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First-order asymptotic perturbation theory for extensions of symmetric operators

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Abstract

This work offers a new prospective on asymptotic perturbation theory for varying self-adjoint extensions of symmetric operators. Employing symplectic formulation of self-adjointness, we use a version of resolvent difference identity for two arbitrary self-adjoint extensions that facilitates asymptotic analysis of resolvent operators via first-order expansion for the family of Lagrangian planes associated with perturbed operators. Specifically, we derive a Riccati-type differential equation and the first-order asymptotic expansion for resolvents of self-adjoint extensions determined by smooth one-parameter families of Lagrangian planes. This asymptotic perturbation theory yields a symplectic version of the abstract Kato selection theorem and Hadamard–Rellich-type variational formula for slopes of multiple eigenvalue curves bifurcating from an eigenvalue of the unperturbed operator. The latter, in turn, gives a general infinitesimal version of the celebrated formula equating the spectral flow of a path of self-adjoint extensions and the Maslov index of the corresponding path of Lagrangian planes. Applications are given to quantum graphs, periodic Kronig–Penney model, elliptic second-order partial differential operators with Robin boundary conditions, and physically relevant heat equations with thermal conductivity.

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Contents

1 | INTRODUCTION

1.1 | Overview

This work concerns first-order asymptotic expansions for resolvents and eigenvalues of self-adjoint extensions of symmetric operators subject to small perturbations of their operator theoretic domains. In the context of elliptic partial differential operators, for instance, the perturbations that we discuss model small variations of the boundary conditions, the spatial domains, and the lower order terms of differential expressions. Our main motivations stem from the Arnold–Keller–Maslov index theory, cf. [8, 9, 29, 35, 84, 103, 114], for self-adjoint elliptic differential operators and from the classical Hadamard–Rayleigh–Rellich [76, 109, 113] variation formulas for their eigenvalues. Our main new technical tool is a strikingly simple formula for the difference of resolvents of two arbitrary self-adjoint extensions of a symmetric operator derived in the context of abstract boundary triplets [13, 15, 50–57, 120] and inspired in part by a recent progress in description of all self-adjoint extensions of the Laplacian [66, 67, 69, 73, 75, 100]. This approach gives a powerful addition to the perturbation theory via quadratic forms as it allows one to control the resolvents and spectral projections of operators with varying domains.

In this paper, we study one-parameter *families* of self-adjoint extensions of densely defined symmetric operators. The main results of this work are twofold. First, we obtain new and quite general asymptotic expansion formulas for resolvents of self-adjoint operators determined by one-parameter differentiable families of Lagrangian planes, and derive a Riccati-type differential equation for the resolvents. From this, we derive a new abstract variational Hadamard-type formula for the slopes of eigenvalue curves bifurcating from a multiple discrete isolated eigenvalue of the unperturbed operator. Motivated by closely related Hadamard variation formulas for partial differential operators on varying domains, we use the term *Hadamard-type* for formulas giving t-derivatives of the eigenvalues of abstract and differential t-dependent operators treated in this paper. Our second major set of results uses the Hadamard-type formulas to bridge the celebrated Atiyah–Patodi–Singer theory and the Maslov index theory as they relate the spectral flow of a family of self-adjoint extensions to the Maslov index of the corresponding path of Lagrangian planes. We give a proof of an infinitesimal version of this relation in a very general abstract setting where all three objects may vary: the domains of the self-adjoint extensions, the boundary traces, and the operators per se. On a more technical level, we systematically use a version of the formula for the difference of resolvent operators of two arbitrary self-adjoint extensions of a given symmetric operator. Specifically, we express this difference in terms of orthogonal projections onto Lagrangian planes uniquely associated with the self-adjoint extensions in question and thus offer a novel point of view on the resolvent difference formulas through the prism of symplectic functional analysis.

The asymptotic perturbation theory is a gem of classical mathematical physics [83, Chapter VIII]. Given a family of, generally, unbounded operators $H_t = H_{t_0} + H^{(1)}_{t_0}(t - t_0) + \dots$ depending on a parameter $t \in [0, 1]$ and considered as perturbations of a fixed operator H_{t_0}, the theory provides, for t near t_0, formulas for the resolvent operators of H_t, for the Riesz projections on a group of isolated eigenvalues of H_t, as well as the asymptotic expansions of the type $\lambda_j(t) = \lambda + \lambda^{(1)}_j(t - t_0) + \dots$ for the semisimple eigenvalues $\lambda_j(t)$, $1 \leqslant j \leqslant m$, of H_t bifurcating from an eigenvalue $\lambda = \lambda(t_0)$ of H_{t_0} of multiplicity m. Of course, it is not always the case that H_t is an additive perturbation of H_{t_0}; a simple example being the Neumann Laplacian considered as a perturbation of the Dirichlet Laplacian posted on the same open set $\Omega \subset \mathbb{R}^n$. Operator-theoretical domains of the two operators are given by the Neumann and Dirichlet boundary traces. The difference of the two operators on the intersection of their domains is zero, and thus, neither of them is an additive perturbation of the other. When the operators are posted on a t-dependent family of open sets Ω_t and, in addition, are subject to perturbations by a family of t-dependent potentials, we are facing the situation when all three objects (the boundary traces, the boundary conditions prescribing the domains of the operators, and the operators per se) are being perturbed. And yet the fundamental questions remain of how to relate their resolvent operators, eigenvalues, and so on.

To answer the questions, we employ the extension theory for symmetric operators that goes back to M. Birman [25], M. Krein [87, 88], and M. Vishik [124], see also [5, 57, 71, 120], and that has been an exceptionally active area of research [1, 7, 14, 18, 20, 30, 55, 71, 102, 106] culminating in the comprehensive monograph [13]. Unlike the classical sesquilinear forms-based approach utilized in analytic perturbation theory, see, for example, [83, Section VII.6.5], the foundational for the current paper result is a very simple formula for the difference of the resolvents of any two self-adjoint extensions of a symmetric operator. The classical Krein's formula going back to [87, 88] expresses the difference of the resolvents of a special, "Dirichlet-type," self-adjoint extension and yet another, arbitrary, self-adjoint extension of a symmetric operator via the γ-field and the abstract Weyl M-function. Given any two arbitrary self-adjoint extensions, the classical Krein's formula is a powerful tool that has been used to prove, for example, that the difference of the resolvents of the two extensions belongs to the appropriate Schatten-von Neumann class, cf. for example, [55, Theorem 2 and Corollary 4].

In the current paper, we give a very elementary and direct proof (without using the Krein's formula) of the resolvent difference formula of any two arbitrary self-adjoint extensions that we were not able to find in the literature. Unlike Krein's resolvent formula, the resolvent difference formula that we offer does not contain the γ-fields nor the Weyl function, and thus is of much lower level than the celebrated Krein's resolvent formula. However, it appears to be a perfect tool for studying *families* of self-adjoint extensions constructed by means of *families* of Lagrangian planes and *families* of trace operators, which is the main objective of our work. Indeed, variation formulas for eigenvalues of differential operators posted on a one-parameter family of domains are typically obtained for differential operators defined via Dirichlet forms, see, for example, [83, Section VII. 6.5], [64], which essentially restricts the set of admissible boundary conditions to Dirichlet, Neumann, and Robin. We drop this restriction by avoiding the quadratic form approach and, instead, dealing with perturbations of self-adjoint extensions through our new symplectic version of the resolvent difference formula thus deriving the Hadamard-type eigenvalue formulas in a quite general setting.

The Hadamard-type formulas are instrumental in applications of spectral theory to differential operators. For example, they recently played a pivotal role in the works of G. Berkolaiko, P. Kuchment, and U. Smilansky [23] and G. Cox, C. Jones, and J. Marzuola [45, 46] on nodal count for eigenfunctions of Schrödinger operators and in the work of A. Hassell [78] on ergodic billiard systems that are not quantum uniquely ergodic. The formulas are also central to the applications that we give, in particular, to our treatment, discussed in more details below, of the periodic Kronig–Penney model, spectral flow formulas for one-parameter families of Robin Laplacians leading to a unified approach to Friedlander's and Rohleder's inequalities, of the heat equation posted on bounded domains, and of one-parameter families of quantum graphs.

1.2 | Description of abstract results

We consider self-adjoint extensions of a closed densely defined symmetric operator A acting in a Hilbert space $\mathcal{H}$. The extensions in question are defined by Lagrangian planes in an auxiliary (boundary) Hilbert space $\mathfrak{H}\times\mathfrak{H}$ by means of a two component trace map $\mathrm{T}=[\Gamma_0,\Gamma_1]^\top$: $\mathrm{dom}(\mathrm{T})\subset\mathcal{H}\to\mathfrak{H}\times\mathfrak{H}$ with dense range and satisfying the abstract Green identity

$$\langle A^*u,v\rangle_{\mathcal{H}}-\langle u,A^*v\rangle_{\mathcal{H}}=\langle J\mathrm{T}u,\mathrm{T}v\rangle_{\mathfrak{H}\times\mathfrak{H}},u,v\in\mathrm{dom}(\mathrm{T}),\ J:=\begin{bmatrix}0 & I_{\mathfrak{H}}\\ -I_{\mathfrak{H}} & 0\end{bmatrix}. \tag{1.1}$$

The trace operator T, geared to facilitate abstract integration by parts arguments, is a central object in our setting.

A typical realization of this setup is given by the Laplace operator $A := -\Delta$ with domain $\mathrm{dom}(A) = H_0^2(\Omega)$ acting in $\mathcal{H} := L^2(\Omega)$ and the trace map $\mathrm{T}u = (u \restriction_{\partial\Omega}, -\Phi\partial_\nu u \restriction_{\partial\Omega})^\dagger$ defined on $\mathrm{dom}(\mathrm{T}) = \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\}$. In this case, $A^* = -\Delta$ with the domain $\mathrm{dom}(A^*) = \{u \in L^2(\Omega) : \Delta u \in L^2(\Omega)\}$, the boundary space $\mathfrak{H} = H^{1/2}(\partial\Omega)$, and (1.1) is the standard Green identity. Equipping $\mathcal{H}_+ := \mathrm{dom}(A^*)$ with the graph norm of the Laplacian and $\mathcal{D} := \mathrm{dom}(T)$ with the norm $(\|u\|^2_{H^1(\Omega)} + \|\Delta u\|^2_{L^2(\Omega)})^{1/2}$, we get a crucial dense embedding $\mathcal{D} \hookrightarrow \mathcal{H}_+$. This embedding becomes equality in the one-dimensional setting when $\Omega = [a, b] \subset \mathbb{R}$; in fact, one has $\mathcal{H}_+ = \mathcal{D} = H^2([a, b])$.

Motivated by this example and returning to the abstract setting, we equip $\mathcal{D} = \mathrm{dom}(\mathrm{T})$ with an abstract Banach norm $\|\cdot\|_{\mathcal{D}}$, the space $\mathcal{H}_+ = \mathrm{dom}(A^*)$ with the graph norm of A^*, and assume that the embedding $\mathcal{D} \hookrightarrow \mathcal{H}_+$ is dense and bounded. Drawing further parallels between the abstract and the PDE/ODE settings, throughout this work, we distinguish between the strict inclusion $\mathcal{D} \subsetneq \mathcal{H}_+$ and the equality $\mathcal{D} = \mathcal{H}_+$. The case when $\mathcal{D}$ is strictly contained in $\mathcal{H}_+$ is closely related to the setting considered in the pioneering paper by V. Derkach and M. Malamud [56], where the concept of generalized (in fact, B–generalized) triplet was originally introduced and applied to the inverse problem of realization of Nevanlinna functions. This case is also closely related to the notion of quasi-boundary triplets extensively studied in the work of J. Behrndt and M. Langer [14, 15], J. Behrndt and T. Micheler [18], and V. Derkach, S. Hassi, M. Malamud, and H. de Snoo [50–54]. In case when $\mathcal{D} = \mathcal{H}_+$, the triplet $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is called the *ordinary boundary triplet*. This case is understood much better and was developed, in particular, in the classical work by V. Gorbachuk and M. Gorbachuk [71] and A. Kochubej, by V. Derkach and M. Malamud [55], and many others, see, for example, [13, 15, 54, 57, 120] and the extensive bibliography therein. The main reason why we consider a nonsurjective embedding $\mathcal{D} \hookrightarrow \mathcal{H}_+$ is that, when applied to elliptic operators, it allows one to use the standard Dirichlet and Neumann trace operators as components of T and therefore discuss physically relevant boundary value problems (e.g., heat equation on bounded domains). The disadvantage of the condition $\mathcal{D} \subsetneq \mathcal{H}_+$, however, is that it restricts the class of admissible self-adjoint extensions of A to those with domains containing in $\mathcal{D}$. We refer to [34, 50–54, 79, 126] for an in-depth study of unbounded traces and stress that abstract results of this type are not the main focus of the current work. On the other hand, the case of ordinary boundary triplets $\mathcal{D} = \mathcal{H}_+$ covers all possible self-adjoint extensions at the expense of dealing with the trace map T which, when considered in the context of second-order elliptic partial differential operators, is a nonlocal first-order operator on the boundary of the spatial domain. The trace maps of this type have been studied, in particular, by G. Grubb [73], H. Abels, G. Grubb, and I. Wood [1], and F. Gesztesy and M. Mitrea [67–69].

The ordinary boundary triplets are particularly well suited for ordinary differential operators and quantum graphs; we will exploit this in Section 4. Our approach allows one to obtain some new results that are not reachable or very hard to obtain using other methods such as the quadratic forms. This includes our arguably new Riccati-type differential equations for the resolvents, our ability to handle quite general boundary conditions for quantum graphs where the form method results are not known, our new and convenient formulas for the slopes of the eigenvalue curves for both quantum graphs with general boundary conditions and the PDE operators, as well as our

† where Φ denotes natural Riesz isomorphism $\Phi \in \mathcal{B}(H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega))$ as defined in (4.21).

ability to handle nonlocal boundary conditions (even of generalized Robbin type but also such as those that appear in describing Krein's self-adjoint extensions of PDE operators).

