A remark on Krein's resolvent formula and boundary conditions

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Abstract
We prove an analogue of Krein's resolvent formula expressing the resolvents of self-adjoint extensions in terms of boundary conditions. Applications to quantum graphs and systems with point interactions are discussed.

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Krein's resolvent formula [1] is a powerful tool in the spectral analysis of self-adjoint extensions, which found numerous applications in many areas of mathematics and physics, including the study of exactly solvable models in quantum physics [2–4]. For the use of this formula in the traditional way one needs a kind of preliminary construction, like finding a maximal common part of two extensions, see [2, appendix A]. While this is enough for many applications, including models with point interactions, there are a number of problems such as the study of quantum graphs or more general hybrid structures, where self-adjoint extensions are suitably described by more complicated boundary conditions, see [5–7], and it is necessary to modify Krein's resolvent formula to take into account these new requirements. This can be done if one either modifies the coordinates in which the boundary data are calculated [6, 8] or considers boundary conditions given in a non-operator way using linear relations [9, 10]. On the other hand, a more attractive idea is to have a resolvent formula taking directly the boundary conditions into account, without changing the coordinates. We describe the realization of this idea in the present paper.

Let S be a closed densely defined symmetric operator with the deficiency indices (n, n), $0 < n < \infty$, acting in a certain Hilbert space $\mathcal{H}$. One says that a triple (V, Γ_1, Γ_2),

where $V = \mathbb{C}^n$ and Γ_1 and Γ_2 are linear maps from the domain dom S^* of the adjoint of S to V, is a *boundary value space* for S if $\langle \phi, S^*\psi \rangle - \langle S^*\phi, \psi \rangle = \langle \Gamma_1\phi, \Gamma_2\psi \rangle - \langle \Gamma_2\phi, \Gamma_1\psi \rangle$ for any $\phi, \psi \in$ dom S^* and the map (Γ_1, Γ_2) : dom $S^* \to V \oplus V$ is surjective. A boundary value space always exists [9, theorem 3.1.5]. All self-adjoint extensions of S are restrictions of S^* to functions $\phi \in$ dom S^* satisfying $A\Gamma_1\phi = B\Gamma_2\phi$, where the matrices A and B must obey the following two properties:

$$AB^* = BA^* \quad \Leftrightarrow \quad AB^* \text{ is self-adjoint,} \tag{1}$$

$$\text{the } n \times 2n \text{ matrix } (A|B) \text{ has maximal rank } n. \tag{2}$$

We denote such an extension of S by $H^{A,B}$. Our aim is to write a formula for the resolvent $R^{A,B}(z) = (H^{A,B} - z)^{-1}$ in terms of these two matrices A and B.

We will need some notions from the theory of linear relations. Let $V = \mathbb{C}^n$. Any linear subspace Λ of $V \oplus V$ will be called a *linear relation* on V. By the *domain* of Λ we mean the set dom $\Lambda = \{x \in V : \exists y \in V \text{ with } (x, y) \in \Lambda\}$. A linear relation $\Lambda^{-1} = \{(x, y) : (y, x) \in \Lambda\}$ is called *inverse* to Λ. For $\alpha \in \mathbb{C}$ we put $\alpha\Lambda = \{(x, \alpha y) : (x, y) \in \Lambda\}$. For two linear relations $\Lambda', \Lambda'' \subset V \oplus V$ one can define the sum $\Lambda' + \Lambda'' = \{(x, y' + y''), (x, y') \in \Lambda', (x, y'') \in \Lambda''\}$; clearly, one has dom $(\Lambda' + \Lambda'') =$ dom $\Lambda' \cap$ dom Λ''. The graph of any linear operator L acting in V is a linear relation, which we denote by gr L. Clearly, if L is an invertible operator, then gr $L^{-1} = (\text{gr } L)^{-1}$. For arbitrary linear operators L', L'' one has gr $L' +$ gr $L'' = $ gr$(L' + L'')$. Therefore, the set of linear operators is naturally imbedded into the set of linear relations.

