \varkappa^1 + \dots + \varkappa^{\mathcal{T}}$. We also assume that every of these waves is given by (3) in Π^q_+ for some q and vanishes in Π^r_+ for $r \neq q$.

The matrix $S(\mu) = \|S_{jl}(\mu)\|$ is unitary; it is called the scattering matrix. The matrix-valued function $\mu \mapsto S(\mu)$ is defined on the continuous spectrum except the thresholds; it is analytic on every interval between neighbouring thresholds.

4. LIMITING ABSORPTION PRINCIPLE. SPECTRAL MEASURE

Denote by ρ_α a smooth positive function in G that coincides with $e^{\alpha|x|}$ in every cylindrical end; here α is the number in (4), independent of μ. We introduce the space $L_{2,\alpha}(G) = \{f : \rho_\alpha f \in L_2(G)\}$. Let $R(\mu)$ be the resolvent $(A - \mu)^{-1}$, $\sigma_c(A)$ is the continuous spectrum, $\mathscr{H}_c$ the continuous subspace of A (i.e., the orthocomplement in $L_2(G)$ to the linear hull of the eigenvectors of the operator A), $E(x)$ is the spectral projection.

Lemma 1. *For any $f \in L_{2,\alpha}(G) \cap \mathscr{H}_c$ and $\mu \in \sigma_c(A)$ different from the thresholds, there exist the limits $R(\mu \pm i0)f$ while*

$$R(\mu \pm i0)f(x) = \sum_{j=1}^{\varkappa(\mu)} c_j^{\mp}(\mu)u_j^{\mp}(x;\mu) + O(e^{-\alpha(\mu)|x|}), \quad |x| \to \infty, \qquad (5)$$

and the coefficients in the asymptotics satisfy

$$c_j^{\pm}(\mu) = \mp i(f, Y_j^{\pm}), \qquad (6)$$

where $Y_j^- = \sum_{k=1}^{\varkappa(\mu)} S_{jk}^* Y_k^+$. Moreover,

$$R(\mu + i0)f - R(\mu - i0)f = -\sum_{j=1}^{\varkappa} c_j^+(\mu)Y_j^+(\cdot,\mu). \qquad (7)$$

Proof. Let us explain the main idea. The right-hand side in (5) gives intrinsic radiation conditions. The statement of problem

$$\mathcal{A}(x, D_x)u(x) - \mu u(x) = f(x), \quad x \in G, \qquad u(x) = 0, \quad x \in \partial G, \qquad (8)$$

with such radiation conditions was justified in [1]. The solutions $u^{\mp}(x;\mu)$ admit analytic continuation into a complex neighborhood of μ [2]. By virtue of (3), the functions $u_j^{\mp}(x;\mu \pm i\varepsilon)$ are exponentially decreasing as $\varepsilon > 0$ and $|x| \to \infty$. Therefore the solutions $u^{\mp}(x;\mu \pm i\varepsilon)$ belong to $L_2(G)$ and coincide with $R(\mu \pm i\varepsilon)$. It remains to verify (7) for large $|x|$. □

Lemma 2. *Let the interval $[\mu', \mu''] \subset \sigma_c(A)$ be free from the thresholds, $[\mu', \mu''] \supset X$ an arbitrary interval, and $f, g \in L_{2,\alpha}(G) \cap \mathscr{H}_c$. Then*

$$(E(X)f,g) = \frac{1}{2\pi}\int_X \sum_{j=1}^{\varkappa}(f,Y_j^+)(Y_j^+,g)d\mu, \qquad (9)$$

and the measure $X \mapsto (E(X)f,g)$ is absolutely continuous.

Proof. According to the Stone formula,

$$(E(X)f,g) = \frac{1}{2\pi i}\int_X (R(\mu+i0)f - R(\mu-i0)f,g)d\mu.$$

Taking into account (7) and (6), we obtain (9). It follows that the measure $X \mapsto (E(X)f,g)$ is absolutely continuous. Indeed, equality (9) extends to arbitrary Borel sets $X \subset [\mu',\mu'']$ and for such X leads to the estimate $|(E(X)f,g)| \le c|X|$, where the constant

$$c = \frac{1}{2\pi}\sup_{\mu\in[\mu',\mu'']}\sum_{j=1}^{\varkappa}|(f,Y_j^+)(Y_j^+,g)|$$

is finite due to analyticity of the functions $\mu \mapsto Y_j^+(\cdot,\mu)$ and independent of X.