Having introduced the notion of an abstract trace map and Green identity (1.1), we switch to a symplectic version of the resolvent difference formula. We note that the right-hand side of (1.1) can be written as $\omega(\mathrm{T}u, \mathrm{T}w)$, where $\omega(\cdot,\,\cdot) = \langle J\cdot,\,\cdot\rangle_{\mathfrak{H}}$ is the natural symplectic form. It is well known that self-adjoint extensions of A in $\mathcal{H}$ can be described by Lagrangian planes in various symplectic Hilbert boundary spaces. W. N. Everitt and W. N. Markus [59] and B. Booss-Bavnbek and K. Furutani [26], for example, relate self-adjoint extensions to Lagrangian subspaces of the symplectic quotient space $\mathrm{dom}(A^*)/\,\mathrm{dom}(A)$, while J. Behrndt and M. Langer [18], K. Pankrashkin [106], and K. Schmüdgen [120, Chapter 14] and [13], on the other hand, discuss self-adjointness in terms of linear relations. Closely following these works, we utilize the abstract Green identity (1.1) assuming (possibly, nonsurjective) embedding $\mathcal{D} \hookrightarrow \mathcal{H}_+$, and associate self-adjoint extensions $\mathcal{A}$ of A to Lagrangian planes $\mathcal{F} \subset \mathfrak{H} \times \mathfrak{H}$ via the mapping $\mathrm{dom}(\mathcal{A}) \mapsto \mathcal{F} := \overline{\mathrm{T}(\mathrm{dom}(\mathcal{A}))}$, see Theorems A.1 and A.2 and Corollary A.5 for more details on this correspondence. This observation brings us one step closer to the perturbation theory for self-adjoint extensions with continuously varying domains of self-adjointness as it allows us to recast this nonadditive perturbation problem in terms of the perturbation of Lagrangian planes, or more specifically, in terms of perturbation of the orthogonal projections onto the planes.

A major issue in perturbation theory for unbounded operators with varying domains is that their difference could be defined on a potentially very small subspace, for example, on the zero subspace. This issue is not as severe when one talks about self-adjoint extensions $\mathcal{A}_1, \mathcal{A}_2$ of the same operator A, since $\mathrm{dom}(A) \subset \mathrm{dom}(\mathcal{A}_1) \cap \mathrm{dom}(\mathcal{A}_2)$ but there is still a caveat: the difference $\mathcal{A}_1 - \mathcal{A}_2$ could be the zero operator; hence, $\mathcal{A}_1$, $\mathcal{A}_2$ could be trivial additive perturbations of one another (again, think about the Dirichlet and Neumann realizations of the second derivative on a segment). To deal with this issue, one considers instead of $\mathcal{A}_1 - \mathcal{A}_2$ the difference of the *resolvents* $(\mathcal{A}_1 - \zeta)^{-1} - (\mathcal{A}_2 - \zeta)^{-1}$ and, classically, expresses it in terms of the abstract Weyl M-function, see Appendix B and, in particular, Proposition B.1 for a brief reminder of this topic. Such an expression is called the *Krein (or Krein–Naimark) resolvent formula*; we refer to [87, 88] and [89, 90].

This foundational result in spectral theory has been studied and derived in various settings by many authors; we refer to the texts [2, 13, 120] where one can find a detailed historical account and further bibliography. Without even attempting to give a review of the vast literature on this subject, we mention here the work by H. Abels, G. Grubb, and I. Wood [1], W.O Amrein and D.B. Pearson [6], S. Albeverio and K. Pankrashkin [4], J. Behrndt and M. Langer [14], S. Clark, F. Gesztesy, R. Nichols, and M. Zinchenko [41], V. Derkcach and M. Malamud [55, 57], F. Gesztesy and M. Mitrea [67–69], G. Grubb [74], A. Posilicano [107], and A. Posilicano and L. Raimondi [108]. We specifically mention important contribution for the case of quasi-boundary triplets in [14, Theorem 5.1] and in more complete form in Theorem 6.16 and Corollary 6.17 of [15]; for generalized boundary triplets of bounded type in Theorem 7.26 and Proposition 7.27 of the paper [54] by V. Derkach, S. Hassi and M. Malamud; for so-called AB-generalized boundary triplets (which covers the previous two cases) in Theorem 4.12, Remark 4.13, and Corollary 4.14 of [51]. In addition, in a recent paper [52] by V. Derkach, S. Hassi, and M. Malamud (see also [50]), the authors studied boundary triplets and gave an analytic characterization of their Weyl functions as form domain invariant Nevanlinna functions. These papers contain applications of boundary triplets techniques closely related to the results in Sections 4.2 and 5.1 of the present paper. Most closely related to our work is the Krein formula for two arbitrary self-adjoint extensions of the Laplace operator expressing the resolvent difference in terms of an operator-valued Herglotz function that has been obtained in [69], see also [66, 67, 100, 105].

However, all above-mentioned Krein-type formulas are not quite suited for the purposes of the current paper as they do not capture quantitatively the perturbations of operator-theoretic domains of the self-adjoint extensions in the form that we need. One of the main objectives of the current work is to address this issue. Specifically, we propose to use a very elementary new *resolvent difference formula* expressing the difference of the resolvents of two arbitrary self-adjoint extensions of a given symmetric operator in terms of the *projections onto the Lagrangian planes* determining the domains of the extensions. As far as we can see this simple but extremely handy version of the formula was not widely used in the literature in the generality that we offer, see, however, already mentioned [55, Theorem 2 and Corollary 4].

Indeed, for arbitrary self-adjoint extensions $\mathcal{A}_1, \mathcal{A}_2$ of a symmetric operator A, we obtain the following symplectic version of the formula for the difference of resolvents $R_1(\zeta) = (\mathcal{A}_1 - \zeta)^{-1}$ and $R_2(\zeta) = (\mathcal{A}_2 - \zeta)^{-1}$,

$$R_1(\zeta) - R_2(\zeta) = (\mathrm{T}R_2(\overline{\zeta}))^* Q_2 J Q_1(\mathrm{T}R_1(\zeta)), \tag{1.2}$$

where $\zeta \notin \mathrm{Spec}(\mathcal{A}_1) \cup \mathrm{Spec}(\mathcal{A}_2)$, J is the symplectic matrix from (1.1), $Q_1, Q_1 \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H})$ are the orthogonal projections onto the Lagrangian planes $\mathcal{F}_1, \mathcal{F}_2 \subset \mathfrak{H} \times \mathfrak{H}$ defining the self-adjoint extensions $\mathcal{A}_1, \mathcal{A}_2$ via $\mathcal{F}_1 = \overline{\mathrm{T}(\mathrm{dom}(\mathcal{A}_1))}$, $\mathcal{F}_2 = \overline{\mathrm{T}(\mathrm{dom}(\mathcal{A}_2))}$. In particular, using the property $Q_1 J Q_1 = 0$, a key property of projections onto Lagrangian planes, formula (1.2) yields

$$R_2(\zeta) - R_1(\zeta) = (\mathrm{T}R_2(\overline{\zeta}))^* (Q_2 - Q_1) J Q_1(\mathrm{T}R_1(\zeta)), \tag{1.3}$$

which indicates that $\|R_2(\zeta) - R_1(\zeta)\|_{\mathcal{B}(\mathcal{H})} \to 0$ whenever $\|Q_2 - Q_1\|_{\mathcal{B}(\mathfrak{H}\times\mathfrak{H})} \to 0$, see Theorem 2.6. Also, we rewrite the resolvent difference formula (1.3) in terms of bounded operators $X_k, Y_k \in \mathcal{B}(\mathfrak{H})$ chosen such that $\mathcal{F}_k = \ker[X_k, Y_k]$, $k = 1, 2$, see (2.15).

Relying on the resolvent difference formula (1.3), we investigate differentiability properties and obtain asymptotic expansion for resolvent operators as functions of a scalar parameter $t \in [0, 1]$ parametrizing sufficiently smooth paths of Lagrangian planes $t \mapsto \mathcal{F}_t$, additive bounded self-adjoint perturbations $t \mapsto V_t \in \mathcal{B}(\mathcal{H})$, and trace maps $t \mapsto \mathrm{T}_t$ satisfying Green identity (1.1). That is, we develop a full-scale first-order asymptotic theory for a one-parameter family of self-adjoint operators $H_t := \mathcal{A}_t + V_t$, with $\mathcal{A}_t$ being a self-adjoint extension of A associated with the Lagrangian plane $\mathcal{F}_t$ via the relation $\overline{\mathrm{T}_t(\mathrm{dom}(\mathcal{A}_t))} = \mathcal{F}_t$. First, we prove that, respectively, continuity, Lipschitz continuity, and differentiability at $t_0 \in [0, 1]$ of the paths of Lagrangian planes, bounded perturbations, and trace maps, yield continuity, Lipschitz continuity, and differentiability, respectively, of the path of resolvent operators $t \mapsto R_t(\zeta) := (H_t - \zeta)^{-1}$, $\zeta \notin \mathrm{Spec}(H_{t_0})$. At the first glance, such results should seemingly follow from the resolvent difference formula (1.3) as it suggests that $R_t(\zeta) - R_{t_0}(\zeta)$ and $Q_t - Q_{t_0}$ are of the same order. It turns out, however, that the boundedness of the appropriate norm of $TR_t(\zeta)$ for t near t_0 could be a subtle issue depending on whether we are dealing with the strict inclusion $\mathcal{D} \subsetneq \mathcal{H}_+$ or the equality $\mathcal{D} = \mathcal{H}_+$.

Let us elaborate on this in more detail. First, the operator $TR_t(\zeta)$ is bounded as a linear mapping from $\mathcal{H}$ to $\mathfrak{H} \times \mathfrak{H}$, that is, $TR_t(\zeta) \in \mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H})$ even without assuming that $\mathcal{D} = \mathrm{dom}(\mathrm{T})$ is equipped with its own Banach norm, see Lemma 2.4. When it is, however, we claim more: $\mathrm{T} \in \mathcal{B}(\mathcal{D}, \mathfrak{H} \times \mathfrak{H})$ and $R_t(\zeta) \in \mathcal{B}(\mathcal{H}, \mathcal{D})$, see Proposition 3.2. The main issue is that in the abstract setting, one does not have a good quantitative control of the norm $\|R_t(\zeta)\|_{\mathcal{B}(\mathcal{H},\mathcal{D})}$ as a function of

t. We therefore impose the assumption

$$\|R_t(\zeta)\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} \underset{t\to t_0}{=} \mathcal{O}(1). \tag{1.4}$$

That being said, condition (1.4) is automatically satisfied when the strict inclusion $\mathcal{D} \subsetneq \mathcal{H}_+$ is replaced by the equality $\mathcal{D} = \mathcal{H}_+$, in which case we show not only boundedness (1.4) but also continuity of the reslovent operators

$$\|R_t(\zeta) - R_{t_0}(\zeta)\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} \underset{t\to t_0}{=} o(1), \tag{1.5}$$

see Proposition 4.4. We stress that (1.4) is a natural assumption for the case when $\mathcal{D} \subsetneq \mathcal{H}_+$. This assumption is satisfied, although not trivially, in many PDE contexts of interest as its proof essentially boils down to controlling $L^2(\Omega)$ to $H^1(\Omega)$ norm of the resolvent of a second-order elliptic operator for t near t_0, see Section 5.2 where we check it for elliptic operators subject to Robin boundary conditions. To sum up, the resolvent difference formula (1.3) together with hypothesis (1.4) yields continuity of the resolvent operators $t \mapsto R_t(\zeta)$. The differentiability requires not only (1.4) but actually (1.5) that we impose as an assumption when $\mathcal{D} \subset \mathcal{H}_+$. As we already pointed out (1.5) holds automatically if $\mathcal{D} = \mathcal{H}_+$ and it holds in most standard PDE realizations of a more general situation $\mathcal{D} \subsetneq \mathcal{H}_+$.

Having discussed differentiability of the mapping $t \mapsto R_t(\zeta)$, we now switch to first-order asymptotic expansions of the resolvents. The main goal of this part of the paper is to derive an Hadamard-type formula[†] for derivatives of the eigenvalues curves of H_t. As a first step, we derive in Theorem 3.18 the following asymptotic expansion for the resolvent:

$$\begin{aligned} R_t(\zeta) \underset{t\to t_0}{=} R_{t_0}(\zeta) + \Big(&-R_{t_0}(\zeta)\dot{V}_{t_0}R_{t_0}(\zeta) + (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}R_{t_0}(\zeta) \\ &+ (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta)\Big)(t-t_0) + o(t-t_0), \text{ in } \mathcal{B}(\mathcal{H}); \end{aligned} \tag{1.6}$$

here and throughout the paper, $\frac{d}{dt}$ is abbreviated by the dot, for example, $\dot{V}_{t_0} = \frac{dV}{dt}|_{t=t_0}$. In particular, we deduce a new Riccati-type differential equation for the resolvents,

$$\begin{aligned} \dot{R}_{t_0}(\zeta) = -R_{t_0}(\zeta)\dot{V}_{t_0}R_{t_0}(\zeta) &+ (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}R_{t_0}(\zeta) \\ &+ (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta). \end{aligned}$$

Next, we compute the slopes of eigenvalue curves $\{\lambda_j(t)\}_{j=1}^m$ bifurcating from an isolated eigenvalue $\lambda \in \operatorname{Spec}(H_{t_0})$ of multiplicity $m \geqslant 1$. Our strategy is to integrate (1.6) over a contour $\gamma \subset \mathbb{C}$ enclosing the eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ for t near t_0, obtain an asymptotic expansion for the m-dimensional operator $P(t)H_tP(t)$, where $P(t)$ is the Riesz projector onto the spectral subspace $\operatorname{ran}(P(t)) = \bigoplus_{j=1}^m \ker(H_t - \lambda_j(t))$, and reduce matters to asymptotic perturbation techniques for finite-dimensional self-adjoint operators. Specifically, we employ the body of finite-dimensional results from Theorem II.5.4 and Theorem II.6.8 of [83]. In the literature

[†] As we have already noted above, we borrow the term *Hadamard-type formula* from the PDE literature on geometric perturbations of spatial domains and use it for general formulas for derivatives of eigenvalues.

on Maslov index and spectral flow, these results are called the *Kato selection theorem*, cf. [114, Theorem 4.28], as they allow one to properly choose the m branches of the eigenvalue curves for $P(t)H_tP(t)$ and compute their slopes. A subtle issue in this scheme, though, is that the finite-dimensional operators $P(t)H_tP(t)$ are defined on varying t-dependent spaces $\operatorname{ran}(P(t))$. As in [96], we remedy this by introducing a differentiable family of unitary operators $t \mapsto U_t$, cf. (3.26), (3.27), mapping $\operatorname{ran}(P(t_0))$ onto $\operatorname{ran}(P(t))$ and obtain the first-order expansion for unitarily equivalent to $P(t)H_tP(t)$ operators acting in a fixed finite-dimensional space $\operatorname{ran}(P(t_0))$, see Lemma 3.24. Finally, utilizing this expansion and the Kato selection theorem, we show that there is a proper labeling of the eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of H_t for t near t_0 and an orthonormal basis $\{u_j\}_{j=1}^m \subset \ker(H_{t_0} - \lambda)$ such that the following Hadamard-type formula holds,

$$\dot{\lambda}_j(t_0) = \langle \dot{V}_{t_0} u_j, u_j \rangle_{\mathcal{H}} + \omega(\dot{Q}_{t_0} \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j) + \omega(\mathrm{T}_{t_0} u_j, \dot{\mathrm{T}}_{t_0} u_j), 1 \leqslant j \leqslant m, \tag{1.7}$$

where $\omega(f, g) = \langle Jf, g \rangle_{\mathfrak{H}\times\mathfrak{H}}$, $f, g \in \mathfrak{H} \times \mathfrak{H}$ is the symplectic form. This quite general result is one of the major points of the paper; we apply it in several particular situations.