Denote by J an operator acting in $V \oplus V$ by the rule $J(x_1, x_2) = (x_2, -x_1)$, $x_1, x_2 \in V$. For a linear relation Λ on V the relation $\Lambda^* = J\Lambda^\perp$ is called *adjoint* to Λ; Λ is called *symmetric* if $\Lambda \subset \Lambda^*$ and is called *self-adjoint* if $\Lambda = \Lambda^*$. The graph of a linear operator L in V is symmetric (respectively, self-adjoint), iff its graph is a symmetric (respectively, self-adjoint) linear relation. In other words, a self-adjoint linear relation (abbreviated as s.a.l.r) is a symmetric linear relation of dimension n. Let A, B be $n \times n$ matrices. We introduce the notation

$$\Lambda^{A,B} = \{(x_1, x_2) \in V \oplus V, Ax_1 = Bx_2\}.$$

A criterion for $\Lambda^{A,B}$ to be self-adjoint was proven in [5]: *a linear relation $\Lambda^{A,B}$ is self-adjoint iff A and B satisfy* (1) *and* (2). It is important to emphasize that *any* s.a.l.r. Λ can be defined by this construction, more precisely, there exists a unitary operator U such that $\Lambda = \Lambda^{i(1+U),1-U}$ [9]. This shows that there is a bijection between s.a.l.r.s and unitary operators; nevertheless, we consider parametrization by the two matrices of coefficients as a more natural way to present s.a.l.r.

The language of linear relations is widely used in the theory of self-adjoint extensions of symmetric operators [3, 8, 11]. Let us return to the symmetric operator S and its boundary value space (V, Γ_1, Γ_2). It is a well-known fact that *there is a bijection between all self-adjoint extensions of S and s.a.l.r.s on V. A self-adjoint extension H^Λ corresponding to a s.a.l.r. Λ is a restriction of S^* to elements $\phi \in$ dom S^* satisfying abstract boundary conditions* $(\Gamma_1\phi, \Gamma_2\phi) \in \Lambda$ [9, theorem 3.1.6]. To carry out the spectral analysis of the operators H^Λ it is useful to know their resolvents, which are provided by the famous Krein's formula [1, 10]. To write this formula we need some additional constructions. For $z \in \mathbb{C} \setminus \mathbb{R}$, let $\mathcal{N}_z$ denote the corresponding deficiency subspace for S, i.e. $\mathcal{N}_z = \ker(S^* - z)$. The restrictions of Γ_1 and Γ_2 onto $\mathcal{N}_z$ are invertible linear maps from $\mathcal{N}_z$ to V. Put $\gamma_z = (\Gamma_1|_{\mathcal{N}_z})^{-1}$ and $Q(z) = \Gamma_2\gamma_z$; these maps form holomorphic families from $\mathbb{C} \setminus \mathbb{R}$ to the spaces $\mathcal{L}(V, \mathcal{H})$ and $\mathcal{L}(V, V)$ of bounded operators from V to $\mathcal{H}$ and from V to V, respectively. Denote by H^0 a self-adjoint extension of S given by the boundary conditions $\Gamma_1\phi = 0$. That is for $A = 1$ and $B = 0$, then the maps

γ_z and $Q(z)$ have analytic continuations to the resolvent set res H^0, and for all $z, \zeta \in$ res H^0 one has [10]

$$Q(z) - Q^*(\zeta) = (z - \overline{\zeta})\gamma_\zeta^* \gamma_z. \tag{3}$$

The maps γ_z and $Q(z)$ are called the Γ-field and the Q-function for the pair (S, H^0), respectively.

For all $z \in$ res $H^0 \cap$ res H^Λ we consider the linear relation gr $Q(z) - \Lambda$. While this set is, generally speaking, not the graph of an operator, the inverse linear relation $(\text{gr } Q(z) - \Lambda)^{-1}$ is the graph of a certain linear operator $C^\Lambda(z)$, so that the resolvent $R^\Lambda(z) = (H^\Lambda - z)^{-1}$ is expressed through the resolvent $R^0(z) = (H^0 - z)^{-1}$ by *Krein's formula* [10, proposition 2]

$$R^\Lambda(z) = R^0(z) - \gamma_z C^\Lambda(z)\gamma_{\overline{z}}^*. \tag{4}$$

