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On the concept of spectral singularities

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Abstract. In this paper, we discuss the concept of spectral singularities for non-Hermitian Hamiltonians. We exihibit spectral singularities of some well-known concrete Hamiltonians with complex-valued coefficients.

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1. Introduction

Spectral singularities, though impossible for Hermitian Hamiltonians, are rather typical for non-Hermitian Hamiltonians with a continuous part of spectrum. Particular role pertaining to the spectral singularities was discovered for the first time by Naimark in [1]. The term 'spectral singularity' itself was introduced later by Schwartz in [2] where the spectral singularities of a certain class of abstract linear operators were studied. Detailed investigation of differential operators with spectral singularities was done by Pavlov [3,4] and Lyantse [5]. Spectral singularities for some class of abstract operators were introduced also by Krein and Langer [6,7]. A general notion of the sets of spectral singularities for closed (bounded or unbounded) linear operators on a Banach space was given by Nagy in [8] and further investigated in [9–11]. We shall not bring in this paper the definition of spectral singularities for general operators given in [8] because of its technical difficulty, referring the interested reader to the original paper [8]. Note only that Nagy shows, in addition, in [8] that the set of spectral singularities defined according to his general definition coincides in the case of differential operators with the set of spectral singularities as defined by Lyantse in [5].

An extensive account of non-Hermitian (non-self-adjoint) problems of mathematical physics considered in the literature till 1960 is given by Dolph in [12]. For the past ten years, non-Hermitian Hamiltonians and complex extension of quantum mechanics have received a lot of attention (see review papers [13,14]). Recently there appeared several papers (see [15–18]) where spectral singularities are identified for some concrete complex scattering potentials and where some physical interpretations for the spectral singularities are offered.

On the other hand, it turns out that (as A Mostafazadeh complained to the author) it is not easy to find in the literature a precise and explicit definition of the spectral singularity. Our intent in the present paper is to try to give an elementary introduction to this specific subject. We describe a definition of the spectral singularity for some class of abstract operators given by Schwartz [2] and a definition widely used for differential operators (whose resolvents are integral operators). We illustrate the definitions by presenting several known examples of operators with spectral singularities.

2. Some preliminaries

Since the concept of spectral singularities is connected to the concepts of spectrum and resolvent of an operator, we start with these concepts.

Let $\mathcal{H}$ be a Hilbert space with an inner product $\langle\cdot|\cdot\rangle$ and A: $D(A) \subset \mathcal{H} \to \mathcal{H}$ a linear operator (unbounded, in general) with the domain $D(A)$ dense in $\mathcal{H}$. The concept of spectrum of A is related to the equation

$$A\psi - \lambda\psi = f, \tag{1}$$

where $f \in \mathcal{H}$ is given, $\psi \in D(A)$ is a desired solution and λ is a given complex number. There are three main problems concerning this equation: uniqueness of the solution, existence of the solution, and continuous dependence of the solution on the right-hand side element (stability property of the solution). The following definition of regular points reflects these three properties of the solution.

A complex number $\lambda \in \mathbb{C}$ is called a regular point of the operator A if the following three conditions are satisfied:

(i) $\ker(A-\lambda I) = \{0\}$ so that there exists the inverse operator $(A-\lambda I)^{-1}$ defined on $\mathrm{ran}(A-\lambda I)$, where I is the identity operator, $\ker(A-\lambda I)$ is the kernel of $A-\lambda I$ consisting of all elements $\psi \in D(A)$ such that $(A-\lambda I)\psi = 0$ and $\mathrm{ran}(A-\lambda I)$ denotes the range of $A-\lambda I$ consisting of all elements $(A-\lambda I)\psi$ for $\psi \in D(A)$.

(ii) The inverse operator $(A-\lambda I)^{-1}$ is bounded on $\mathrm{ran}(A-\lambda I)$, i.e. there is a finite positive constant C such that

$$||(A-\lambda I)^{-1}f|| \le C||f|| \quad \text{for all } f \in \ \mathrm{ran}(A-\lambda I)$$

(iii) $\mathrm{ran}(A-\lambda I)$ is dense in $\mathcal{H}$.

The condition (iii) means that eq. (1) is solvable for 'almost all' right-hand sides f. The condition (i) means that solution of eq. (1) is unique. Finally, the condition (ii) means that the solution of eq. (1) depends continuously on the right-hand side f.

The set of all regular points of the operator A is called the resolvent set of A and is denoted by $\rho(A)$. The operator $(A-\lambda I)^{-1}$ defined for regular points λ is called the resolvent of A and is denoted by $R_\lambda(A)$ or briefly R_λ. It follows by (iii) and (ii) that R_λ is uniquely extended as a linear and bounded operator to the whole space $\mathcal{H}$.

The set

$$\sigma(A) = \mathbb{C} \setminus \rho A,$$

the complement of $\rho(A)$ in the complex plane $\mathbb{C}$, is called the spectrum of the operator A. So a point λ in $\mathbb{C}$ belongs to the spectrum of A if and only if at least one of the above conditions (i), (ii) and (iii) fails to hold.

The spectrum $\sigma(A)$ of the operator A can be splitted into three mutually disjont subsets $\sigma_{\mathrm{p}}(A)$, $\sigma_{\mathrm{c}}(A)$ and $\sigma_{\mathrm{r}}(A)$ as follows:

The set $\sigma_{\mathrm{p}}(A)$ consists of all eigenvalues of A and is called the point spectrum of A:

$$\sigma_{\mathrm{p}}(A) = \{\lambda \in \mathbb{C} \colon \ker(A - \lambda I) \neq \{0\}\}.$$

The set $\sigma_{\mathrm{c}}(A)$ consists of all $\lambda \in \mathbb{C}$ for which the operator $A - \lambda I$ has the inverse with the domain dense in $\mathcal{H}$ (i.e. $\ker(A-\lambda I) = \{0\}$ and $\operatorname{ran}(A-\lambda I)$ is dense in $\mathcal{H}$), but the inverse operator $(A-\lambda I)^{-1}$ is unbounded. This set is called the continuous spectrum of A.