Also, we use this computation to give an infinitesimal version of a general abstract analog of the classical formula, cf. [26, 29, 35], relating the following two quantities: (1) the Maslov index of the path $t \mapsto \mathcal{F}_t \oplus \mathrm{T}\big(\ker\big(A^* + V_t - \lambda\big)\big)$ relative to the diagonal plane in $\mathfrak{H} \times \mathfrak{H}$, and (2) the spectral flow of the family $t \mapsto H_t$ through λ for t near t_0. Heuristically, the latter quantity is given by the difference between the number of monotonically increasing and decreasing eigenvalue curves of H_t bifurcating from λ. The former quantity is equal to the signature of the Maslov form that is a certain bilinear form defined on $\mathrm{T}\big(\ker(H_{t_0} - \lambda)\big)$, see Sections 4.5 and 5.5. In order to relate the two, we prove by computation that, in fact, the value of the Maslov crossing form coincides with the right-hand side of (1.7), cf. Theorem 4.22 and Proposition 5.8. Similar relations have been established, in particular, by G. Cox, C.K.R.T. Jones, and J. Marzuola in [45, 46], B. Booß-Bavnbek, C. Zhu [29], B. Booß-Bavnbek, K. Furutani [26], and P. Howard and A. Sukhtayev [81, 82]. The computational and applied aspects of the Maslov index theory have recently been considered by F. Chardard, F. Dias, and T. J. Bridges [36–39]

In a later part of the paper, we also give a generalization of the resolvent difference formula to the case of *adjoint pair* of operators, see, for example, [1, 30, 32] and the literature cited therein. Important contributions to the theory of adjoint pairs can be found in [7, 31, 102]. It allows one to describe nonselfadjoint extensions for an adjoint pair of densely defined closed (but not necessarily symmetric) operators. A typical example of the adjoint pair is given by a nonsymmetric elliptic second-order partial differential operator and its formal adjoint; this example is also discussed in the paper.

1.3 | Summary of applications

Our applications are given in Sections 4 and 5. In Section 4, we collected all results pertaining the ordinary boundary triplets (covering the case of metric graphs, and “rough” PDE traces). This section also provides more applications of the asymptotic expansions of resolvents in the context of ordinary boundary triplets obtained by the authors in [94]. In Section 5, we deal with more general case of densely defined not surjective traces (which covers the “weak” PDE traces). Our main applications are to spectral count for Robin Laplacians on bounded domains, periodic Kronig–Penney models, Hadamard-type formulas for Schrödinger operators on metric graphs, and heat equation posted on bounded Lipschitz domains. Let us succinctly describe relevant results.

• We prove that for Baire almost every periodic sequence of coupling constants $\alpha = \{\alpha_k\}_{k=1}^{\infty} \in \ell^{\infty}(\mathbb{Z}, \mathbb{R})$, the spectrum of the Schrödinger operator H_α acting in $L^2(\mathbb{R})$ and given by

$$H_\alpha := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{k\in\mathbb{Z}} \alpha_k \delta(x-k),$$

has no closed gaps, see Section 4.4. The analogous assertion for Schrödinger operators $H_V = -\frac{d^2}{dx^2} + V$ for periodic $V \in C^{\infty}(\mathbb{R})$ (due to B. Simon [121]) and their discrete versions have been instrumental in the works of D. Damanik, J. Fillman, and M. Lukic [48] and A. Avila [11], correspondingly, on Cantor spectra for generic limit-periodic Schrödinger operators. As in [121], we prove this statement by perturbation arguments applied to the Hill equation on a finite interval associated with H_α (an alternative approach covering a wide class second-order differential operators is proposed in the work of D. Damanik, J. Fillman, and the second author).

• For a general elliptic second-order operator $\mathcal{L} := -\operatorname{div}(\mathtt{A}\nabla) + \mathtt{a}\cdot\nabla - \nabla\cdot\mathtt{a} + \mathtt{q}$ posted on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^d$, $d \geqslant 2$, see Section 5.1, and subject to a one-parameter family of Robin conditions $\partial_\nu u = \Theta_t u$ on $\partial\Omega$, we derive Hadamard- and resolvent difference formulas, see Theorem 5.2, and use these results to discuss in Section 5.2 a unified approach to L. Friedlander's and J. Rohleder's inequalities via a spectral flow argument, see [62, 116] and [46].

• For an arbitrary compact metric graph $\mathcal{G}$ and the Schrödinger operator $H_t = -\frac{d^2}{dx^2} + V$ subject to parameter-dependent vertex conditions $X_t u + Y_t \partial_n u = 0$ (here $\partial_n u$ is the derivative of u taken in the inward direction along each edge), we derive the following Hadamard-type formula for the slopes of eigenvalue curves $\{\lambda_j(t)\}_{j=1}^m$ bifurcating from an eigenvalue of H_{t_0} of multiplicity $m \geqslant 1$,

$$\dot{\lambda}_j(t_0) = \langle \dot{V}_{t_0} u_j, u_j \rangle_{L^2(\mathcal{G})} + \left\langle (X_{t_0}\dot{Y}_{t_0}^* - Y_{t_0}\dot{X}_{t_0}^*)\phi_j, \phi_j \right\rangle_{L^2(\partial\mathcal{G})}, \tag{1.8}$$

where $\{u_j\}_{j=1}^m$ is a certain orthonormal basis of $\ker(H_{t_0} - \lambda(t_0))$, ϕ_j is a unique vector in $L^2(\partial\mathcal{G})$ satisfying $u_j = -Y_{t_0}^*\phi_j$ and $\partial_n u_j = X_{t_0}^*\phi_j$, $1 \leqslant j \leqslant m$, see Section 4.3. In the theory of quantum graphs, Hadamard-type formulas are often derived on a case-by-case basis for simple eigenvalue curves, see, for example, a classical monograph by G. Berkolaiko and P. Kuchment [21, Section 3.1.4.]; (1.8) closes this gap in the literature. In addition, we derive a resolvent difference formula expressing the difference of two arbitrary self-adjoint realizations of the Schrödinger operator in terms of the vertex matrices X_j, Y_j, $j = 1, 2$.

• For the heat equation

$$\begin{cases} u_{\mathrm{t}}(\mathrm{t}, x) = \kappa\rho(x)\Delta_x u(\mathrm{t}, x), x \in \Omega, \mathrm{t} \geqslant 0, \\ -\kappa\frac{\partial u}{\partial n} = u, \text{ on } \partial\Omega, \end{cases}$$

describing the temperature u of a material in the region $\Omega \subset \mathbb{R}^3$ with thermal conductivity κ immersed in a surrounding medium of zero temperature (here $1/\rho(x)$ is the product of the density of the material times its heat capacity), we give a new proof of continuous dependence of u on κ with respect to $L^2(\Omega)$ norm, see Section 5.3.

The symplectic (Lagrangian) point of view on self-adjoint extensions and boundary triplets systematically used in this paper (and a more general approach via Krein spaces, cf. [53]) is a quite powerful tool that, of course, brings up many new and unresolved issues. Among the open questions we mention: finding a symplectic interpretation of the abstract Weyl's function; describing exit-space extensions using symplectic approach; studying (in the context of self-adjoint extensions) so-called lateral perturbations introduced in [22]; and relating Hadamard-type formulas to the secular equations [21] for quantum graphs.

Organization of the paper. In Section 2, we begin with basic setup and discuss properties of the trace operators and their composition with the resolvents for the general case when the embedding $\mathcal{D} \hookrightarrow \mathcal{H}_+$ is not surjective. The most general symplectic resolvent difference formula for the difference of resolvents of any two self-adjoint extensions is proven in Theorem 2.6. In Section 3.1, we discuss our main setup and assumptions on one-parameter families of traces, self-adjoint extensions, and bounded perturbations, and provide typical examples when our assumptions are satisfied. The examples include: Schrödinger operators with Robin-type boundary conditions on families of star-shaped domains, second-order operators on infinite cylinders with variable multidimensional cross-sections, operators arising as Floquet–Bloch decomposition of periodic Hamiltonians, and first-order elliptic operators of Cauchy–Riemann type on cylinders. In Section 3.2, we obtain general resolvent expansions and derive the Riccati equations for the resolvent operators. The variational Hadamard-type formula for the eigenvalue curves is proven in Section 3.3. This section also contains resolvent difference formulas for families of self-adjoint extensions given by either families of projections in the boundary space $\mathfrak{H} \times \mathfrak{H}$ or as kernels of the bounded row operators $[X_t, Y_t]$. In Section 4.1, we formulate our major results for the case $\mathcal{D} = \mathcal{H}_+$, that is, for the ordinary boundary triplets. As an example, we treat the ODE case of Robin boundary conditions on a segment. In Section 4.2, we study Robin Laplacian on multidimensional domains in the framework of the boundary triplets that requires the use of the "rough" traces. Section 4.3 is devoted to applications to quantum graphs, here, in particular, we derive Hadamard-type formula (1.8). The periodic Kronig–Penney model is considered in Section 4.4. In Section 4.5, we begin discussion on connections to the Maslov index and prove a general result relating the value of the Maslov crossing form and the slope of the eigenvalue curves for ordinary boundary triplets. In Section 5.1, we switch to the second-order elliptic operators, return back to the case $\mathcal{D} \subsetneq \mathcal{H}_+$, and use weak boundary traces. Hadamard-type and resolvent difference formulas for Robin realizations, Friedlander's, and Rohleder's theorems are discussed in Section 5.2. Applications to the heat equation are given in Section 5.3. In Section 5.4, we derive from our general results the classical Hadamard–Rellich formula for the eigenvalues of the Schrödinger operator posted on a family of star-shaped domains. The Maslov crossing form for elliptic operators defined by means of the weak solutions is studied in Section 5.5. In Section 6, we provide generalizations of the resolvent difference formula to the case of an *adjoin pair* of operators. The results are applied to the example of an elliptic second-order partial differential operator and its formal adjoint. In Appendix A, we give a detailed discussion of the correspondence between the Lagrangian planes in the boundary space $\mathfrak{H} \times \mathfrak{H}$ and the domains of the self-adjoint extensions. We introduce and study the notion of *aligned subspaces* and show that for these the correspondence is a bijection. Appendix B shows how to derive the classical Krein's formulas involving the M-function from the new symplectic version of the resolvent difference formula that we offered in the paper.

Notation. We denote the space of bounded linear operators acting between two Banach spaces $\mathcal{X}$ and $\mathcal{Y}$ by $\mathcal{B}(\mathcal{X}, \mathcal{Y})$ and let $\mathcal{B}(\mathcal{X}) := \mathcal{B}(\mathcal{X}, \mathcal{X})$. The closure of an operator $T : \mathcal{X} \to \mathcal{Y}$ is denoted by $\overline{T}$. We denote by $\mathrm{Spec}(T)$ the spectrum, by $\mathrm{Spec}_{\mathrm{disc}}(T)$ the set of isolated eigenvalues of finite algebraic multiplicity, and by $\mathrm{Spec}_{\mathrm{ess}}(T) = \mathrm{Spec}(T) \setminus \mathrm{Spec}_{\mathrm{disc}}(T)$ the essential spectrum of T. The scalar product (linear with respect to the *first* argument) and the norm on a Hilbert space $\mathcal{H}$ are denoted by $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ and $\| \cdot \|_{\mathcal{H}}$, respectively. When $\mathcal{H}$ is a Hilbert space, we denote the space of bounded *linear* functionals on $\mathcal{H}$ by $\mathcal{H}^*$ and define a *conjugate-linear* Riesz isomorphism by

$\Phi : \mathcal{H}^* \mapsto \mathcal{H}$, $\mathcal{H}^* \ni \psi \mapsto \Phi_\psi \in \mathcal{H}$ so that ${}_{\mathcal{H}}\langle f, \psi\rangle_{\mathcal{H}^*} := \psi(f) = \langle f, \Phi_\psi\rangle_{\mathcal{H}}, f \in \mathcal{H}$. In the special case of Sobolev spaces $\mathcal{H} = H^{1/2}(\partial\Omega)$, we set $\mathcal{H}^* = H^{-1/2}(\partial\Omega)$ and denote $\langle f, \psi\rangle_{-1/2} :={}_{H^{1/2}(\partial\Omega)} \langle f, \psi\rangle_{H^{-1/2}(\partial\Omega)}$ for $f \in H^{1/2}(\partial\Omega), \psi \in H^{-1/2}(\partial\Omega)$. The closure of a subspace $S \subset \mathcal{H}$ with respect to $\|\cdot\|_{\mathcal{H}}$ is denoted by $\overline{S}^{\mathcal{H}}$, while its orthogonal complement by $S^{\perp_{\mathcal{H}}}$. For operators $A, B \in \mathcal{B}(\mathcal{X}, \mathcal{Y})$, we let $[A, B] \in \mathcal{B}(\mathcal{X} \times \mathcal{X}, \mathcal{Y})$, $[A, B](h_1, h_2)^\top := Ah_1 + Bh_2$, $h_1, h_2 \in \mathcal{X}$ and $[A, B]^\top \in \mathcal{B}(\mathcal{X}, \mathcal{Y} \times \mathcal{Y})$, $[A, B]^\top(h) := (Ah, Bh)^\top$, $h \in \mathcal{X}$, where $\top$ stands for transposition. We denote by $\Lambda(\mathcal{X} \times \mathcal{X})$ the set of Lagrangian subspaces in $\mathcal{X} \times \mathcal{X}$ equipped with the symplectic form ω induced by the operator $J = \begin{bmatrix} 0 & I_{\mathcal{X}} \\ -I_{\mathcal{X}} & 0 \end{bmatrix} \in \mathcal{B}(\mathcal{X} \times \mathcal{X})$. Given an operator valued function $f : \mathbb{R} \to \mathcal{B}(\mathcal{X})$, we write $f(t) = o((t - t_0)^n)$ as $t \to t_0$ if $\|f(t)\|_{\mathcal{B}(\mathcal{X})}|t - t_0|^{-n} \to 0$ as $t \to t_0$. Similarly, $f(t) = \mathcal{O}((t - t_0)^n)$ as $t \to t_0$ whenever $\|f(t)\|_{\mathcal{B}(\mathcal{X})}|t - t_0|^{-n} \leqslant c$ for some $c > 0$ and all $t \neq t_0$ in some open interval containing t_0. We denote by $\mathbb{B}_r(\zeta)$ the disc in $\mathbb{C}$ of radius r centered at ζ and by $\mathbb{B}_r^n$ the ball in $\mathbb{R}^n$ of radius r centered at zero.