Corollary 1. The absolutely continuous spectrum $\sigma_{ac}(A)$ of A coincides with $[\tau_1, +\infty)$, while the singularly continuous spectrum is absent.

5. THE SPECTRAL REPRESENTATION OF THE OPERATOR *A*

Let $\{\tau_j\}_{j=1}^{\infty}$ be the thresholds of the operator A in G numbered in order of increasing, $\varkappa_j$ the multiplicity of continuous spectrum on (τ_j,τ_{j+1}), while $\{Y_{jk}^+\}_{k=1}^{\varkappa_j}$ and $\{Y_{jk}^-\}_{k=1}^{\varkappa_j}$ the bases of the continuous spectrum eigenfunctions. For $f \in L_{2,\alpha}(G)\cap\mathcal{H}_c$ and $\mu\in(\tau_j,\tau_{j+1})$ we introduce the column vector

$$(\Phi^{\pm}f)(\mu) = \frac{1}{\sqrt{2\pi}}\{(f,Y_{jk}^{\pm}(\cdot,\mu))\}_{k=1}^{\varkappa_j}.$$

The function $\mu \mapsto (\Phi^{\pm}f)(\mu)$ is given on $\sigma_{ac}(A)$, except the thresholds. We denote by $\mathfrak{h}$ the Hilbert space of vector-functions $g \in \bigoplus_{j=1}^{\infty} L_2((\tau_j,\tau_{j+1});\mathbb{C}^{\varkappa_j})$ with inner product

$$(g,h)_{\mathfrak{h}} = \sum_{j=1}^{\infty}\int_{\tau_j}^{\tau_{j+1}}\sum_{k=1}^{\varkappa_j} g_{jk}(\mu)\overline{h_{jk}(\mu)}d\mu.$$

By definition, the absolutely continuous subspace $\mathcal{H}_{ac}$ of the operator A consists of such elements $f\in\mathcal{H}_c$ that the function $\mu\mapsto(E(-\infty,\mu)f,f)$ is absolutely continuous. According to Colollary 1, we have $\mathcal{H}_{ac} = \mathcal{H}_c$. Let us denote by P_{ac} the orthogonal projection on $\mathcal{H}_{ac}$.

Lemma 3. *For any $f,g \in L_{2,\alpha}(G)\cap\mathcal{H}_{ac}$ there holds the equality*

$$(\Phi^{\pm}f,\Phi^{\pm}g)_{\mathfrak{h}} = (f,g)_{L_2(G)}.$$

Proof. Let τ_j and τ_{j+1} be some neighbouring thresholds. Since the function $\mu\mapsto(E(\tau_1,\mu)f,f)$ is absolutely continuous, its derivative is summable on the interval (τ_j,τ_{j+1}). From (9) with $g=f$ it follows that

$$\frac{d}{d\mu}(E(\tau_1,\mu)f,f) = \frac{1}{2\pi}\sum_{k=1}^{\varkappa_j}|(f,Y_{jk}^+(\cdot,\mu))|^2.$$

The summability of the left-hand side on (τ_j,τ_{j+1}) means that the function $\mu\mapsto(f,Y_{jk}^+(\cdot,\mu))$ can have at the thresholds a square integrable singularity only.

In (9) we put $X = (\tau_j,\tau_{j+1})$ and sum the obtained equalities over j from 1 to J. We have

$$(E(\tau_1,\tau_{J+1})f,g) = \frac{1}{2\pi}\sum_{j=1}^{J}\int_{\tau_j}^{\tau_{j+1}}\sum_{k=1}^{\varkappa_j}(f,Y_{jk}^+)(Y_{jk}^+,g)d\mu.$$

Since $E(\tau_1,+\infty)P_{ac} = P_{ac}$ and $f,g\in\mathcal{H}_{ac}$, there exists the limit as $J\to\infty$:

$$(f,g) = \frac{1}{2\pi}\sum_{j=1}^{\infty}\int_{\tau_j}^{\tau_{j+1}}\sum_{k=1}^{\varkappa_j}(f,Y_{jk}^+)(Y_{jk}^+,g)d\mu = (\Phi^{\pm}f,\Phi^{\pm}g)_{\mathfrak{h}}.$$

The maps $\Phi^{\pm}$ can be extended by continuity to the whole subspace $\mathcal{H}_{ac}$. Since the continuous spectrum eigenfunctions $Y_{jk}^{\pm}$ are orthogonal to any eigenfunction, the $\Phi^{\pm}$ are defined on $\mathcal{H}_p$, while $\Phi^{\pm}|_{\mathcal{H}_p} = 0$.