Finally, the set $\sigma_{\mathrm{r}}(A)$, which is called the remainder (or residual) spectrum of A, consists of all $\lambda \in \mathbb{C}$ for which $A - \lambda I$ has the (bounded or unbounded) inverse (i.e. $\ker(A - \lambda I) = \{0\}$) whose domain however is not dense in $\mathcal{H}$ (i.e. $\operatorname{ran}(A - \lambda I)$ is not dense in $\mathcal{H}$). Note that for self-adjoint operators the remainder spectrum is always empty.

Now we are going to formulate the famous spectral theorem for self-adjoint operators.

The adjoint operator $A^\dagger \colon D(A^\dagger) \subset \mathcal{H} \to \mathcal{H}$ is defined as follows:

$$D(A^\dagger) = \{g \in \mathcal{H} \colon \exists g^\dagger \in \mathcal{H},\ \langle g|Af\rangle = \left\langle g^\dagger|f\right\rangle,\ \forall f \in D(A)\}.$$

Since $D(A)$ is dense in $\mathcal{H}$, for each $g \in D(A^\dagger)$ the corresponding element $g^\dagger \in \mathcal{H}$ is unique. We put

$$A^\dagger g = g^\dagger \quad \text{for } g \in D(A^\dagger).$$

Thus,

$$\langle g|Af\rangle = \langle A^\dagger g|f\rangle \quad \text{for all } f \in D(A) \text{ and } g \in D(A^\dagger).$$

The operator A is called self-adjoint (Hermitian) if $A = A^\dagger$. Otherwise A is called non-self-adjoint (non-Hermitian).

An operator A with the domain $D(A)$ dense in $\mathcal{H}$ is called symmetric if

$$\langle g|Af\rangle = \langle Ag|f\rangle \quad \text{for all } f, g \in D(A).$$

For any symmetric operator A we have $A \subset A^\dagger$, that is, $D(A) \subset D(A^\dagger)$ and $Af = A^\dagger f$ for $f \in D(A)$. In general, a symmetric operator need not be self-adjoint.

Next, remember that a linear bounded operator $P \colon \mathcal{H} \to \mathcal{H}$ defined on the whole space $\mathcal{H}$ is called a projection, if $P = P^2$. If in addition $P = P^\dagger$, then P is called an orthogonal projection.

Let $A \colon D(A) \subset \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator with the domain $D(A)$ dense in $\mathcal{H}$. Then the spectrum of A is real and the well-known spectral theorem for self-adjoint operators states that for the operator A there is a unique family (spectral family) of orthogonal projection operators E_λ, $-\infty < \lambda < \infty$, having the properties:

(1) E_λ is non-decreasing: $E_\lambda \leq E_\mu$ for $\lambda < \mu$, that is,

$$\langle E_\lambda \psi | \psi \rangle \leq \langle E_\mu \psi | \psi \rangle \quad \text{for } \lambda < \mu \text{ and all } \psi \in \mathcal{H}.$$

(2) E_λ is continuous from the left in the strong limit sense, that is,

$$\lim_{\varepsilon \to 0^+} \| E_{\lambda - \varepsilon} \psi - E_\lambda \psi \| = 0 \quad \text{for all } \psi \in \mathcal{H}.$$

(3) $E_{-\infty} = 0$, $E_\infty = I$, that is,

$$\lim_{\lambda \to -\infty} \| E_\lambda \psi \| = 0 \quad \text{and} \quad \lim_{\lambda \to \infty} \| E_\lambda \psi - \psi \| = 0 \quad \text{for all } \psi \in \mathcal{H}.$$

(4) The element ψ belongs to $D(A)$ if and only if

$$\int_{-\infty}^{\infty} \lambda^2 \mathrm{d} \langle \psi | E_\lambda \psi \rangle < \infty.$$

For these elements ψ,

$$A\psi = \int_{-\infty}^{\infty} \lambda \mathrm{d} E_\lambda \psi \quad \text{and} \quad \| A\psi \|^2 = \int_{-\infty}^{\infty} \lambda^2 \mathrm{d} \langle \psi | E_\lambda \psi \rangle .$$

The operator function E_λ is called the spectral function of A (or the resolution of the identity for A).

The point $\lambda_0 \in (-\infty, \infty)$ is called a point of constancy of E_λ if there exists an $\varepsilon > 0$ such that

$$E_{\lambda_0 + \varepsilon} - E_{\lambda_0 - \varepsilon} = 0,$$

and a point of growth otherwise. Furthemore, the point λ_0 is called a jump point if

$$E_{\lambda_0^+} - E_{\lambda_0} \neq 0.$$

Continuity points which are also points of growth are called points of continuous growth.

If E_λ is the spectral function of a self-adjoint operator A, then

(a) A real number λ_0 is a regular point of A if and only if λ_0 is a point of constancy of E_λ.

(b) A real number λ_0 is an eigenvalue of A if and only if λ_0 is a jump point of E_λ.

From the propositions (a) and (b) it follows that each point of the continuous growth of spectral function of a self-adjoint operator belongs to its continuous spectrum.

We shall use the following notation: Let Δ be one of the intervals

$$(\alpha, \beta), [\alpha, \beta), (\alpha, \beta], [\alpha, \beta];$$

then E_Δ denotes the operators

$$E_\beta - E_{\alpha^+}, E_\beta - E_\alpha, E_{\beta^+} - E_{\alpha^+}, E_{\beta^+} - E_\alpha,$$

respectively. Note that E_Δ is also an orthogonal projection operator.