2 | A SYMPLECTIC RESOLVENT DIFFERENCE FORMULA

Let $\mathcal{H}, \mathfrak{H}$ be complex, separable Hilbert spaces. Let A be a densely defined, closed, symmetric operator acting in $\mathcal{H}$ and having equal (possibly infinite) deficiency indices, that is,

$$\dim\ker(A^* - \mathbf{i}) = \dim\ker(A^* + \mathbf{i}).$$

We denote $\mathcal{H}_+ = \mathrm{dom}(A^*)$ and equip this Hilbert space with the graph scalar product

$$\langle u, v\rangle_{\mathcal{H}_+} := \langle u, v\rangle_{\mathcal{H}} + \langle A^*u, A^*u\rangle_{\mathcal{H}},\ u, v \in \mathrm{dom}(A^*).$$

Let $\mathcal{H}_- = (\mathcal{H}_+)^*$ denote the space adjoint to $\mathcal{H}_+$ with

$$\mathcal{H}_+ \hookrightarrow \mathcal{H} \hookrightarrow \mathcal{H}_-, \tag{2.1}$$

where the first embedding is given by $\mathcal{H}_+ \ni u \mapsto u \in \mathcal{H}$, and the second embedding is given by $\mathcal{H} \ni v \mapsto \langle\cdot, v\rangle_{\mathcal{H}}$. Let $\Phi^{-1} : \mathcal{H}_+ \to \mathcal{H}_-$ be the Riesz isomorphism such that

$${}_{\mathcal{H}_+}\langle u, \Phi^{-1}w\rangle_{\mathcal{H}_-} = \langle u, w\rangle_{\mathcal{H}_+} = \langle u, w\rangle_{\mathcal{H}} + \langle A^*u, A^*w\rangle_{\mathcal{H}}, u, w \in \mathcal{H}_+.$$

The following hypothesis will be assumed throughout the rest of the paper.

Hypothesis 2.1. We assume that A is a densely defined, closed, symmetric operator acting in $\mathcal{H}$ and having equal (possibly infinite) deficiency indices. Suppose that $\mathcal{D}$ is a core for A^*, that is, $\mathcal{D}$ is a dense subspace of $\mathcal{H}_+$ with respect to the graph norm of A^*, and assume that $\mathrm{dom}(A) \subset \mathcal{D}$. Consider a linear operator

$$\mathrm{T} := [\Gamma_0, \Gamma_1]^\top : \mathcal{H}_+ \to \mathfrak{H} \times \mathfrak{H} \text{ such that } \mathrm{dom}(\mathrm{T}) = \mathcal{D}, \overline{\mathrm{ran}(\mathrm{T})} = \mathfrak{H} \times \mathfrak{H} \tag{2.2}$$

called the *trace operator*. Assume that T satisfies the following abstract Green identity:

$$\langle A^*u, v\rangle_{\mathcal{H}} - \langle u, A^*v\rangle_{\mathcal{H}} = \langle \Gamma_1 u, \Gamma_0 v\rangle_{\mathfrak{H}} - \langle \Gamma_0 u, \Gamma_1 v\rangle_{\mathfrak{H}} \text{ for all } u, v \in \mathcal{D}. \tag{2.3}$$

A simple but very important setting satisfying Hypothesis 2.1 is given by ordinary boundary triplets, cf. for example, [13, 56], in which case one lets $\mathcal{D} = \operatorname{dom}(A^*) = \mathcal{H}_+$ and one can always define a Hilbert space $\mathfrak{H}$ and a trace operator T satisfying (2.3). This scenario is discussed in Section 4 below. Yet, more elaborate setting, which is more suitable for PDEs, is discussed in Section 5 where Hypothesis 2.1 holds with $\mathcal{D} \subsetneq \operatorname{dom}(A^*)$ being a proper subset of $\mathcal{H}_+$.

Remark 2.2. The notion of ordinary boundary triplets has been modified and generalized in several (similar but not equivalent) directions and applied to elliptic differential operators by multiple authors. The pioneering paper [56] offered the first such generalization where Γ_0 was assumed to be surjective and the operator $A^*|_{\ker \Gamma_0}$ self-adjoint, see also [14, 15, 18, 50–55].

In the following propositions, we collect some properties of the operator T and its composition with the resolvent $R(\zeta, \mathcal{A}) = (\mathcal{A} - \zeta)^{-1}$ of a self-adjoint extension $\mathcal{A}$ of A.

Lemma 2.3. *Under Hypothesis 2.1, the following assertions hold.*

(1) $\operatorname{dom}(A) = \ker(\mathrm{T})$.
(2) *The operator* $\mathrm{T} : \mathcal{D} \subset \mathcal{H}_+ \to \mathfrak{H} \times \mathfrak{H}$ *defined in (2.2) is closable.*

Lemma 2.4. *Assume Hypothesis 2.1 and assume that there exists a self-adjoint extension $\mathcal{A}$ of A satisfying* $\operatorname{dom}(\mathcal{A}) \subset \mathcal{D}$*. Then, the resolvent operator $R(\zeta, \mathcal{A}) := (\mathcal{A} - \zeta)^{-1} \in \mathcal{B}(\mathcal{H})$, $\zeta \in \mathbb{C} \setminus \operatorname{Spec}(\mathcal{A})$, can be viewed as a bounded operator from $\mathcal{H}$ to $\mathcal{H}_+$. Furthermore,*

$$\mathrm{T}R(\zeta, \mathcal{A}) \in \mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H}). \tag{2.4}$$

The elementary proofs of Lemmas 2.3 and 2.4 are provided in the electronic version of this paper available on ArXiv [92].

Remark 2.5. In Lemma 2.4 (and everywhere when needed below), in addition to Hypothesis 2.1, we *assume* the existence of a self-adjoint extension $\mathcal{A}$ of A with $\operatorname{dom}(\mathcal{A}) \subset \mathcal{D}$. The question of the existence of such a self-adjoint extension under merely Hypothesis 2.1 is a subtle one. The nontrivial issue of whether or not, and under which additional minimal assumptions, this indeed happens is beyond the scope of this paper. (We refer interested readers to [13, 50, 53, 54] where closely related questions are discussed and relevant bibliography is provided. In this regard, we highlight an ingenious relevant work [34] that was rediscovered and further developed in [79, 126].) That said, the condition $\operatorname{dom}(\mathcal{A}) \subset \mathcal{D}$ is indeed prevalent in the settings related to elliptic partial differential operators, ordinary differential operators, and quantum graphs covering our principal applications, see Sections 4.2, 4.3, and 5.1–5.4 where relevant PDE models satisfying all abstract assumptions are discussed in detail.

We stress that the main objective of our work is to develop first-order asymptotic perturbation theory for *given* one parametric families of self-adjoint extensions $t \mapsto \mathcal{A}_t$ of the operator A with the additional property $\operatorname{dom}(\mathcal{A}_t) \subset \mathcal{D}$. In the current paper, the operator-theoretic setting described by Hypothesis 2.1 and the condition $\operatorname{dom}(\mathcal{A}_t) \subset \mathcal{D}$ mainly serves as the vehicle for unifying several important classes of partial differential elliptic operators and ordinary differential operators on metric graphs.

As it is well known, the domains of self-adjoint extensions of A are closely related to Lagrangian planes in $\mathfrak{H} \times \mathfrak{H}$, see, for example, [71, Theorem 3.1.6], [77, 106, 120, Proposition 14.7], and Theorems A.1 and A.2 below. The main results of this section are a resolvent difference formula for two given extensions corresponding to two arbitrary Lagrangian planes, see Theorem 2.6. To proceed, we will need to recall some basic definitions from symplectic functional analysis. First, we note that the abstract Green identity (2.3) gives rise to a symplectic form ω defined by

$$\begin{aligned}\omega\big((f_1,f_2)^\top,(g_1,g_2)^\top\big) &:= \langle f_2,g_1\rangle_{\mathfrak{H}} - \langle f_1,g_2\rangle_{\mathfrak{H}}\\ &= \big\langle J(f_1,f_2)^\top,(g_1,g_2)^\top\big\rangle_{\mathfrak{H}\times\mathfrak{H}},\ J := \begin{bmatrix} 0 & I_{\mathfrak{H}}\\ -I_{\mathfrak{H}} & 0\end{bmatrix},\end{aligned}\tag{2.5}$$

$f_k, g_k \in \mathfrak{H}, k = 1,2$. Indeed, using this notation (2.3) can be rewritten as follows:

$$\langle A^*u,v\rangle_{\mathcal{H}} - \langle u,A^*v\rangle_{\mathcal{H}} = \omega(\mathrm{T}u,\mathrm{T}v) \text{ for all } u,v\in\mathcal{D}.$$

We denote the annihilator of a subspace $\mathcal{F}\subset\mathfrak{H}\times\mathfrak{H}$ by

$$\mathcal{F}^\circ := \{(f_1,f_2)^\top\in\mathfrak{H}\times\mathfrak{H} : \omega\big((f_1,f_2)^\top,(g_1,g_2)^\top\big) = 0 \text{ for all } (g_1,g_2)^\top\in\mathcal{F}\},\tag{2.6}$$

and recall that the subspace $\mathcal{F}$ is called *Lagrangian* if $\mathcal{F}=\mathcal{F}^\circ$. We denote by $\Lambda(\mathfrak{H}\times\mathfrak{H})$ the metric space of Lagrangian subspaces of $\mathfrak{H}\times\mathfrak{H}$ equipped with the metric

$$d(\mathcal{F}_1,\mathcal{F}_2) := \|Q_1-Q_2\|_{\mathcal{B}(\mathfrak{H}\times\mathfrak{H})},\ \mathcal{F}_1,\mathcal{F}_2\in\Lambda(\mathfrak{H}\times\mathfrak{H}),$$

where Q_j is the orthogonal projection onto $\mathcal{F}_j$ acting in $\mathfrak{H}\times\mathfrak{H}$, $j=1,2$.

Next, we recall a well-known fact (originally due to Rofe–Beketov, see [57, Chapter 7], [106, Proposition 4(b)][†], [115, 120, Chapter 14]) that any Lagrangian plane $\mathcal{F}\in\Lambda(\mathfrak{H}\times\mathfrak{H})$ can be written as follows:

$$\mathcal{F} = \{(f_1,f_2)^\top\in\mathfrak{H}\times\mathfrak{H} : Xf_1+Yf_2=0\} = \ker([X,Y]),\tag{2.7}$$

where $[X,Y]$ is a (1×2) block operator matrix with X,Y satisfying

$$XY^* = YX^*,\quad X,Y\in\mathcal{B}(\mathfrak{H}),\tag{2.8}$$

$$0\notin\operatorname{Spec}(M^{X,Y}) \text{ for the operator block-matrix } M^{X,Y} := \begin{bmatrix} X & Y\\ -Y & X\end{bmatrix}.\tag{2.9}$$

We note that

$$M^{X,Y}(M^{X,Y})^* = (XX^*+YY^*)\oplus(XX^*+YY^*).$$

In particular, $0\notin\operatorname{Spec}(M^{X,Y})$ if and only if $0\notin\operatorname{Spec}(XX^*+YY^*)$. Using this observation, we write the orthogonal projection Q onto $\mathcal{F}$ from (2.7) as follows:

$$Q = \begin{bmatrix} -Y^*\\ X^*\end{bmatrix}(XX^*+YY^*)^{-1}[-Y,X] = [-Y^*,X^*]^\top W(X,Y).\tag{2.10}$$

[†] Pankrashkin [106] refers to Lagrangian planes as *self-adjoint linear relations* (s.a.l.r.), see [106, Remark 1], and describes $\mathcal{F}$ by means of the equation $Xf_1 = Yf_2$ rather than $Xf_1+Yf_2=0$ used in (2.7). We choose the latter to be consistent with [21, Theorem 1.4.4 A].