Lemma 4. *There hold the relations*

$$(\Phi^{\pm})^*\Phi^{\pm} = P_{ac}, \quad \Phi^{\pm}(\Phi^{\pm})^* = I, \quad \Phi^{\pm}A = \mu\Phi^{\pm}.$$

6. WAVE OPERATOR. SCATTERING OPERATOR

Let $G_0^q \subset G\cap\Pi_+^q$ have a smooth boundary and coincide with $G\cap\Pi_+^q$ at sufficiently large distance. Set $G_0 := \cup_q G_0^q$. Let A_0 be the operator in $L_2(G_0)$ given by the differential expression $\mathcal{A}(x,D_x)$ on the domain $\mathfrak{D}(A_0) = H^2(G_0)\cap H_0^1(G_0)$; in what follows, A_0 plays the role of nonperturbed operator. The sets of thresholds, multiplicities of continuous spectra, and the sets of incoming and outgoing waves coincide for the waveguides G and G_0. We denote by $Y_{0jk}^{\pm}$ the continuous spectrum eigenfunctions in the waveguide G_0 and by $\Phi_0^{\pm}$ the corresponding spectral transforms.

Let χ be a smooth cut-off function in G_0, equal to 1 for $|x|\ge t_0$ and to zero for $|x|\le t_0-1$, where t_0 is a sufficiently large positive number. The identification operator $J : L_2(G_0) \to L_2(G)$ acts as the composition of multiplication by χ and extension by zero to G. The wave operators $W^{\pm}$ are defined by $W^{\pm} f := \lim_{t\to\pm\infty} e^{iAt} J e^{-iA_0 t} f$.

Theorem 1. *There holds the equality* $W^{\pm} f = (\Phi^{\mp})^* \Phi_0^{\mp} f$.

Let us calculate the scattering operator:

$$\mathbf{S} = (W^+)^* W^- = ((\Phi^-)^* \Phi_0^-)^* (\Phi^+)^* \Phi_0^+ = (\Phi_0^-)^* S^t \Phi_0^+;$$

here we take into account the relations $(\Phi^- f)(\mu) = S^t(\mu)(\Phi^+ f)(\mu)$ and $\Phi^+(\Phi^+)^* = I$. Note that $S^t(\mu) = S(\mu)$ provided the coefficients of $\mathcal{A}(x, D_x)$ are real. Since

$$(\Phi_0^-)^* g = \sum_{j=1}^{\infty} \int_{\tau_j}^{\tau_{j+1}} \sum_{k=1}^{\varkappa_j} Y_{0jk}^-(\cdot,\mu) g_{jk}(\mu) d\mu,$$

the operator $\mathbf{S}$ is the integral one with kernel

$$G(x, y) = \sum_{j=1}^{\infty} \int_{\tau_j}^{\tau_{j+1}} \sum_{k,l=1}^{\varkappa_j} S_{lk}(\mu) Y_{0jk}^-(x,\mu) \overline{Y_{0jl}^+(y,\mu)} d\mu.$$

From Lemma 4 it follows that the wave operators are complete and the scattering operator is unitary on the absolutely continuous subspace of the operator A_0.

7. BIBLIOGRAPHIC REMARKS

The papers by Lyford [3, 4] are devoted to scattering theory for wave equation in waveguides with several cylindrical ends. A gap in Lyfords arguments was indicated and corrected in [5]. We develop another approach to the spectral analysis of the stationary problem in the waveguide without using the specifics of the Laplacian and the methods of perturbation theory, in particular the Lippmann–Schwinger equation. This allows us to consider operators with variable coefficients.

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