The use of self-adjoint operators in quantum mechanics is realized as follows. Let S be a quantum-mechanical system (an object consisting of very small particles). In quantum mechanics every state of the system S is described by a certain element ψ of the Hilbert space $\mathcal{H}$. Every physical quantity (observable) is described by a particular self-adjoint operator on the space $\mathcal{H}$. If, for instance, a certain physical quantity a is described by means of an operator A (note that if a denotes the energy of the system, then the corresponding operator A is called the Hamiltonian of the system), the physical interpretations of this circumstance are the following:

(i) Suppose that the system S is in a certain state ψ and $\psi \in D(A)$; then $\langle\psi|A\psi\rangle$ is the mathematical expectation for the quantity a in this state.

(ii) If E_λ denotes the spectral family for the operator A, then $\langle\psi|E_\Delta\psi\rangle$ is the probability that in the state ψ the value of the quantity a lies in the interval Δ. In other words, $\langle\psi|E_\lambda\psi\rangle$ is the distribution function for the quantity a in this state.

The spectral theorem

$$\langle\psi|A\psi\rangle = \int_{-\infty}^{\infty} \lambda \mathrm{d}\, \langle\psi|E_\lambda\psi\rangle \tag{2}$$

may be interpreted here as the familiar integral representation of the mathematical expectation by means of a distribution function. It follows from this that only the points at which the spectral family E_λ increases, i.e. the points of the spectrum of A, enter into the picture as possible values for the quantity a.

If, in particular, $\psi_0 \in D(A)$, $\|\psi_0\| = 1$, is an eigenvector of the operator A and corresponds to the eigenvalue λ_0 ($A\psi_0 = \lambda_0\psi_0$), then

$$\langle\psi_0|E_\lambda\psi_0\rangle = \begin{cases} 0 & \text{for } \lambda \le \lambda_0, \\ 1 & \text{for } \lambda > \lambda_0. \end{cases}$$

Therefore, in the state ψ_0 the quantity a takes the value λ_0 with probability equal to 1, i.e. in state ψ_0 the quantity a certainly is equal to λ_0.

If the spectrum of the operator A is discrete, if $\psi_1, \psi_2, \ldots$ form a complete orthonormal system of its eigenvectors, and if $\lambda_1, \lambda_2, \ldots$ are the corresponding eigenvalues, then the possible values of the quantity a form a discrete system $\lambda_1, \lambda_2, \ldots$. The quantity a takes each of these values with certainty only in the corresponding states $\psi_1, \psi_2, \ldots$. In any other state, the distribution function for the quantity a can be given. If ψ is an arbitrary state of the system, it can be expressed as an expansion in terms of the orthonormal system:

$$\psi = \sum_{n=1}^{\infty} c_n\psi_n, \quad c_n = \langle\psi_n|\psi\rangle,$$

and here (2) takes the form

$$\langle\psi|A\psi\rangle = \sum_{n=1}^{\infty} \lambda_n |c_n|^2.$$

Hence $|c_n|^2$ is the probability that in the state ψ the quantity a is equal to λ_n. (It has been assumed here that λ_n is a simple eigenvalue of the operator A; but if λ_n is a multiple eigenvalue, then the required probability is equal to the sum of all the $|c_k|^2$ for which the corresponding λ_k are equal to λ_n.)

We see that finding the spectral family E_Δ of a given self-adjoint operator A turns out to be an important mathematical problem. Known proofs of the spectral theorem, which imply the existence of the spectral family E_λ for the operator A, tell very little about the structure of E_λ (because this structure strongly depends on the concrete operator A). In practice, one often uses the following formula for the spectral family of general self-adjoint operators. If $R_\lambda = (A - \lambda I)^{-1}$ is the resolvent of the self-adjoint operator A, then

$$E_\Delta = \lim_{\varepsilon \to 0^+} \frac{1}{2\pi i} \int_\Delta (R_{\lambda+i\varepsilon} - R_{\lambda-i\varepsilon}) \mathrm{d}\lambda, \tag{3}$$

where the limit is taken in the strong limit sense.

As a rule, for differential operators the resolvent is an integral operator and hence according to (3) their spectral projectors turn out to be integral operators whose kernels are expressed in terms of special solutions of the corresponding differential equation.

3. Spectral singularities for a class of abstract operators

We have seen in the previous section that the concept of spectral family of a self-adjoint operator is very important for quantum-mechanical applications. Therefore, in the theory of non-self-adjoint operators it was natural to try to define a generalization of the spectral family, even if, it was for some classes of non-self-adjoint operators. It turns out that the possibility of existence of spectral singularities is a serious obstacle for constructing a reasonable spectral family for non-self-adjoint operators.

In the Schwartz's paper [2] the following definition of spectral singularities is used.

DEFINITION 1

Let A: $D(A) \subset \mathcal{H} \to \mathcal{H}$ be a non-self-adjoint operator such that its spectrum $\sigma(A)$ consists of an interval J of the real axis and a finite number of complex numbers outside J. Let J_0 be a finite subset of J. Assume that for any finite subinterval Δ of J, whose closure do not contain any point of the set J_0, the limit operator

$$E_\Delta = \lim_{\varepsilon \to 0^+} \frac{1}{2\pi i} \int_\Delta (R_{\lambda+i\varepsilon} - R_{\lambda-i\varepsilon}) \mathrm{d}\lambda \tag{4}$$

exists in the strong limit sense, so that E_Δ is a linear bounded operator on $\mathcal{H}$. Denote by d the distance from the interval Δ to the set J_0. If

$$\|E(\Delta)\| \to \infty \quad \text{as } d \to 0,$$

then any point of the set J_0 is called a spectral singularity of the operator A.