Here and below, for brevity, for any $X, Y, X_j, Y_j \in \mathcal{B}(\mathfrak{H})$, $j = 1, 2$, we use notation W and $Z_{1,2}$ for the operators

$$\begin{aligned} W(X, Y) &:= (XX^* + YY^*)^{-1}[-Y, X], \quad W(X, Y) \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H}, \mathfrak{H}), \\ Z_{2,1} &:= (W(X_2, Y_2))^*(X_2Y_1^* - Y_2X_1^*)W(X_1, Y_1), \quad Z_{2,1} \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H}). \end{aligned} \tag{2.11}$$

We are ready to formulate the principal result of this section—a symplectic resolvent difference formula for any two arbitrary self-adjoint extensions of A. We refer to Appendix A for connections of the self-adjoint properties of the extensions and Lagrangian properties of the traces of their domains. Also, we refer to Appendix B and, in particular, to Proposition B.1 for the classical Krein–Naimark formula, cf. [2, 13, Theorem 2.6.1], [57, Chapter 7], [55, 120, Theorem 14.18]. Finally, a more general version of the symplectic resolvent difference formula that holds for *adjoint pairs* of operators is given in Theorem 6.2 below.

In the next theorem, we assume the existence of two self-adjoint extensions of A with domains in $\mathcal{D}$. As we have pointed out in Remark 2.5, this assumption is nontrivial in the abstract setting of Hypothesis 2.1 but holds for many PDE and quantum graph scenarios, as discussed in Sections 4.2, 4.3, 5.1, 5.2, 5.3, and 5.4 below.

Theorem 2.6. *Assume Hypothesis 2.1 and suppose that there exist two self-adjoint extensions $\mathcal{A}_1$ and $\mathcal{A}_2$ of A with domains containing in $\mathcal{D}$. Then, for any $\zeta \notin (\operatorname{Spec}(\mathcal{A}_1) \cup \operatorname{Spec}(\mathcal{A}_2))$, we have*

$$R_2(\zeta) - R_1(\zeta) = \left(\Gamma_0 R_2(\overline{\zeta})\right)^* \Gamma_1 R_1(\zeta) - \left(\Gamma_1 R_2(\overline{\zeta})\right)^* \Gamma_0 R_1(\zeta), \tag{2.12}$$

$$R_2(\zeta) - R_1(\zeta) = (\mathrm{T} R_2(\overline{\zeta}))^* J \mathrm{T} R_1(\zeta), \tag{2.13}$$

where $R_j(\zeta) := (\mathcal{A}_j - \zeta)^{-1}$ and $\mathrm{T}R_j(\overline{\zeta}) = \left(\Gamma_0 R_j(\overline{\zeta}), \Gamma_1 R_j(\overline{\zeta})\right)$ is considered as an operator in $\mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H})$, $j = 1, 2$.

Assume, further, that $\overline{\mathrm{T}(\operatorname{dom} \mathcal{A}_j)}$ is a Lagrangian plane in $\mathfrak{H} \times \mathfrak{H}$ and

$$\overline{\mathrm{T}(\operatorname{dom} \mathcal{A}_j)} = \ker([X_j, Y_j])$$

with X_j, Y_j satisfying (2.8) and (2.9), and let Q_j denote the orthogonal projection onto $\overline{\mathrm{T}(\operatorname{dom} \mathcal{A}_j)}$ for $j = 1, 2$. Then

$$R_2(\zeta) - R_1(\zeta) = (\mathrm{T} R_2(\overline{\zeta}))^* Q_2 J Q_1 \mathrm{T} R_1(\zeta), \tag{2.14}$$

$$R_2(\zeta) - R_1(\zeta) = (\mathrm{T} R_2(\overline{\zeta}))^* Z_{2,1} \mathrm{T}\, R_1(\zeta), \tag{2.15}$$

where the operators $Z_{2,1} = (W(X_2, Y_2))^*(X_2Y_1^* - Y_2X_1^*)W(X_1, Y_1)$ and $W(X_j, Y_j)$ are defined in (2.11).

Proof. By Lemma 2.4, we have $\Gamma_0 R_2(\overline{\zeta}), \Gamma_1 R_2(\overline{\zeta}) \in \mathcal{B}(\mathcal{H}, \mathfrak{H})$. In particular, the adjoint operators appearing in (2.12) are also bounded. Next, using $(\mathcal{A}_j - \zeta)R_j(\zeta) = (A^* - \zeta)R_j(\zeta)$, $\mathcal{A}_2 = \mathcal{A}_2^*$, and the Green identity (2.3), for arbitrary $u, v \in \mathcal{H}$, we infer

$$\begin{aligned}\langle R_2(\zeta)u - R_1(\zeta)u, v\rangle_{\mathcal{H}} &= \langle R_2(\zeta)u - R_1(\zeta)u, (\mathcal{A}_2 - \overline{\zeta})R_2(\overline{\zeta})v\rangle_{\mathcal{H}}\\ &= \langle(\mathcal{A}_2 - \zeta)R_2(\zeta)u, R_2(\overline{\zeta})v\rangle_{\mathcal{H}} - \langle R_1(\zeta)u, (A^* - \overline{\zeta})R_2(\overline{\zeta})v\rangle_{\mathcal{H}}\\ &= \langle u, R_2(\overline{\zeta})v\rangle_{\mathcal{H}} - \langle(A^* - \zeta)R_1(\zeta)u, R_2(\overline{\zeta})v\rangle_{\mathcal{H}}\\ &\quad + \langle\Gamma_1 R_1(\zeta)u, \Gamma_0 R_2(\overline{\zeta})v\rangle_{\mathfrak{H}} - \langle\Gamma_0 R_1(\zeta)u, \Gamma_1 R_2(\overline{\zeta})v\rangle_{\mathfrak{H}}\\ &= \langle\Gamma_1 R_1(\zeta)u, \Gamma_0 R_2(\overline{\zeta})v\rangle_{\mathfrak{H}} - \langle\Gamma_0 R_1(\zeta)u, \Gamma_1 R_2(\overline{\zeta})v\rangle_{\mathfrak{H}}\\ &= \Big\langle\Big((\Gamma_0 R_2(\overline{\zeta}))^*\Gamma_1 R_1(\zeta) - (\Gamma_1 R_2(\overline{\zeta}))^*\Gamma_0 R_1(\zeta)\Big)u, v\Big\rangle_{\mathcal{H}}.\end{aligned}$$

This yields (2.12). Rewriting (2.12) using J introduced in (2.5) yields (2.13). For all $u \in \mathcal{H}$, we have $\mathrm{T}R_j(\zeta)u \in \mathrm{T}(\operatorname{dom}\mathcal{A}_j)$ and thus $Q_j\mathrm{T}R_j(\zeta) = \mathrm{T}R_j(\zeta)$; so, Equation (2.13) implies (2.14) since $Q_2^* = Q_2$. Equation (2.15) follows from (2.10), (2.11), and (2.14). □

Remark 2.7. As it is easy to see from the proof of Theorem 2.6, the symplectic resolvent difference formulas (2.13) and (2.14) hold even if $\mathcal{A}_1$ is a nonself-adjoint restriction of A^*; the only assertion used was $\operatorname{dom}(\mathcal{A}_j) \subset \operatorname{dom}(\mathrm{T})$, $j = 1, 2$. We further recall that the classical Krein's resolvent formula, see, for example, [13, 120] and Appendix B, gives an expression of the difference of the resolvents of an *arbitrary* self-adjoint extension $\mathcal{A}$ of A and a *special*, "Dirichlet"-type extension $\mathcal{A}_0$ whose domain is $\ker(\Gamma_0)$. The difference of the resolvents of the two extensions is expressed in terms of the γ-field and the abstract Weyl's function; we recall this in Proposition B.1. The symplectic resolvent difference formula offered in Theorem 2.6 does not contain of course that much information as Krein's resolvent formula as it does not involve, for example, the Weyl function. We stress, however, that Theorem 2.6 works for any two *arbitrary* self-adjoint extensions $\mathcal{A}_1$ and $\mathcal{A}_2$; the domains of neither of them should be the kernels of Γ_0 or Γ_1. Also, as we will see below in Section 3, the symplectic resolvent difference formula in Theorem 2.6 appears to be very useful, for instance, in establishing continuity and differentiability properties of the resolvents of *families* of self-adjoint extensions. Clearly, the resolvent difference formula in Theorem 2.6 can be easily obtained by applying the classical Krein's formula, first, to $\mathcal{A}_1$ and $\mathcal{A}_0$ and, next, to $\mathcal{A}_2$ and $\mathcal{A}_0$ and then by subtracting the two formulas, cf. Remark B.2. This way of computing the difference of resolvents of two arbitrary extensions was often used since very classical work to show, for instance, that the difference belongs to the Schatten-von Neumann ideal, see, for example, [55, Theorem 2 and Corollary 4]. Finally, as we demonstrate in the proof of Proposition B.1, the resolvent difference formula can also be used as the first step in proving the classical Krein's formula (of course, several more steps are required for the proof to dig out the wealth of information that the classical formula contains).

Remark 2.8. We note that (2.13) in Theorem 2.6 yields a new streamlined proof† of the classical Krein's resolvent formula, see [2, Section VIII.106], [41, Appendix A, eq. (A.36)] in the case of finite deficiency indices. It can also be used to derive the classical Krein–Naimark resolvent formula in the case of infinite deficiency indices as demonstrated in Appendix B below.

† Provided in the electronic version of this manuscript [92, Proposition B.3].

We conclude this section with a series of auxiliary assertions aiming to place the above results in the vast literature on the theory of boundary relations in Krein spaces and discuss further the adjoint operators $(\mathrm{T}R_j(\zeta))^*$ appearing in (2.14) and (2.15). Although the assertions could of independent interests, they are not being used in the remainder of the paper.

Remark 2.9. We now briefly mention how to recast Hypothesis 2.1 using Krein's spaces in the context of boundary triplets as discussed in the inspirational paper [53] whose authors are dealing with very general but still closely related to our setting. Let $J_{\mathfrak{H}} = \mathbf{i}J$, cf. (2.5), and define in $\mathfrak{H} \times \mathfrak{H}$ an indefinite scalar product

$$\begin{aligned}\langle\langle (f_1, f_2)^\top, (g_1, g_2)^\top \rangle\rangle_{\mathfrak{H}\times\mathfrak{H}} &:= \langle J_{\mathfrak{H}}(f_1, f_2)^\top, (g_1, g_2)^\top \rangle_{\mathfrak{H}\times\mathfrak{H}} \\ &= \mathbf{i}\omega((f_1, f_2)^\top, (g_1, g_2)^\top),\ f_1, f_2, g_1, g_2 \in \mathfrak{H}.\end{aligned}$$

Let $J_{\mathcal{H}}$ be an analogous operator in $\mathcal{H} \times \mathcal{H}$ yielding the corresponding indefinite scalar product $\langle\langle (u_1, u_2)^\top, (v_1, v_2)^\top \rangle\rangle_{\mathcal{H}}$. Then $(\mathcal{H} \times \mathcal{H}, \langle\langle \cdot, \cdot \rangle\rangle_{\mathcal{H}\times\mathcal{H}})$ and $(\mathfrak{H} \times \mathfrak{H}, \langle\langle \cdot, \cdot \rangle\rangle_{\mathfrak{H}\times\mathfrak{H}})$ are Krein spaces and the operator T induces an isometry between them. To define the latter in precise terms, let $G(A^*)$ denote the graph of A^* in $\mathcal{H} \times \mathcal{H}$ and introduce an operator

$$\mathcal{T} : \mathcal{H} \times \mathcal{H} \to \mathfrak{H} \times \mathfrak{H}, \mathrm{dom}(\mathcal{T}) = \{(u, A^*u)^\top : u \in \mathcal{D}\} \subset G(A^*),\ \mathcal{T}(u, A^*u)^\top := (\Gamma_0 u, \Gamma_1 u)^\top.$$

Then Green's identity (2.3) yields

$$\langle\langle (u, A^*u)^\top, (v, A^*v)^\top \rangle\rangle_{\mathcal{H}} = \langle\langle \mathcal{T}(u, A^*u)^\top, \mathcal{T}(v, A^*v)^\top \rangle\rangle_{\mathfrak{H}} \text{ for all } u, v \in \mathcal{D},$$

and so, $\mathcal{T}$ is an isometry between the Krein spaces $(\mathcal{H} \times \mathcal{H}, \langle\langle \cdot, \cdot \rangle\rangle_{\mathcal{H}})$ and $(\mathfrak{H} \times \mathfrak{H}, \langle\langle \cdot, \cdot \rangle\rangle_{\mathfrak{H}})$. Following [53], we will identify the graph of $\mathcal{T}$ with $\mathcal{T}$ and treat it as a linear relation in $\mathcal{H} \times \mathcal{H} \times \mathfrak{H} \times \mathfrak{H}$, see [13] for a comprehensive introduction into spectral theory of linear relations. In particular, $\mathcal{T}^{-1} \subset \mathcal{T}^{[*]}$, where the inverse is understood in the sense of relations and $\mathcal{T}^{[*]}$ denotes the adjoint relation with respect to the Krein inner products. An important question is whether $\mathcal{T}$ is unitary, that is, $\mathcal{T}^{-1} = \mathcal{T}^{[*]}$. [53, Proposition 2.5] gives sufficient conditions for an isometric map $\mathcal{T}$ to be unitary. The conditions are: (i) $G(A^*)^{[\perp]} \subset G(A^*)$, (ii) $(\mathrm{ran}\mathcal{T})^{[\perp]} \subset \mathrm{mul}(\mathcal{T})$ (here ${}^{[\perp]}$ denotes the orthogonal complement in the Krein space, and mul is the multivalued part of the relation), and (iii) dom $\mathcal{T}^{[*]} \subset \mathrm{ran}(\mathcal{T})$. We note that (i) and (ii) follow from Hypothesis 2.1, while (iii) does not (in general), even in the more restrictive setting of quasi-boundary triples studied in [14]. A deep characterization of the equality $\mathcal{T}^{-1} = \mathcal{T}^{[*]}$ in terms of the Nevanlinna property of the Weyl function is given in [53, Theorem 3.9], see also [54, Theorem 7.57 and Corollary 7.58]. We stress that Hypothesis 2.1 alone is not sufficient for $\mathcal{T}$ being unitary! To further compare the setting of [53] with that given by Hypothesis 2.1, we note that the latter deals with *densely* defined symmetric operator A and the linear relation $\mathcal{T}$ with dense range. These density assumptions model elliptic differential operators on bounded domains and ordinary differential operators on metric graphs, and, at the same time, yield natural relations between self-adjoint extensions of A and Lagrangian planes in $\mathfrak{H} \times \mathfrak{H}$ as described in Theorems A.1 and A.2. In the more general setting of [53], these relations do not always take place, cf. Remark A.3.