The calculation of $C^\Lambda(z)$ is a rather difficult technical problem, as it involves 'generalized' operations with linear relations. Such difficulties do not arise if Λ is a graph of a certain linear operator L; the corresponding boundary conditions can be presented by

$$\Gamma_2 \phi = L\Gamma_1 \phi, \tag{5}$$

and such extensions are called *disjoint with respect to H^0* because they satisfy the equality dom $H^\Lambda \cap$ dom $H^0 =$ dom S [1] (the operator S is then called the *maximal part* of H^0 and H^Λ). Then the subspace gr $Q(z) - \Lambda$ is the graph of the invertible *operator* $Q(z) - L$, and $C^\Lambda(z) = (Q(z) - L)^{-1}$. Actually, for a *given* self-adjoint extension H one can find a boundary value space (which is, of course, not unique) such that H corresponds to the boundary conditions (5) with a suitable L [6, 8]. But finding such boundary value space involves a lot of other problems, in particular, the operators $Q(z)$ and γ_z must be changed [8, 10, 12]. On the other hand, any boundary conditions can be represented with the help of two matrices by

$$A\Gamma_1 \phi = B\Gamma_2 \phi \quad \Leftrightarrow \quad (\Gamma_1 \phi, \Gamma_2 \phi) \in \Lambda^{A,B} \tag{6}$$

with A and B satisfying (1) and (2). Our aim is to show that the resolvent formula admits a simple form in terms of these two boundary matrices. Here is the main result of our paper.

Proposition (modified Krein's resolvent formula). *Let $H^{A,B}$ be the self-adjoint extension of S corresponding to the boundary conditions (6) with A, B satisfying (1) and (2), and $z \in$ res $H^0 \cap$ res $H^{A,B}$, then*

(a) the matrices $Q(z)B^* - A^*$ and $BQ(z) - A$ are non-degenerate,
(b) the resolvent $R^{A,B}(z) = (H^{A,B} - z)^{-1}$ is connected with $R^0(z)$ by

$$R^{A,B}(z) = R^0(z) - \gamma_z B^*(Q(z)B^* - A^*)^{-1}\gamma_{\overline{z}}^*, \tag{7}$$

or

$$R^{A,B}(z) = R^0(z) - \gamma_z (BQ(z) - A)^{-1}B\gamma_{\overline{z}}^*. \tag{8}$$

Remark. Formulae (7) and (8) are equivalent. To obtain them from each other one should replace z by $\overline{z}$ and take in both sides adjoint operators taking into account the resolvent property $R(\overline{z}) = R^*(z)$ and the equality $Q(\overline{z}) = Q^*(z)$ which follows from (3).

First we prove some simple properties of the matrices A and B:

Lemma. *Let A, B satisfy (1) and (2), then*

(a) ker $A^* \cap$ ker $B^* = 0$,
(b) $\Lambda^{A,B} = \{(B^*x, A^*x), x \in V\}$.

Proof of lemma. (a) We first remark that condition (2) is equivalent to $\operatorname{ran} A + \operatorname{ran} B = V$. Then $\ker A^* \cap \ker B^* = (\operatorname{ran} A)^\perp \cap (\operatorname{ran} B)^\perp = (\operatorname{ran} A + \operatorname{ran} B)^\perp = V^\perp = 0$.

(b) Equation (1) says that $\{(B^*x, A^*x), x \in V\} \subset \Lambda^{A,B}$. At the same time, it follows from (a) that the linear subspace on the left-hand side has dimension n, which coincides with the dimension of $\Lambda^{A,B}$. Therefore, these two linear subspaces coincide. $\square$

Proof of proposition. (a) The matrices in question are adjoint to each other, therefore, it suffices to prove that one of them is non-degenerate.

Consider first the case $z \in \mathbb{C} \setminus \mathbb{R}$. As follows from (3), for such z the matrix $\operatorname{Im} z \cdot \operatorname{Im} Q(z)$ is positive definite (Here $\operatorname{Im} Q = (Q - Q^*)/(2\mathrm{i})$.) Assume that $\det(Q(z)B^* - A^*) = 0$, then there exists a non-zero $x \in V$ with

$$(Q(z)B^* - A^*)x = 0. \tag{9}$$

If $B^*x = 0$, then, due to item (a) of lemma, we would have $A^*x \neq 0$, and (9) would be impossible. Therefore, $B^*x \neq 0$. Taking the scalar product of B^*x with both sides of (9) we get $\langle Q(z)B^*x, B^*x \rangle = \langle x, AB^*x \rangle$. The number on the left-hand side has non-zero imaginary part, while the number on the right-hand side is real due to (2). This contradiction proves the requested non-degeneracy for non-real z.