Note that for self-adjoint operators $\|E(\Delta)\| \leq 1$ for all intervals Δ of the real axis so that self-adjoint operators have no spectral singularities.

Example 2. Consider in the Hilbert space $L^2(-1,1)$ the linear bounded operator A defined by

$$Af(x) = xf(x) + cx\int_{-1}^{1} f(t)\mathrm{d}t, \quad f \in L^2(-1,1), \tag{5}$$

where c is a complex number.

The adjoint $A^\dagger$ of the operator A is

$$A^\dagger f(x) = xf(x) + c^* x\int_{-1}^{1} f(t)\mathrm{d}t, \quad f \in L^2(-1,1),$$

where c^* denotes the complex conjugate of the number c. Therefore, the operator A is self-adjoint if and only if the number c is real.

It can be verified directly that the resolvent $R_\lambda = (A - \lambda I)^{-1}$ of A has the form

$$R_\lambda f(x) = \frac{f(x)}{x-\lambda} - \frac{cx}{\omega(\lambda)(x-\lambda)}\int_{-1}^{1} \frac{f(t)}{t-\lambda}\mathrm{d}t, \quad f \in L^2(-1,1),$$

where

$$\omega(\lambda) = 1 + c\int_{-1}^{1} \frac{t}{t-\lambda}\mathrm{d}t. \tag{6}$$

The spectrum $\sigma(A)$ of the operator A coincides with the real axis interval $[-1,1]$. If $c \neq -\frac{1}{2}$, then $\sigma(A)$ is purely continuous. But if $c = -\frac{1}{2}$, then $\lambda = 0$ is an eigenvalue of A with the corresponding eigenfunction $f(x) \equiv 1$ and the union $[-1,0) \cup (0,1]$ forms the continuous spectrum of A. If

$$\lambda_0 \in (-1,1) \quad \text{and} \quad \omega(\lambda_0) = 0,$$

then λ_0 is a spectral singularity of the operator A (see [2] for details). Using (6) we can see that any $\lambda_0 \in (-1,1)$ is a spectral singularity of A if we take

$$c = -\left(2 + \lambda_0 \log\frac{1-\lambda_0}{1+\lambda_0} \pm \pi i\lambda_0\right)^{-1}$$

in Definition (5) of A. In the case $c = -\frac{1}{2}$, the eigenvalue $\lambda = 0$ is a spectral singularity of A.

Example 3. In the same paper [2], Schwartz considered also the following example A of linear unbounded operators:

$$D(A) = \{f \in L^2(0,\infty)\colon f'' \in L^2(0,\infty), \quad f(0) = hf'(0)\},$$

$$Af = -f''(x), \quad f \in D(A),$$

where h is a complex number.

The adjoint $A^\dagger$ of the operator A is given by

$$D(A^\dagger) = \{f \in L^2(0,\infty)\colon f'' \in L^2(0,\infty), f(0) = h^* f'(0)\},$$

$$A^\dagger f = -f''(x), \quad f \in D(A^\dagger),$$

where h^* is the complex conjugate of the number h. It follows that the operator A is self-adjoint if and only if the number h is real.

Consider the equation

$$-y''(x) = \lambda y(x), \quad 0 < x < \infty, \tag{7}$$

with $\lambda = k^2$, $\operatorname{Im} k \geq 0$. Denote by $\varphi(x,\lambda)$ the solution of eq. (7) satisfying the initial conditions

$$\varphi(0,\lambda) = h, \quad \varphi'(0,\lambda) = 1,$$

that is,

$$\varphi(x,\lambda) = \frac{\sin kx}{k} + h\cos kx.$$

Note that the solution $\varphi(x,\lambda)$ is chosen so that it satisfies the boundary condition $f(0) = hf'(0)$. All numbers λ of the form $\lambda = k^2$, $\operatorname{Im} k > 0$, $1 - hik \neq 0$ belong to the resolvent set of the operator A. The resolvent $R_\lambda = (L - \lambda I)^{-1}$ is an integral operator of the form

$$R_\lambda f(x) = \int_0^\infty R(x,\xi,\lambda) f(\xi) \mathrm{d}\xi$$

with the kernel

$$R(x,\xi,\lambda) = \frac{1}{1 - hik} \begin{cases} \varphi(x,\lambda)\mathrm{e}^{ik\xi} & \text{for } 0 \leq x \leq \xi < \infty, \\ \varphi(\xi,\lambda)\mathrm{e}^{ikx} & \text{for } 0 \leq \xi \leq x < \infty. \end{cases}$$

If $\operatorname{Re} h > 0$ and $h = 0$, then the spectrum $\sigma(A)$ of the operator A is purely continuous and coincides with the real axis interval $[0,\infty)$. Further, if $\operatorname{Re} h < 0$, then the spectrum of A consists of the continuous part coincided with the real interval $[0,\infty)$ and a single eigenvalue $\lambda_0 = (ih)^{-2} = -h^{-2}$ with the corresponding eigenfunction $y_0(x) = \mathrm{e}^{x/h}$. Finally, if $\operatorname{Re} h = 0$ and $\operatorname{Im} h \neq 0$, then the spectrum of A is purely continuous and coincides with the interval $[0,\infty)$, but in this case the number $\lambda_0 = (ih)^{-2} = -h^{-2}$ comes to lie in the continuous spectrum $[0,\infty)$ and it is a spectral singularity of A in the sense of Definition 1 (see [2] for the details).

In the next section we describe a definition of the spectral singularities for differential operators, frequently used in the literature.