Remark 2.10. We choose to use Lagrangian (symplectic) language throughout the paper. Alternatively, Lagrangian plains are called *self-adjoint linear relations*, and we refer to [13, 120] for a detailed account of the topic, see also [106]. Another way to describe the same object is to involve the Krein spaces introduced in Remark 2.9. We notice that $\mathcal{F}^{\circ}$ defined in (2.6) is just $\mathcal{F}^{[\perp]}$, the $\langle\langle\cdot,\cdot\rangle\rangle_{\mathfrak{H}}$-orthogonal to $\mathcal{F}$ subspace of $\mathfrak{H}\times\mathfrak{H}$, and $\mathcal{F}$ is Lagrangian if and only if $\mathcal{F}=\mathcal{F}^{[\perp]}$.

Next, we discuss the operator $(\mathrm{T}R_2(\zeta))^*$ appearing in Theorem 2.6. Let us first record the following useful fact about T^*.

Proposition 2.11. *The domain of the adjoint operator* $\mathrm{T}^*:\mathrm{dom}(\mathrm{T}^*)\subset\mathfrak{H}\times\mathfrak{H}\to\mathcal{H}_-$*, cf. (2.1), satisfies* $J(\mathrm{T}(\mathcal{D}))\subseteq\mathrm{dom}(\mathrm{T}^*)$.

Proof. By the general definition of adjoint operator, $\mathrm{dom}((\mathrm{T})^*)$ is the set of $h\in\mathfrak{H}\times\mathfrak{H}$ such that there exists a $w\in\mathcal{H}_+$ so that for all $u\in\mathcal{D}=\mathrm{dom}(\mathrm{T})$, one has

$$\langle \mathrm{T}u,h\rangle_{\mathfrak{H}\times\mathfrak{H}}={}_{\mathcal{H}_+}\langle u,\Phi^{-1}w\rangle_{\mathcal{H}_-}=\langle u,w\rangle_{\mathcal{H}_+}=\langle u,w\rangle_{\mathcal{H}}+\langle A^*u,A^*w\rangle_{\mathcal{H}}; \tag{2.16}$$

if this is the case, then $(\mathrm{T})^*h:=\Phi^{-1}w$. We recall the orthogonal direct sum decomposition $\mathcal{H}_+=\mathrm{dom}(A)\dotplus(\mathrm{dom}(A))^{\perp_{\mathcal{H}_+}}$ where, by [26, Lemma 3.1(a)],

$$(\mathrm{dom}(A))^{\perp_{\mathcal{H}_+}}=\big\{v\in\mathcal{H}_+ : A^*v\in\mathcal{H}_+ \text{ and } v=-A^*(A^*v)\big\}. \tag{2.17}$$

Since $\mathrm{dom}(A)\subset\mathcal{D}$ and $\ker(\mathrm{T})=\mathrm{dom}(A)$ by part (1) of the proposition, we have

$$\mathrm{T}(\mathcal{D})=\mathrm{T}\Big((\mathrm{dom}(A))^{\perp_{\mathcal{H}_+}}\cap\mathcal{D}\Big).$$

If $h:=(h_1,h_2)^\top=J\mathrm{T}v$ for some $v\in(\mathrm{dom}(A))^{\perp_{\mathcal{H}_+}}\cap\mathcal{D}$, then

$$\begin{aligned}\langle \mathrm{T}u,h\rangle_{\mathfrak{H}\times\mathfrak{H}}&=\langle\Gamma_0u,h_1\rangle_{\mathfrak{H}}+\langle\Gamma_1u,h_2\rangle_{\mathfrak{H}}=\langle\Gamma_0u,\Gamma_1v\rangle_{\mathfrak{H}}-\langle\Gamma_1u,\Gamma_0v\rangle_{\mathfrak{H}}\\&=\langle u,A^*v\rangle_{\mathcal{H}}-\langle A^*u,v\rangle_{\mathcal{H}}\end{aligned}$$

by the Green identity (2.3). Letting $w=A^*v$, we derive (2.16) from (2.17) and thus $J(\mathrm{T}(\mathcal{D}))\subseteq\mathrm{dom}((\mathrm{T})^*)$. □

It is tempting to rewrite the prefactor $(\mathrm{T}R_2(\overline{\zeta}))^*$ in the right-hand side of (2.13) in terms of the product of the operators adjoint to T and $R_2(\overline{\zeta})$. To that end, we first prove an auxiliary result about the product of the adjoints.

Proposition 2.12. *Assume Hypothesis 2.1 and recall (2.1). Assume that there exists a self-adjoint extension $\mathcal{A}$ of A satisfying* $\mathrm{dom}(\mathcal{A})\subset\mathcal{D}$ *and denote $R(\zeta,\mathcal{A}):=(\mathcal{A}-\zeta)^{-1}\in\mathcal{B}(\mathcal{H})$ for all $\zeta\in\mathbb{C}\setminus$* $\mathrm{Spec}(\mathcal{A})$*. The operator $R(\overline{\zeta},\mathcal{A})\in\mathcal{B}(\mathcal{H})$ can be uniquely extended to a bounded linear operator in $\mathcal{B}(\mathcal{H}_-,\mathcal{H})$ that we will denote by $\mathcal{R}(\overline{\zeta},\mathcal{A})$. This extension is given by the operator $(R(\zeta,\mathcal{A}))^*\in\mathcal{B}(\mathcal{H}_-,\mathcal{H})$ adjoint to $R(\zeta,\mathcal{A})\in\mathcal{B}(\mathcal{H},\mathcal{H}_+)$. With this notational conventions, the operator* $\big(\mathrm{T}R(\zeta,\mathcal{A})\big)^*\in\mathcal{B}(\mathfrak{H}\times\mathfrak{H},\mathcal{H})$ *can be written as*

$$(\mathrm{T}R(\zeta,\mathcal{A}))^*h=\mathcal{R}(\overline{\zeta},\mathcal{A})(\mathrm{T})^*h \text{ for all } h\in J(\mathrm{T}(\mathcal{D})). \tag{2.18}$$

Proof. For the sake of the proof, we will denote by $\widehat{R}(\zeta,\mathcal{A})\in\mathcal{B}(\mathcal{H},\mathcal{H}_+)$ the resolvent operator $R(\zeta,\mathcal{A})$ viewed as an operator acting from $\mathcal{H}$ to $\mathcal{H}_+$; thus, $(\widehat{R}(\zeta,\mathcal{A}))^*\in\mathcal{B}(\mathcal{H}_-,\mathcal{H})$. We let $i\in\mathcal{B}(\mathcal{H}_+,\mathcal{H})$ denote the first embedding $i: w\mapsto w$ in (2.1) and let $j=(i)^*\in\mathcal{B}(\mathcal{H},\mathcal{H}_-)$ denote the second embedding in (2.1) so that $\langle iu, w\rangle_{\mathcal{H}} = {}_{\mathcal{H}_+}\langle u, jw\rangle_{\mathcal{H}_-}$ for all $u \in \mathcal{H}_+ \hookrightarrow \mathcal{H}$ and $w \in \mathcal{H} \hookrightarrow \mathcal{H}_-$. In this notation, $i\widehat{R}(\zeta, \mathcal{A}) = R(\zeta, \mathcal{A})$, and, in order to prove the first part of the proposition, we have to show that

$$(\widehat{R}(\zeta, \mathcal{A}))^* jw = R(\overline{\zeta}, \mathcal{A})w \text{ for all } w \in \mathcal{H}, \tag{2.19}$$

and so, $\mathcal{R}(\overline{\zeta}, \mathcal{A}) := (\widehat{R}(\zeta, \mathcal{A}))^* \in \mathcal{B}(\mathcal{H}_-, \mathcal{H})$ is indeed a bounded extension to $\mathcal{H}_-$ of $R(\overline{\zeta}, \mathcal{A}) \in \mathcal{B}(\mathcal{H})$. For any $u \in \mathcal{H}_+$ and $w \in \mathcal{H}$, we infer

$$\begin{aligned}
\langle iu, (\widehat{R}(\zeta, \mathcal{A}))^* jw\rangle_{\mathcal{H}} &= {}_{\mathcal{H}_+}\langle u, j(\widehat{R}(\zeta, \mathcal{A}))^* jw\rangle_{\mathcal{H}_-} && \text{(because } i^* = j\text{)}\\
&= \langle \big(j(\widehat{R}(\zeta, \mathcal{A}))^* j\big)^* u, w\rangle_{\mathcal{H}} && \text{(because } j(\widehat{R}(\zeta, \mathcal{A}))^* j \in \mathcal{B}(\mathcal{H}, \mathcal{H}_-)\text{)}\\
&= \langle i\widehat{R}(\zeta, \mathcal{A}) iu, w\rangle_{\mathcal{H}} && \text{(because } i^* = j\text{)}\\
&= \langle R(\zeta, \mathcal{A}) iu, w\rangle_{\mathcal{H}} && \text{(because } i\widehat{R}(\zeta, \mathcal{A}) = R(\zeta, \mathcal{A})\text{)}\\
&= \langle iu, R(\overline{\zeta}, \mathcal{A})w\rangle_{\mathcal{H}} && \text{(because } \mathcal{A} = \mathcal{A}^* \text{ in } \mathcal{H}\text{).}
\end{aligned}$$

Since $\operatorname{ran}(i)$ is dense in $\mathcal{H}$, we have (2.19).

It remains to prove (2.18), that is, in the notation of the current proof, that

$$(\mathrm{T}\widehat{R}(\zeta, \mathcal{A}))^* h = (\widehat{R}(\zeta, \mathcal{A}))^* (\mathrm{T})^* h \text{ for all } h \in J(\mathrm{T}(\mathcal{D})). \tag{2.20}$$

By [83, Problem III.5.26], we have $(\widehat{R}(\zeta, \mathcal{A}))^*(\mathrm{T})^* \subseteq (\mathrm{T}\widehat{R}(\zeta, \mathcal{A}))^*$, where the domain of the product $(\widehat{R}(\zeta, \mathcal{A}))^*(\mathrm{T})^*$ is set to be equal to $\operatorname{dom}(\mathrm{T}^*)$. Since $J(\mathrm{T}(\mathcal{D})) \subseteq \operatorname{dom}(\mathrm{T}^*)$ by Proposition 2.11, we infer (2.20). □

Corollary 2.13. *Resolvent difference formula formulas (2.12) and (2.13) can be also rewritten as*

$$R_2(\zeta) - R_1(\zeta) = \mathcal{R}_2(\zeta)\mathrm{T}^* J\mathrm{T}R_1(\zeta), \tag{2.21}$$

where the operator $\mathcal{R}_2(\zeta)$ in the right-hand side is viewed as a unique extension of the resolvent $R_2(\zeta) \in \mathcal{B}(\mathcal{H})$ to an element of $\mathcal{B}(\mathcal{H}_-, \mathcal{H})$ as in Proposition 2.12 and, in fact, is given by $(R_2(\overline{\zeta}))^* \in \mathcal{B}(\mathcal{H}_-, \mathcal{H})$. Indeed, (2.21) follows from (2.13), (2.18), and the fact that $\operatorname{ran}\big(J\mathrm{T}R_1(\zeta)\big) \subseteq J(\mathrm{T}(\mathcal{D})) \subseteq \operatorname{dom}(\mathrm{T}^*)$, by Proposition 2.11 (3).

Remark 2.14. We conclude this preliminary section with a slight generalization,[†] see (2.23) below, of the resolvent difference formula in Theorem 2.6. To formulate it, we will freely use elementary facts on (linear) relations as nicely described in [13, Chapter 1]. In particular, we will identify the operators on a Hilbert space $\mathcal{H}$ with their graphs in $\mathcal{H} \times \mathcal{H}$. In this remark (and only in this remark) instead of Hypothesis 2.1, we will impose the following assumptions. Let $A \subset A^*$ be a symmetric relation in $\mathcal{H} \times \mathcal{H}$ (not necessarily densely defined), and $\mathrm{T} = [\Gamma_0, \Gamma_1]^\top : \operatorname{dom}(\mathrm{T}) \subseteq A^* \to \mathfrak{H} \times \mathfrak{H}$ be a linear operator (possibly unbounded) with a dense in A^* domain and such that the following abstract Green's identity holds:

$$\langle u_2, v_1\rangle_{\mathcal{H}} - \langle u_1, v_2\rangle_{\mathcal{H}} = \langle \Gamma_1\widehat{u}, \Gamma_0\widehat{v}\rangle_{\mathfrak{H}} - \langle \Gamma_0\widehat{u}, \Gamma_1\widehat{v}\rangle_{\mathfrak{H}} \text{ for all } \widehat{u} = (u_1, u_2), \widehat{v} = (v_1, v_2) \in \operatorname{dom}(\mathrm{T}).$$

[†] We thank the referee of an earlier version of the paper for suggesting this generalization.