Now let $z \in \mathbb{R} \cap \operatorname{res} H^0$ and $\det(Q(z)B^* - A^*) = 0$. Let us show that $z \in \operatorname{spec} H^{A,B}$. Equation (3) says that $Q(z)$ is now self-adjoint. As the matrix $Q(z)B^* - A^*$ is non-invertible, there is a non-zero $x \in \operatorname{ran}(Q(z)B^* - A^*)^\perp = \ker(BQ(z) - A)$. By definition, the element $\phi = \gamma_z x$ is an eigenvector of S^* corresponding to the eigenvalue z. Let us show that $\phi \in \operatorname{dom} H^{A,B}$ (and then z is an eigenvalue of $H^{A,B}$). In fact, one has $\Gamma_1 \phi = \Gamma_1 \gamma_z x = \Gamma_1 \Gamma_1^{-1} x = x$, $\Gamma_2 \phi = \Gamma_2 \gamma_z x = Q(z)x$, and, therefore, $A\Gamma_1 \phi - B\Gamma_2 \phi = -(BQ(z) - A)x = 0$, which means that $\phi \in \operatorname{dom} H^{A,B}$.

(b) Taking into account the remark after proposition it is enough to prove only (7). Actually, we must only show that for $z \in \operatorname{res} H^0 \cap \operatorname{res} H^{A,B}$ the linear relation inverse to $\operatorname{gr} Q(z) - \Lambda^{A,B}$ is the graph of $B^*(Q(z)B^* - A^*)^{-1}$. Taking into account item (b) of lemma, we conclude that $\operatorname{dom} Q(z) \cap \operatorname{dom} \Lambda^{A,B} = \operatorname{ran} B^*$ and $\operatorname{gr} Q(z) - \Lambda^{A,B} = \{(B^*u, (Q(z)B^* - A^*)u), u \in V\} = \{(B^*(Q(z)B^* - A^*)^{-1}w, w), w \in V\}$. $\square$

Let us consider some examples from the point of view of the resolvent formula.

Example (graph with a single vertex). Let $\mathcal{H} = \oplus_{j=1}^n \mathcal{H}_j$ with $\mathcal{H}_j = \mathcal{L}^2(\mathbb{R}_+^{(j)})$, where each $\mathbb{R}_+^{(j)}$ is a copy of the positive half-line $[0, +\infty)$. We will write the elements of $\phi \in \mathcal{H}$ in the vector form, $\phi(x) = (\phi_j(x_j))$, $\phi_j \in \mathcal{H}_j$, $x_j \in \mathbb{R}_+^{(j)}$. By S we denote an operator which acts on each $\mathcal{H}_j$ as $-\mathrm{d}^2/\mathrm{d}x_j^2$ with the domain $\operatorname{dom} S = \{\phi = (\phi_j), \phi_j \in W^{2,2}(\mathbb{R}_+^{(j)}), \phi_j(0) = \phi_j'(0) = 0, j = 1, \ldots, n\}$. Then S^* is the direct sum $\oplus_{j=1}^n \mathrm{d}^2/\mathrm{d}x_j^2$ with the domain $\oplus_{j=1}^n W^{2,2}(\mathbb{R}_+^{(j)})$. An integration by parts shows that as a boundary value space one can take $(\mathbb{C}^n, \Gamma_1, \Gamma_2)$ with $\Gamma_1 \phi = \Gamma_1(\phi_j) = (-\phi_j'(0)) \equiv -\phi'(0)$, $\Gamma_2 \phi = \Gamma_2(\phi_j) = (\phi_j(0)) \equiv \phi(0)$; details may be found in [5–7]. Then any self-adjoint extension of S involves the boundary conditions $A\phi'(0) + B\phi(0) = 0$ with suitable A and B, which describes the coupling of n half-lines at the origin. The operator H^0 defined by $\phi'(0) = 0$ is the direct sum of Neumann Laplacians, and its Green function (the resolvent integral kernel) $G^0(x, y; z)$ is given by