4. Spectral singularities of differential operators

Let (a, b) be a finite or infinite interval of the real axis $\mathbb{R}$ and $p_0, p_1, \ldots, p_n \colon (a, b) \to \mathbb{C}$ be complex-valued functions. Consider the differential expression

$$l(y) = p_0(x)y^{(n)} + p_1(x)y^{(n-1)} + \cdots + p_n(x)y, \quad a < x < b, \tag{8}$$

and assume that the functions $1/p_0(x), p_1(x), \ldots, p_n(x)$ are integrable on any finite subinterval of the interval (a, b). In the case when the interval (a, b) has one or two finite end points we take some linear homogeneous boundary conditions at the finite end points of the interval (a, b). Let us present such needed boundary conditions in the form

$$U(y) = 0. \tag{9}$$

With the differential expression (8) and the boundary condition (9) we associate an operator A acting in the Hilbert space $L^2(a, b)$ as follows. The domain of definition $D(A)$ of the operator A consists of all functions $y \in L^2(a, b)$ such that:

(1) y has a derivative $y^{(n-1)}$ absolutely continuous on every finite subinterval of the interval (a, b) (hence the derivative $y^{(n)}$ exists almost everywhere) and $l(y) \in L^2(a, b)$.
(2) $U(y) = 0$ (in the case of finite end points of the interval (a, b)).

If $y \in D(A)$, then we set

$$Ay = l(y).$$

Since we do not assume that $p_0(x), p_1(x), \ldots, p_n(x)$ are real-valued, the operator A is, in general, non-self-adjoint.

It is known [19] that for $\lambda \in \rho(A)$ the resolvent $R_\lambda = (A - \lambda I)^{-1}$ is an integral operator of the form

$$R_\lambda f(x) = \int_a^b R(x, \xi, \lambda) f(\xi) \mathrm{d}\xi, \tag{10}$$

where $R(x, \xi, \lambda)$ is a kernel function which is an analytic (holomorphic) function of the variable $\lambda \in \rho(A)$. Note that if λ_0 is an isolated eigenvalue of A (that is, λ_0 is an eigenvalue of A and it is an isolated point in $\sigma(A)$), then λ_0 is a pole of the kernel function $R(x, \xi, \lambda)$ with respect to λ so that

$$R(x, \xi, \lambda) \to \infty \quad \text{as } \lambda \in \rho(A) \text{ and } \lambda \to \lambda_0. \tag{11}$$

However, (11) may be held also for some points $\lambda_0 \in \sigma(A)$ that are not isolated eigenvalues of A. We call such a point $\lambda_0 \in \sigma(A)$ as a spectral singularity of the operator A. Thus we can introduce the following definition.

DEFINITION 4

We call a point $\lambda_0 \in \sigma(A)$ as a spectral singularity of the operator A, if it is not an isolated eigenvalue of A, but (11) holds.

Note that such a definition is enough in applications as the resolvent of almost all differential operators (including partial differential operators) is an integral operator of type (10). Since the resolvent kernel is unbounded in any small neighbourhood of the spectral singularity, often spectral singularity is interpreted as a certain 'pole' of the resolvent kernel as a function of λ and one says that the spectral singularities are those poles of the resolvent kernel which are not isolated eigenvalues of the operator. If the interval (a, b) is finite, then the spectrum of the operator A consists only of isolated eigenvalues and therefore in this case there are no spectral singularities. As usual, spectral singularities of differential operators are embedded in the continuous spectrum of the operator. Note also that in order to determine the spectral singularities of a given operator by using the above definition one needs to construct the resolvent kernel of the operator.

It can be seen using formulas (4), (10), and the reasonings of Schwartz's paper [2] that if for a differential operator A both Definitions 1 and 4 are applicable, then these definitions are equivalent.

5. Operators on the semi-axis

Example 5 (see [19], Appendix II). Consider the operator A generated in the Hilbert space $L^2(0, \infty)$ by the differential expression

$$l(y) = -y'' + p(x)y, \quad 0 < x < \infty, \tag{12}$$

with the boundary condition

$$y(0) = 0. \tag{13}$$

Under the condition

$$\int_0^\infty (1 + x)\,|p(x)|\,\mathrm{d}x < \infty,$$

the equation

$$-y'' + p(x)y = \lambda y, \quad 0 < x < \infty, \tag{14}$$

with $\lambda = k^2$ ($\operatorname{Im} k \geq 0$), has a solution $e(x, k)$ (Jost solution) such that

$$e(x, k) = \mathrm{e}^{ixk}[1 + o(1)] \quad \text{as } x \to \infty \text{ and } \operatorname{Im} k \geq 0.$$

For every $x \geq 0$, the solution $e(x, k)$ is continuous with respect to k for $\operatorname{Im} k \geq 0$, and is holomorphic with respect to k for $\operatorname{Im} k > 0$. Denote by $\varphi(x, \lambda)$ the solution of eq. (14) satisfying the initial conditions

$$\varphi(0,\lambda) = 0, \quad \varphi'(0,\lambda) = 1.$$

Note that $\varphi(x,\lambda)$ satisfies the boundary condition (13) and is an entire function of $\lambda \in \mathbb{C}$. Let us set

$$\begin{aligned}\omega(\lambda) = W_x(\varphi, e) &= \varphi(x,\lambda)e'(x,k) - \varphi'(x,\lambda)e(x,k) \\ &= \varphi(0,\lambda)e'(0,k) - \varphi'(0,\lambda)e(0,k) = -e(0,k),\end{aligned}$$

the Wronskian of the solutions $\varphi(x,\lambda)$ and $e(x,k)$, which does not depend on x.