(Clearly, if A^* is an operator, then $u_2 = A^*u_1$, $v_2 = A^*v_1$ and so this becomes (2.3) upon setting $\Gamma_0 u_1 = \Gamma_0\widehat{u}$ and $\Gamma_1 u_1 = \Gamma_1\widehat{u}$, cf. [13, Section 2.1]). Furthermore, let $\mathcal{A}_1$ and $\mathcal{A}_2$ be two relations such that $A \subset \mathcal{A}_j \subset A^*$ and $\rho(\mathcal{A}_j) \neq \emptyset$, $j = 1, 2$, and assume that $\mathcal{A}_1 \subset \mathrm{dom}(\mathrm{T})$ and $\mathcal{A}_2^* \subset \mathrm{dom}(\mathrm{T})$. Let us fix $\zeta \in \rho(\mathcal{A}_1) \cap \rho(\mathcal{A}_2)$ and use the resolvents $R_1(\zeta)$ and $R_2(\zeta)^* = (\mathcal{A}_2^* - \overline{\zeta})^{-1}$ of $\mathcal{A}_1$ and $\mathcal{A}_2^*$ to write the relations $\mathcal{A}_1$ and $\mathcal{A}_2^*$ as follows:

$$\begin{aligned}\mathcal{A}_1 &= \big\{\widehat{u} := \big(R_1(\zeta)u, (I_{\mathcal{H}} + \zeta R_1(\zeta))u\big) \,:\, u \in \mathcal{H}\big\},\\ \mathcal{A}_2^* &= \big\{\widehat{v} := (R_2(\zeta)^*v, (I_{\mathcal{H}} + \overline{\zeta} R_2(\zeta)^*)v) \,:\, v \in \mathcal{H}\big\}.\end{aligned} \tag{2.22}$$

Using Green's identity then yields

$$\langle \Gamma_1\widehat{u}, \Gamma_0\widehat{v}\rangle_{\mathfrak{H}} - \langle \Gamma_0\widehat{u}, \Gamma_1\widehat{v}\rangle_{\mathfrak{H}} = \langle (I_{\mathcal{H}} + \zeta R_1(\zeta))u, R_2(\zeta)^*v\rangle_{\mathcal{H}} - \langle R_1(\zeta)u, (I_{\mathcal{H}} + \overline{\zeta} R_2(\zeta)^*)v\rangle_{\mathcal{H}},$$

and so, rearranging the right-hand side of the last formula gives the desired generalization of the resolvent difference formula,

$$\langle (R_2(\zeta) - R_1(\zeta))u, v\rangle_{\mathcal{H}} = \langle \Gamma_1\widehat{u}, \Gamma_0\widehat{v}\rangle_{\mathfrak{H}} - \langle \Gamma_0\widehat{u}, \Gamma_1\widehat{v}\rangle_{\mathfrak{H}} \text{ for all } u, v \in \mathcal{H} \tag{2.23}$$

and $\widehat{u}, \widehat{v}$ as defined in (2.22). (Clearly, when A, $\mathcal{A}_1$, $\mathcal{A}_2$ are operators, the resolvent difference Equation (2.23) becomes (2.12)).

3 | RICCATI EQUATION FOR RESOLVENTS AND HADAMARD-TYPE FORMULAS FOR EIGENVALUES

In this section, we consider a one-parameter family of self-adjoint extensions of a given symmetric operator perturbed by a family of bounded operators. In turn, the extensions are constructed using families of Lagrangian subspaces in a boundary space and boundary traces that also depend on the parameter. Our final objective is to derive a differential (Riccati-type) equation for the resolvents of the perturbed operators and formulas for the derivatives of their isolated eigenvalues with respect to the parameter. The latter abstract formulas generalize, on the one side, the classical perturbation results from the case of additive perturbations, see, for example, [83, Section II.5], and, on another, the Rayleigh–Hadamard-type variational formulas for eigenvalues of partial differential operators depending on a parameter, see, for example, [72, 80].

3.1 | Parametric families of operators

We continue to assume that A is a densely defined closed symmetric operator with equal (possibly infinite) deficiency indices, that $\mathcal{H}_+ = \mathrm{dom}(A^*)$ is equipped with graph norm of A^*, and that $\mathcal{D}$, the domain of the trace operator, is a dense subspace of $\mathcal{H}_+$. The following hypothesis will be assumed throughout this section.

Hypothesis 3.1. We assume that Hypothesis 2.1 holds for the trace operator T and a subspace $\mathcal{D} \subset \mathcal{H}_+$ with $\mathrm{dom}(\mathrm{T}) = \mathcal{D}$, and, in addition, we assume that the subspace $\mathcal{D}$ of $\mathcal{H}_+$ is equipped with a Banach norm $\|\cdot\|_{\mathcal{D}}$ such that the (injective) embedding $\jmath$ of $\mathcal{D}$ into $\mathcal{H}_+$ is continuous with respect to this norm, that is, $\jmath \in \mathcal{B}(\mathcal{D}, \mathcal{H}_+)$.

A typical example that we have in mind is the Laplacian $A = -\Delta$ on $L^2(\Omega)$ with $\mathrm{dom}(A) = H_0^2(\Omega)$ for an open bounded $\Omega \subset \mathbb{R}^n$ with smooth boundary. In this case, we have

$$A^* = -\Delta,\ \mathcal{H}_+ = \mathrm{dom}(A^*) := \{u \in L^2(\Omega) : \Delta u \in L^2(\Omega)\},$$

$\mathcal{D} := \mathcal{D}^1(\Omega)$, where the space

$$\mathcal{D}^1(\Omega) := \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\}$$

is equipped with the norm $\|u\|_{\mathcal{D}} := (\|u\|^2_{H^1(\Omega)} + \|\Delta u\|^2_{L^2(\Omega)})^{1/2}$.

For $u \in \mathcal{D}$, the trace operator is given by

$$\mathrm{T}u = [\gamma_{_D} u, -\Phi\gamma_{_N} u]^\top \in \mathfrak{H} \times \mathfrak{H} \text{ with } \mathfrak{H} := H^{1/2}(\partial\Omega),$$

here $\gamma_{_D}$ is the Dirichlet and $\gamma_{_N} = \nu \cdot \gamma_{_D} \nabla u$ is the (weak) Neumann trace maps, and Φ is the Riesz isomorphism between $H^{-1/2}(\partial\Omega) = (H^{1/2}(\partial\Omega))^*$ and $H^{1/2}(\partial\Omega)$, cf. (4.21) below.

Proposition 3.2. *Under Hypothesis 3.1, one has* $\mathrm{T} \in \mathcal{B}(\mathcal{D}, \mathfrak{H} \times \mathfrak{H})$*. In addition, if $\mathcal{A}$ is a self-adjoint extension of A with* $\mathrm{dom}(\mathcal{A}) \subset \mathcal{D}$*, then there exist $c, C > 0$ such that*

$$c\|u\|_{\mathcal{H}_+} \leqslant \|u\|_{\mathcal{D}} \leqslant C\|u\|_{\mathcal{H}_+} \textit{ for all } u \in \mathrm{dom}(\mathcal{A}). \tag{3.1}$$

In other words, the norms in $\mathcal{H}_+$ and $\mathcal{D}$ are equivalent on $\mathrm{dom}(\mathcal{A})$ *for any self-adjoint extension $\mathcal{A}$ of A with* $\mathrm{dom}(\mathcal{A}) \subset \mathcal{D}$*. Furthermore, if $V = V^* \in \mathcal{B}(\mathcal{H})$ and $\zeta \notin \mathrm{Spec}(\mathcal{A} + V)$, then*

$$(\mathcal{A} + V - \zeta)^{-1} \in \mathcal{B}(\mathcal{H}, \mathcal{D}). \tag{3.2}$$

Proof. The operator T is bounded as an everywhere defined on the Banach space $\mathcal{D}$ closable operator (see Lemma 2.4). We claim that $\mathrm{dom}(\mathcal{A})$ is a $\|\cdot\|_{\mathcal{D}}$-closed subspace of the Banach space $\mathcal{D}$. Indeed, suppose that $u_n \to u$ in $\mathcal{D}$ for some $u_n \in \mathrm{dom}(\mathcal{A})$. Since $\mathcal{D}$ is continuously embedded into $\mathcal{H}_+$, the sequence $\{u_n\}_{n\in\mathbb{N}}$ is Cauchy in $\mathcal{H}_+$, that is, it is Cauchy with respect to the graph norm of A^*. Hence, $\{u_n\}$ is convergent to u in $\mathcal{H}$ and the sequence of vectors $A^*u_n = \mathcal{A}u_n$ converges in $\mathcal{H}$. Since $\mathcal{A}$ is a closed operator, we conclude that $u \in \mathrm{dom}(\mathcal{A})$, as claimed. Now, we will consider $\jmath$ as a mapping from the Banach space $(\mathrm{dom}(\mathcal{A}), \|\cdot\|_{\mathcal{D}})$ into the Banach space $(\mathrm{dom}(\mathcal{A}), \|\cdot\|_{\mathcal{H}_+})$. This mapping is bounded and bijective; hence, its inverse is also bounded yielding (3.1). Assertion (3.2) follows from Lemma 2.4 and (3.1). □

Remark 3.3. It is worth comparing Lemma 2.4 and 3.2: indeed, (2.4) says that the product $\mathrm{T}R(\zeta, \mathcal{A})$ is a bounded operator, while Proposition 3.2 gives that each factor in this product is bounded. The latter fact will be used in the proof of Theorem 3.18 below (specifically, see (3.21)) and it comes at the expense of assuming Hypothesis 3.1.

Hypothesis 3.4. We assume that

$$\mathrm{T} : [0, 1] \to \mathcal{B}(\mathcal{D}, \mathfrak{H} \times \mathfrak{H}) : t \mapsto \mathrm{T}_t$$

is a one-parameter family of trace operators and $\mathcal{D} \subset \mathcal{H}_+$ is a t-independent subspace such that T_t and $\mathcal{D} = \mathrm{dom}(\mathrm{T}_t)$ satisfy Hypothesis 3.1 (and thus, in particular, Hypothesis 2.1) for each $t \in [0, 1]$. Let $Q : [0, 1] \to \mathcal{B}(\mathfrak{H} \times \mathfrak{H})$, $t \mapsto Q_t$, be a one-parameter family of orthogonal projections.

We assume that $\mathrm{ran}(Q_t) \in \Lambda(\mathfrak{H} \times \mathfrak{H})$ is a Lagrangian plane for each $t \in [0,1]$. We further assume that there exists a family $\mathcal{A}_t$, $t \in [0,1]$, of self-adjoint extensions of A satisfying

$$\mathrm{dom}(\mathcal{A}_t) \subset \mathcal{D}, \tag{3.3}$$

$$\overline{\mathrm{T}_t(\mathrm{dom}(\mathcal{A}_t))} = \mathrm{ran}(Q_t).$$

Let $V : [0,1] \to \mathcal{B}(\mathcal{H})$, $t \mapsto V_t$ be a one-parameter family of self-adjoint bounded operators. We denote $H_t := \mathcal{A}_t + V_t$ and $R_t(\zeta) := (H_t - \zeta)^{-1} \in \mathcal{B}(\mathcal{H})$ for $\zeta \notin \mathrm{Spec}(H_t)$ and $t \in [0,1]$.

Hypothesis 3.4 gives a rather general setup for boundary value problems parameterized by a one-dimensional variable. We briefly list several families of operators for which the operators per se, their domains, and respective traces depend on a given parameter. Our immediate objective is just to give a glimpse of the typical situations of the setup described in Hypothesis 3.4. More examples with detailed analysis are given below, see Subsections 4.2, 4.3, 4.4, 5.2, 5.3, and 5.4.

Example 3.5. A well-studied model that fits Hypothesis 3.4 is the family of Schrödinger operators equipped with Robin-type boundary conditions considered on a family of subdomains $\Omega_t \subset \Omega$ obtained by linear shrinking of a bounded star-shaped domain $\Omega \subset \mathbb{R}^n$ to its center. The linear rescaling of Ω_t back to Ω leads to a one-parameter family of Schrödinger operators $H_t := -\Delta_t + V$ in $L^2(\Omega)$ subject to Robin boundary conditions $(\theta_t u - t^{-1}\frac{\partial u}{\partial \nu}) \restriction_{\partial\Omega} = 0$, where $\theta_t \in L^\infty(\partial\Omega, \mathbb{R})$ is the rescaled boundary function. In this case, the minimal symmetric operator is given by the Laplacian considered on $H^2_0(\Omega)$, and its self-adjoint extensions $-\Delta_t$ are determined by the boundary condition $(\theta_t u - t^{-1}\frac{\partial u}{\partial \nu}) \restriction_{\partial\Omega} = 0$ that, in turn, corresponds to the Lagrangian planes $\{(f,g)^\top \in H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega) : \theta_t f = g\}$ in $H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$. That is, we have

$$\mathcal{H} := L^2(\Omega), \mathfrak{H} := H^{1/2}(\partial\Omega), \mathrm{T}_t := [\gamma_{_D}, -t^{-1}\Phi\gamma_{_N}]^\top,$$

$$A := -\Delta, \mathrm{dom}(A) = H^2_0(\Omega), \mathcal{D} = \mathcal{D}^1(\Omega) := \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\},$$

$$\mathrm{dom}(\mathcal{A}_t) := \{u \in \mathcal{D}^1(\Omega) : \theta_t \gamma_{_D} u = t^{-1}\gamma_{_N} u\},$$

$$\mathrm{ran}(Q_t) := \{(f,g)^\top \in H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega) : \theta_t f = g\},$$

here $\gamma_{_D}$ and $\gamma_{_N}$ denote the Dirichlet and (weak) Neumann traces and $\Phi : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ denotes the Riesz isomorphism, see (4.21). Similar models are systematically studied in [44, 45, 49] and discussed in some details in a more general setting in Section 5.4 below.