$$G^0(x, y; z) = \frac{1}{2\sqrt{-z}} \operatorname{diag}(\mathrm{e}^{-\sqrt{-z}|x_j - y_j|} + \mathrm{e}^{-\sqrt{-z}(x_j + y_j)}),$$

where the continuous branch of the square root is chosen by the rule $\operatorname{Re} \sqrt{z} > 0$ for $z \notin (-\infty, 0]$, and $x = (x_j)$, $y = (y_j)$, $x_j, y_j \in \mathbb{R}_+^{(j)}$. Then the elements $g_z^j = G^0(\cdot, 0; z)e_j = \mathrm{e}^{-\sqrt{-z}x}/\sqrt{-z}\, e_j$, (e_j) is the standard basis in $\mathbb{C}^n$, $j = 1, \ldots, n$, form a

basis in $\mathcal{N}_z = \ker(S^* - z)$, and the map γ_z defined by $\mathbb{C}^n \ni v = (v_j) \mapsto (v_j g_z^j)$ is the corresponding Γ-field, because $\Gamma_1 \gamma_z v = v$ for any $v \in \mathbb{C}^n$, and the Q-function has the simple form $Q(z) = 1/\sqrt{-z} E_n$, where E_n is the unit matrix of order n. Therefore, the resolvent for $H^{A,B}$ takes the form

$$R^{A,B}(z) = R^0(z) - \sum_{j,k=1}^{n} C_{jk}(z) \langle g_z^k, \cdot \rangle g_z^j$$

with $C(z) = (BQ(z) - A)^{-1} B = \sqrt{-z}(B - \sqrt{-z}A)^{-1} B$. A similar formula was obtained in [5].

Example (point interactions with mixed boundary conditions). Here we consider the well-known example of point interactions in three dimensions [2]. Let $Y = (y_1, \ldots, y_n) \subset \mathbb{R}^3$. Denote by S the Laplacian with the domain dom $S = \{\phi \in W^{2,2}(\mathbb{R}^3), \phi(Y) = 0\}$. This operator has deficiency indices (n, n), and the adjoint operator S^* is the Laplacian with the domain dom $S^* = W^{2,2}(\mathbb{R}^3 \backslash Y)$. Each function $\phi \in$ dom S^* has the following asymptotics near each point y_j, $j = 1, \ldots, n$:

$$\phi(x) = \frac{1}{4\pi |x - y_j|} \phi_j^1 + \phi_j^2 + o(1), \qquad x \to y_j, \quad \phi_j^1, \phi_j^2 \in \mathbb{C},$$

and the vectors $\Gamma_1 \phi = (\phi_j^1)$ and $\Gamma_2 \phi = (\phi_j^2)$ can be considered as boundary values of ϕ, see [3, 6, 13] for details. The operator H^0 is just the free Laplacian in $\mathbb{R}^3$. Denote by $G^0(x, y; z)$ its Green function, $G^0(x, y; z) = e^{-\sqrt{-z}|x-y|}/(4\pi |x - y|)$, then the functions $g_z^j = G^0(\cdot, y_j; z)$, $j = 1, \ldots, n$, form a basis in $\ker(S^* - z)$, and the map $\gamma_z : \mathbb{C}^n \ni v = (v_j) \mapsto \sum v_j g_z^j$ is the Γ-field (it is easy to check that $\Gamma_1 \gamma_z v = v$), and the Q-function is given by the $n \times n$ matrix

$$Q_{jk}(z) = G^0(y_j, y_k; z) = \frac{e^{-\sqrt{-z}|y_j - y_k|}}{4\pi |y_j - y_k|}, j \neq k, \qquad Q_{jj}(z) = -\frac{\sqrt{-z}}{4\pi}.$$

Therefore, the resolvent of the operator $H^{A,B}$ given by the boundary conditions $A\phi^1 = B\phi^2$ can be defined by its integral kernel

$$G^{A,B}(x, y; z) = G^0(x, y; z) - \sum_{j,k=1}^{n} C_{jk}(z) G^0(x, y_j; z) G^0(y_k, y; z)$$

with $C(z) = (BQ(z) - A)^{-1} B$. We remark that the class of interactions described by this formula is wider than the one studied in [2]. Some properties of $H^{A,B}$ in its dependence on A and B were studied recently in [13].

Acknowledgments

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