All numbers λ of the form $\lambda = k^2$, $\operatorname{Im} k > 0$, $e(0,k) \neq 0$ belong to the resolvent set of the operator A. The resolvent $R_\lambda = (L - \lambda I)^{-1}$ is an integral operator of the form

$$R_\lambda f(x) = \int_0^\infty R(x,\xi,\lambda) f(\xi) \mathrm{d}\xi$$

with the kernel

$$R(x,\xi,\lambda) = \frac{R_1(x,\xi,\lambda)}{\omega(\lambda)},$$

where

$$R_1(x,\xi,\lambda) = -\begin{cases} \varphi(x,\lambda)e(\xi,k) & \text{for } 0 \le x \le \xi < \infty, \\ \varphi(\xi,\lambda)e(x,k) & \text{for } 0 \le \xi \le x < \infty. \end{cases}$$

Therefore, spectral singularities of A are those points $\lambda_0 = k_0^2$ ($\operatorname{Im} k_0 \ge 0$) for which $e(0,k_0) = 0$ but $\lambda_0 = k_0^2$ is not an isolated eigenvalue of the operator A.

For every $l > 0$ there is a number $C_l > 0$ such that

$$\|R_{k^2}\| \ge \frac{C_l}{|e(0,k)|\sqrt{\operatorname{Im} k}}$$

for all k in the domain $\operatorname{Im} k > 0$, $|k| \le l$. This shows that the resolvent grows in norm more faster than in the absence of spectral singularities, when $\lambda = k^2$ approaches a spectral singularity.

For given $f \in L^2(0,\infty)$ the solution ψ of the equation

$$-\psi'' + p(x)\psi = \lambda\psi + f, \quad 0 < x < \infty,$$

$$\psi(0) = 0,$$

is given by the formula

$$\psi(x) = \int_0^\infty R(x,\xi,\lambda) f(\xi)\mathrm{d}\xi = -\frac{1}{e(0,k)} \int_0^\infty R_1(x,\xi,\lambda) f(\xi)\mathrm{d}\xi. \tag{15}$$

If λ is in the continuous spectrum of the operator A, then the integral operator

$$R_1 f(x) = \int_0^\infty R_1(x,\xi,\lambda) f(\xi)\mathrm{d}\xi$$

is an unbounded operator causing an instability of the solution. If at the point λ we have, besides, a spectral singularity ($e(0,k)=0$), then eq. (15) shows that we will have a 'resonance' phenomenon at the spectral singularity.

An expansion formula in eigenfunctions (including 'generalized eigenfunctions' corresponding to the continuous spectrum) of a differential operator A, not necessarily self-adjoint, is derived in practice very often by applying the technique of contour integration as follows. Often one can establish that for any $f \in \mathcal{H}$

$$R_\lambda f = -\frac{f}{\lambda} + r_\lambda,$$

where r_λ tends to zero as $|\lambda| \to \infty$ faster than λ^{-1}. Hence

$$f = -\frac{1}{2\pi i}\int_{\Gamma_N} R_\lambda f \mathrm{d}\lambda + \frac{1}{2\pi i}\int_{\Gamma_N} r_\lambda \mathrm{d}\lambda,$$

where Γ_N is the circle in the complex λ-plane of radius N centred at the origin. If

$$\lim_{N\to\infty}\int_{\Gamma_N} r_\lambda \mathrm{d}\lambda = 0,$$

which holds in most cases, we get

$$f = -\lim_{N\to\infty}\frac{1}{2\pi i}\int_{\Gamma_N} R_\lambda f \mathrm{d}\lambda. \tag{16}$$

Next the main job is to carry the integral in (16) onto the spectrum of A using the concrete structure and analytical properties of the resolvent R_λ.

Assume that in eq. (14) the potential $p(x)$ satisfies the condition

$$\int_0^\infty \mathrm{e}^{\varepsilon x}\,|p(x)|\,\mathrm{d}x < \infty$$

for some $\varepsilon > 0$. Then the function $e(0,k)$ is holomorphic in the half-plane $\operatorname{Im} k > -\varepsilon/2$ and therefore it may have only a finite number roots (zeros) in the closed upper half-plane $\operatorname{Im} k \geq 0$. Let

$$e(0,k_j) = 0\,(\operatorname{Im} k_j > 0), \quad j = 1,\ldots,N,$$

and

$$e(0,r_j) = 0\,(\operatorname{Im} r_j = 0), \quad j = 1,\ldots,N'.$$

The numbers $\lambda_j = k_j^2$, $j = 1,\ldots,N$, are eigenvalues of the operator A, and this operator has no other eigenvalues. The real axis interval $[0,\infty)$ forms the continuous spectrum of the operator A and the remainder spectrum of A is empty. The numbers $\mu_j = r_j^2$, $j = 1,\ldots,N'$, are spectral singularities of the operator A. If the potential $p(x)$ is real-valued, then $e(0,k) \neq 0$ for $-\infty < k < \infty$ and hence a self-adjoint operator A has no spectral singularities. The functions $\varphi(x,\lambda_j)$ and $e(x,k_j)$, as well as the functions $\varphi(x,r_j)$ and $e(x,r_j)$, are linearly dependent. Let m_j denote the multiplicity of the root k_j of the equation $e(0,k)=0$. Then $e^{(m)}(0,k_j) = 0$ for $m = 0,1,\ldots,m_j-1$ (the derivative with respect to k) and

$$\varphi^{(m)}(x,\lambda_j) = \left(\frac{\mathrm{d}}{\mathrm{d}\lambda}\right)^m \varphi(x,\lambda)|_{\lambda=\lambda_j} \in L^2(0,\infty),$$

$$\varphi^{(m)}(0,\lambda_j) = 0 \quad \text{for } m = 0,1,\ldots,m_j-1.$$

Therefore, the functions $\varphi^{(m)}(x,\lambda_j)$, $m = 0,1,\ldots,m_j-1$, are eigenfunction and associated functions (Jordan functions) of the operator A, corresponding to the eigenvalue λ_j:

$$A\varphi^{(0)} = \lambda_j\varphi^{(0)}, \quad A\varphi^{(m)} = \lambda_j\varphi^{(m)} + \varphi^{(m-1)}, \quad m = 1,\ldots,m_j-1.$$

Let m_j' denote the multiplicity of the root r_j of the equation $e(0,k) = 0$. Then $\varphi^{(m)}(0,\mu_j) = 0$, $m = 0,1,\ldots,m_j'-1$, but the functions $\varphi^{(m)}(x,\mu_j)$ are not now in $L^2(0,\infty)$, we can state only that

$$\sup_{0\le x<\infty} \frac{\left|\varphi^{(m)}(x,\mu_j)\right|}{(1+x)^m} < \infty, \quad m = 0,1,\ldots\ .$$

The functions $\varphi^{(m)}(x,\mu_j)$, $m = 0,1,\ldots,m_j'-1$, are Jordan functions of the operator A, corresponding to the spectral singularity μ_j.

For a function $f \in L^2(0,\infty)$ the following expansion in eigenfunctions holds:

$$\begin{aligned} f(x) = {} & \frac{1}{\pi}\int_0^\infty F(\lambda)[\mathcal{B}\varphi(x,\lambda)]\frac{\sqrt{\lambda}\,\mathrm{d}\lambda}{e(0,\sqrt{\lambda})e(0,-\sqrt{\lambda})} \\ & + \sum_{j=1}^{N}\sum_{m=0}^{m_j-1} M_{jm}(f)\varphi^{(m)}(x,\lambda_j) \\ & + \sum_{j=1}^{N'}\sum_{m=0}^{m_j'-1} M_{jm}'(f)\varphi^{(m)}(x,\mu_j), \end{aligned} \tag{17}$$

where

$$F(\lambda) = \int_0^\infty f(x)\varphi(x,\lambda)\,\mathrm{d}x$$

and $M_{jm}(f)$, $M_{jm}'(f)$ are some numbers depending on the function f. Note that the integral

$$\int_0^\infty F(\lambda)\varphi(x,\lambda)\frac{\sqrt{\lambda}\,\mathrm{d}\lambda}{e(0,\sqrt{\lambda})e(0,-\sqrt{\lambda})} \tag{18}$$

does not, in general, converge if there are spectral singularities (at which $e(0,\sqrt{\lambda}) = 0$). The operation $\mathcal{B}$ used in (17) regularizes the divergent integral (18) as follows. For an arbitrary function $\Phi(\lambda)$ which is differentiable sufficiently often at the points $\mu_1,\ldots,\mu_{N'}$, we put

$$[\mathcal{B}\Phi(\lambda)] = \Phi(\lambda) - \sum_{j=1}^{N'}\sum_{m=0}^{m_j'-1} B_{jm}(\lambda)\Phi^{(m)}(\mu_j),$$

where

$$B_{jm}(\lambda) = \begin{cases} \frac{(\lambda-\mu_j)^m}{m!} & \text{for } |\lambda-\mu_j| < \delta, \\ 0 & \text{for } |\lambda-\mu_j| \geq \delta, \end{cases}$$

in which $\delta > 0$ is a sufficiently small number. Note also that the expansion (17) converges to $f(x)$, in general, in a norm weaker than the norm of $L^2(0,\infty)$ (see [19], Appendix II for details).

The expansion formula (17) shows that if the operator A has spectral singularities, then the eigenfunctions corresponding to the eigenvalues and the continuous spectrum are not complete and one should include the eigenfunctions corresponding to the spectral singularities as well to get a complete system of eigenfunctions.

Example 6. Operator with a given spectral singularity.

Take an arbitrary real number $k_0 \neq 0$ and put

$$p(x) = \frac{u''(x)}{u(x)} + k_0^2 \quad \text{for } 0 \leq x \leq b$$

and

$$p(x) = 0 \quad \text{for } b < x < \infty, \tag{19}$$

where $u(x)$ is a twice continuously differentiable function on $0 \leq x \leq b$ such that

$$u(0) = 0, \quad u(b) = \mathrm{e}^{ibk_0}, \quad u'(b) = ik_0\mathrm{e}^{ibk_0}.$$

Then the Jost solution $e(x,k)$ introduced in Example 5 has the form, for $k = k_0$,

$$e(x,k_0) = \begin{cases} u(x) & \text{for } 0 \leq x \leq b, \\ \mathrm{e}^{ixk_0} & \text{for } b < x < \infty. \end{cases}$$

Therefore, $e(0,k_0) = u(0) = 0$ and hence the point $\lambda_0 = k_0^2$ is a spectral singularity for the operator A defined in Example 5 with the potential $p(x)$ given in (19).

Example 7 (see [1]). Consider the same operator A as in Example 5, but replace the boundary condition (13) by

$$y'(0) - \theta y(0) = 0, \tag{20}$$

where θ is a complex number.

Let $e(x,k)$ be the same solution of eq. (14) as in Example 5, but $\varphi(x,\lambda)$ be the solution of eq. (14) satisfying the initial conditions

$$\varphi(0,\lambda) = 1, \quad \varphi'(0,\lambda) = \theta.$$

Note that $\varphi(x,\lambda)$ satisfies the boundary condition (20).

The resolvent $R_\lambda = (A - \lambda I)^{-1}$ is an integral operator of the form

$$R_\lambda f(x) = \int_0^\infty R(x,\xi,\lambda) f(\xi)\mathrm{d}\xi$$

with the kernel

$$R(x,\xi,\lambda)=\frac{R_1(x,\xi,\lambda)}{\omega(\lambda)},$$

where $\omega(\lambda)$ is equal to the Wronskian of the solutions $\varphi(x,\lambda)$ and $e(x,k)$,

$$\omega(\lambda)=W_x(\varphi,e)=\varphi(x,\lambda)e'(x,k)-\varphi'(x,\lambda)e(x,k)$$

$$=\varphi(0,\lambda)e'(0,k)-\varphi'(0,\lambda)e(0,k)=e'(0,k)-\theta e(0,k),$$

and

$$R_1(x,\xi,\lambda)=-\begin{cases}\varphi(x,\lambda)e(\xi,k) & \text{for } 0\le x\le\xi<\infty,\\ \varphi(\xi,\lambda)e(x,k) & \text{for } 0\le\xi\le x<\infty.\end{cases}$$

Therefore, spectral singularities of A are those points $\lambda_0=k_0^2$ $(\operatorname{Im}k_0\ge 0)$ for which $e'(0,k_0)-\theta e(0,k_0)=0$ but $\lambda_0=k_0^2$ is not an isolated eigenvalue of the operator A.

Example 8. Another operator with a given spectral singularity.

Consider the operator A generated in $L^2(0,\infty)$ by the differential expression

$$l(y)=-y''(x),\quad 0<x<\infty,$$

subject to the boundary condition

$$y'(0)-\theta y(0)=0.$$

Then we have

$$e(x,k)=\mathrm{e}^{ixk}\quad\text{and}\quad e'(0,k)-\theta e(0,k)=ik-\theta.$$

Therefore, if θ is a pure imaginary complex number, then $\lambda=(-i\theta)^2=-\theta^2\in[0,\infty)$ is a spectral singularity for the operator A.

6. Operators on the whole axis

Example 9 (see [20]). Consider the operator A generated in the Hilbert space $L^2(-\infty,\infty)$ by the differential expression

$$l(y)=-y''+p(x)y,\quad -\infty<x<\infty,$$

and suppose that

$$\int_{-\infty}^{\infty}(1+|x|)\,|p(x)|\,\mathrm{d}x<\infty.$$

The equation

$$-y''+p(x)y=k^2y,\quad -\infty<x<\infty,$$

has the solutions (Jost solutions) $e_+(x,k)$ and $e_-(x,k)$ for $\operatorname{Im} k \geq 0$ such that

$$e_+(x,k) = \mathrm{e}^{ixk}[1+o(1)] \quad \text{as } x \to \infty,$$

$$e_-(x,s) = \mathrm{e}^{-ixk}[1+o(1)] \quad \text{as } x \to -\infty.$$

The resolvent $R_\lambda = (A - \lambda I)^{-1}$ is the integral operator

$$R_\lambda f(x) = \int_{-\infty}^{\infty} R(x,\xi,\lambda) f(\xi)\mathrm{d}\xi$$

with the kernel

$$R(x,\xi,\lambda) = \frac{R_1(x,\xi,\lambda)}{\omega(\lambda)},$$

where $\omega(\lambda)$, with $\lambda = k^2$, is equal to the Wronskian of the solutions $e_-(x,k)$ and $e_+(x,k)$,

$$\omega(\lambda) = W_x(e_-, e_+) = e_-(x,k)e'_+(x,k) - e'_-(x,k)e_+(x,k)$$

$$= e_-(0,k)e'_+(0,k) - e'_-(0,k)e_+(0,k),$$

and

$$R_1(x,\xi,\lambda) = -\begin{cases} e_-(x,k)e_+(\xi,k) & \text{for } -\infty < x \leq \xi < \infty, \\ e_-(\xi,k)e_+(x,k) & \text{for } -\infty < \xi \leq x < \infty. \end{cases}$$

Therefore, spectral singularities of A are those points $\lambda_0 = k_0^2$ ($\operatorname{Im} k_0 \geq 0$) for which $e_-(0,k_0)e'_+(0,k_0) - e'_-(0,k_0)e_+(0,k_0) = 0$ but $\lambda_0 = k_0^2$ is not an isolated eigenvalue of the operator A.

Example 10 (see [21]). Consider the operator A generated in the Hilbert space $L^2(-\infty,\infty)$ by the differential expression

$$l(y) = -y'' + p(x)y, \quad -\infty < x < \infty,$$

with the complex periodic potential

$$p(x) = \sum_{n=1}^{\infty} p_n \mathrm{e}^{inx}, \quad p_n \in \mathbb{C}, \quad \sum_{n=1}^{\infty} |p_n| < \infty.$$

The equation

$$-y'' + p(x)y = k^2 y, \quad -\infty < x < \infty,$$

has a solution φ of the form

$$\varphi(x,k) = \mathrm{e}^{ixk}\left(1 + \sum_{n=1}^{\infty} \frac{1}{n+2k} \sum_{\alpha=n}^{\infty} v_{n\alpha}\mathrm{e}^{i\alpha x}\right). \tag{21}$$

The resolvent $R_\lambda = (A - \lambda I)^{-1}$ is the integral operator

$$R_\lambda f(x) = \int_{-\infty}^{\infty} R(x, \xi, \lambda) f(\xi) \mathrm{d}\xi$$

with the kernel

$$R(x, \xi, \lambda) = \frac{1}{2ik} \begin{cases} \varphi(x, -k)\varphi(\xi, k) & \text{for } -\infty < x \leq \xi < \infty, \\ \varphi(x, k)\varphi(\xi, -k) & \text{for } -\infty < \xi \leq x < \infty, \end{cases} \tag{22}$$

where $\lambda = k^2$. The spectrum of the operator A is purely continuous and coincides with the real interval $[0, \infty)$. Since the solution $\varphi(x, k)$ defined by (21) may have singularities at the points $k = -n/2$ for $n = 1, 2, \ldots$, we see from (22) that the resolvent kernel $R(x, \xi, \lambda)$ may have singularities at these points. Therefore, the points $\lambda_n = (-n/2)^2 = n^2/4$, $n = 1, 2, \ldots$, which belong to the interval $[0, \infty)$, may be spectral singularities for the operator A. Note that these points certainly are spectral singularities for the one-term potential $p(x) = \mathrm{e}^{ix}$.

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