Example 3.6. Our next example is a matrix second-order operator posted on a multidimensional infinite cylinder with variable cross sections. We denote by $t \in \mathbb{R}$ the axial and by x the transversal variables, that is, we set

$$\Omega := \left\{(t,x) \in \mathbb{R}^{n+1} : t \in \mathbb{R}, x \in \mathbb{B}^n_{r(t)}\right\} \subset \mathbb{R}^{n+1},$$

where, for instance, $r(t) = 1 + t/(1+t^2)$, and $\mathbb{B}^n_r$ is the ball in $\mathbb{R}^n$ of radius r centered at zero. Denoting $\Delta_{(t,x)} = \partial^2_t + \Delta_x$ and $\Delta_x = \sum_{j=1}^n \partial^2_{x_j}$, we will consider in $L^2(\Omega; \mathbb{C}^N)$ the Schrödinger operator

$$-\Delta_{(t,x)} + V = -\partial^2_t + B_t, \text{ where } B_t = -\Delta_x(t) + V \text{ and } V = V(t,x)$$

is a smooth-bounded $(N \times N)$-matrix-valued potential taking symmetric values, while the x-Laplace operator $-\Delta_x(t)$ is acting in $L^2(\mathbb{B}^n_{r(t)}; \mathbb{C}^N)$ and equipped with the following domain:

$$\mathrm{dom}(-\Delta_x(t)) := \big\{ u \in \mathcal{D}^1(\mathbb{B}^n_{r(t)}) : \mathrm{T}u := (\gamma_{D,\partial\mathbb{B}^n_{r(t)}} u, -\Phi\gamma_{N,\partial\mathbb{B}^n_{r(t)}} u) \in \mathcal{F}_t \big\},$$

where $\mathcal{F} : t \mapsto \mathcal{F}_t$ is a given smooth family of Lagrangian subspaces in the boundary space $H^{1/2}(\partial\mathbb{B}^n_{r(t)}) \times H^{1/2}(\partial\mathbb{B}^n_{r(t)})$. We note parenthetically that the spectral flow of the family $\{B_t\}_{t=-\infty}^{\infty}$ of the self-adjoint operators B_t is of interest as it is related to the spectrum of the Schrödinger operator $-\Delta_{(t,x)} + V$ in $L^2(\Omega; \mathbb{C}^N)$; this relation could be established using spatial dynamics, cf. [91, 118, 119], via a connection to a first-order differential operator, cf. [97] and [65]. Rescaling $x \mapsto z = x/r(t)$ of $\mathbb{B}^n_{r(t)}$ onto $\mathbb{B}^n_1$ gives rise to a family of operators H_t defined analogously to B_t by

$$H_t = -(r(t))^{-2}\Delta_z(t) + V_t, \ \text{ where } z \in \mathbb{B}^n_1, V_t(z) = V(t, r(t)z), \tag{3.4}$$

the Lagrangian subspace $\widehat{\mathcal{F}}_t$ is obtained from $\mathcal{F}_t$ by rescaling as well, and the z-Laplacian $-\Delta_z(t)$ acting in $L^2(\mathbb{B}^n_1; \mathbb{C}^N)$ is equipped with the domain

$$\mathrm{dom}(-\Delta_z(t)) := \big\{ w \in \mathcal{D}^1(\mathbb{B}^n_1) : \mathrm{T}_t w := (\gamma_{D,\partial\mathbb{B}^n_1} w, -(r(t))^{-1}\Phi\gamma_{N,\partial\mathbb{B}^n_1} w) \in \widehat{\mathcal{F}}_t \big\}. \tag{3.5}$$

The family of operators H_t can be considered within the setting of Hypothesis 3.4 with T_t given in (3.5), V_t given in (3.4), and Q_t being the projection onto $\widehat{\mathcal{F}}_t$.

Example 3.7. The next example is given by a one-parameter family of operators arising in Floquet–Bloch decomposition of periodic Hamiltonians on $\mathbb{R}$, see [111, Theorem XII.88] and Example 4.18 below. We consider the Schrödinger operator $A := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on (0,1) with domain $H^2_0(0,1)$ and its sefl-adjoint extensions determined by the following boundary conditions $u(1) = e^{\mathrm{i}t}u(0), u'(1) = e^{\mathrm{i}t}u'(0), t \in [0, 2\pi)$. In this case, the setup described in Hypothesis 3.4 is as follows:

$$\mathcal{H} := L^2(0,1), \mathfrak{H} := \mathbb{C}^2, \Gamma_0 u = (u(0), u(1)), \Gamma_1 u = (u'(0), -u'(1)),$$

$$A := -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \mathrm{dom}(A) = H^2_0(0,1), \mathcal{D} = H^2(0,1);$$

$$\mathrm{dom}(\mathcal{A}_t) := \{u \in H^2(\Omega) : u(1) = e^{\mathrm{i}t}u(0), u'(1) = e^{\mathrm{i}t}u'(0)\},$$

$$\mathrm{ran}(Q_t) := \{(z_1, z_2, z_3, z_4) \in \mathbb{C}^4 : z_2 = e^{\mathrm{i}t}z_1, z_3 = -e^{\mathrm{i}t}z_4\}.$$

Example 3.8. This example concerns a *first-order* operator related to the perturbed Cauchy–Riemann operator on a two-dimensional infinite cylinder, cf. [114, Section 7]. Let $a, b : \mathbb{R} \to \mathbb{R}$ be smooth functions having limits $a_\pm < b_\pm$ at $\pm\infty$ and such that $a(t) < b(t)$ for all $t \in \mathbb{R}$, and consider the two-dimensional cylinder

$$\Omega = \{(t, x) \in \mathbb{R}^2 : a(t) < x < b(t), t \in \mathbb{R}\}.$$

For $N \geqslant 1$, we consider the perturbed Cauchy–Riemann operator $\bar{\partial}_{S,\mathcal{F}} = \partial_t + B_t$ acting in the space $L^2(\Omega;\mathbb{R}^{2N})$ of real vector-valued functions, where

$$B_t = -J_N \partial_x(t) + S, t \in \mathbb{R}, J_N = \begin{bmatrix} 0 & I_{\mathbb{R}^N} \\ -I_{\mathbb{R}^N} & 0 \end{bmatrix},$$

and $S = S(t,x) \in \mathbb{R}^{2N\times 2N}$ is a given smooth-bounded matrix-valued function taking symmetric values and having limits $S_\pm(x)$ as $t \to \pm\infty$. Here and below for each $t \in \mathbb{R}$, we denote by $\partial_x(t)$ the operator of x-differentiation in $L^2\big((a(t), b(t));\mathbb{R}^{2N}\big)$ with the domain

$$\operatorname{dom}(\partial_x(t)) = \big\{u \in H^1\big((a(t), b(t));\mathbb{R}^{2N}\big) : \mathrm{T}_t u := (u(a(t)), u(b(t))) \in \mathcal{F}_t\big\}, \tag{3.6}$$

where $\mathcal{F} : t \mapsto \mathcal{F}_t \in \Lambda(2N)$ is a given smooth family of Lagrangian subspaces in $\mathbb{R}^{4N}$ having limits $\mathcal{F}_\pm$ as $t \to \pm\infty$. Again, we note that the spectral flow of the family $\{B_t\}_{t=-\infty}^{+\infty}$ of the self-adjoint operators B_t is of interest since, in particular, it is equal (see, e.g., [65, 97]) to the Fredholm index of the Cauchy–Riemann operator $\bar{\partial}_{S,\mathcal{F}}$, see a detailed discussion and various implications of this fact in [114, Section 7]. Rescaling $u(t,x) \mapsto w(t,z) := u(t, z(b(t) - a(t)) + a(t))$, $z \in (0,1)$, gives rise to an analogous to B_t operator H_t acting in $L^2([0,1];\mathbb{R}^{2N})$ as

$$H_t = -J_N \partial_z(t) + V_t, t \in \mathbb{R}, z \in (0,1), \text{where } V_t(z) = S(t, (b(t) - a(t))z + a(t)), \tag{3.7}$$

and $\partial_z(t) = (b(t) - a(t))\frac{\partial}{\partial z}$ is the operator in $L^2([0,1];\mathbb{R}^{2N})$ with the domain

$$\operatorname{dom}(\partial_z(t)) = \big\{w \in H^1([0,1];\mathbb{R}^{2N})) : \mathrm{T}w := (w(0), w(1)) \in \mathcal{F}_t\big\}.$$

The family of operators H_t can be considered within the setting of Hypothesis 3.4 with the trace given in (3.6), with Q_t being the projection onto $\mathcal{F}_t$, and V_t given in (3.7).

Example 3.9. Parameter-depended Hamiltonians satisfying Hypothesis 3.4 play an important role in the theory of quantum graphs. For example, the well-known eigenvalue bracketing, see [21, Section 3.1.6], is established by studying the dependence of eigenvalues of the δ-type graph Laplacian on the coupling constant. We refer the reader to Section 4.3 for an in-depth discussion of parameter-depended quantum graphs satisfying Hypothesis 3.4.

Remark 3.10. Hypothesis 3.4 is satisfied, for example, when $\operatorname{ran}(Q_t) \in \Lambda(\mathfrak{H}\times\mathfrak{H})$ is $(\mathcal{D}, \mathrm{T}_t)$ aligned, cf. Definition A.4, and $\mathcal{A}_t$ is the operator associated with $\operatorname{ran}(Q_t)$ and $\operatorname{dom}(\mathcal{A}_t) \subset \mathcal{D}$, $t \in [0,1]$, see Theorem A.1. Conversely, if $\mathcal{A}_t$ is a self-adjoint extension of A with $\operatorname{dom}(\mathcal{A}_t) \subset \mathcal{D}$, $t \in [0,1]$, which is $(\mathcal{D}, \mathrm{T}_t)$ aligned and $\operatorname{ran}(Q_t)$ is a subspace associated with $\mathcal{A}_t$ then $\operatorname{ran}(Q_t) \in \Lambda(\mathfrak{H}\times\mathfrak{H})$, $t \in [0,1]$, see Theorem A.2.

3.2 | Resolvent expansion

Our first major result in the setting of Hypothesis 3.4 is a symplectic formula for the difference of the resolvents $R_t(\zeta) = (H_t - \zeta)^{-1}$ of the operators H_t at different values of t.

Theorem 3.11. *Assume Hypothesis 3.4 and let $t, s, \tau \in [0,1]$, $\zeta \notin \operatorname{Spec}(H_t) \cup \operatorname{Spec}(H_s)$. Then for $R_t(\zeta) := (H_t - \zeta)^{-1}$ and $H_t = \mathcal{A}_t + V_t$, one has*

$$R_t(\zeta) - R_s(\zeta) = R_t(\zeta)(V_s - V_t)R_s(\zeta) + (\mathrm{T}_\tau R_t(\overline{\zeta}))^* J \mathrm{T}_\tau R_s(\zeta) \tag{3.8}$$

$$= R_t(\zeta)(V_s - V_t)R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^*(Q_t - Q_s) J \mathrm{T}_s R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta). \tag{3.9}$$

The operators whose adjoints enter (3.8), (3.9) are being considered as elements of $\mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H})$ (cf. Proposition 3.2), and thus, their adjoints are elements of $\mathcal{B}(\mathfrak{H} \times \mathfrak{H}, \mathcal{H})$.

Proof. As in the proof of Theorem 2.6 for arbitrary $u, v \in \mathcal{H}$ and $\mathrm{T}_\tau = [\Gamma_0, \Gamma_1]^\top$, one has

$$\langle R_t(\zeta)u - R_s(\zeta)u, v\rangle_{\mathcal{H}} = \langle R_t(\zeta)u - R_s(\zeta)u, (H_t - \overline{\zeta})R_t(\overline{\zeta})v\rangle_{\mathcal{H}}$$

$$= \langle (H_t - \zeta)R_t(\zeta)u, R_t(\overline{\zeta})v\rangle_{\mathcal{H}} - \langle R_s(\zeta)u, (A^* + V_t - \overline{\zeta})R_t(\overline{\zeta})v\rangle_{\mathcal{H}}$$

$$= \langle u, R_t(\overline{\zeta})v\rangle_{\mathcal{H}} + \langle R_s(\zeta)u, (V_s - V_t)R_t(\overline{\zeta})v\rangle_{\mathcal{H}} - \langle (A^* + V_s - \zeta)R_s(\zeta)u, R_t(\overline{\zeta})v\rangle_{\mathcal{H}}$$

$$+ \langle \Gamma_1 R_s(\zeta)u, \Gamma_0 R_t(\overline{\zeta})v\rangle_{\mathfrak{H}} - \langle \Gamma_0 R_s(\zeta)u, \Gamma_1 R_t(\overline{\zeta})v\rangle_{\mathfrak{H}}$$

$$= \langle R_s(\zeta)u, (V_s - V_t)R_t(\overline{\zeta})v\rangle_{\mathcal{H}} + \langle \Gamma_1 R_s(\zeta)u, \Gamma_0 R_t(\overline{\zeta})v\rangle_{\mathfrak{H}} - \langle \Gamma_0 R_s(\zeta)u, \Gamma_1 R_t(\overline{\zeta})v\rangle_{\mathfrak{H}}$$

$$= \Big\langle \Big(R_t(\zeta)(V_s - V_t)R_s(\zeta) + (\Gamma_0 R_t(\overline{\zeta}))^* \Gamma_1 R_s - (\Gamma_1 R_t(\overline{\zeta}))^* \Gamma_0 R_s \Big) u, v \Big\rangle_{\mathcal{H}}.$$

Thus,

$$R_t(\zeta) - R_s(\zeta) = R_t(\zeta)(V_s - V_t)R_s(\zeta) + (\Gamma_0 R_t(\overline{\zeta}))^* \Gamma_1 R_s(\zeta) - (\Gamma_1 R_t(\overline{\zeta}))^* \Gamma_0 R_s(\zeta),$$

yielding (3.8). In order to prove (3.9), we note that

$$\mathrm{T}_s R_s(\zeta) = Q_s \mathrm{T}_s R_s(\zeta) \text{ and } \mathrm{T}_t R_t(\zeta) = Q_t \mathrm{T}_t R_t(\zeta).$$

In addition, we have $Q_s J Q_s = 0$ since $\operatorname{ran}(Q_s)$ is Lagrangian. This implies

$$(\mathrm{T}_t R_t(\overline{\zeta}))^* J \mathrm{T}_t R_s(\zeta) = (\mathrm{T}_t R_t(\overline{\zeta}))^* J \mathrm{T}_s R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta)$$

$$= (\mathrm{T}_t R_t(\overline{\zeta}))^* Q_t J Q_s \mathrm{T}_s R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta)$$

$$= (\mathrm{T}_t R_t(\overline{\zeta}))^*(Q_t - Q_s) J \mathrm{T}_s R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta).$$

Utilizing this and letting $\tau = t$ in (3.8) yields (3.9). □

Remark 3.12. We note that (3.8) holds even if $\mathcal{A}_s$ is a nonself-adjoint restriction of A.

Next, given the one-parameter families of self-adjoint extensions $\mathcal{A}_t$, traces T_t and operators V_t described in Hypothesis 3.4, we will show that the resolvent operators for $H_t = \mathcal{A}_t + V_t$ are continuous (differentiable) at a given point $t = t_0$ whenever the mappings $t \mapsto Q_t$, $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$ are continuous (differentiable) at t_0.

To introduce appropriate assumptions, we recall from Proposition 3.2 (replacing $\operatorname{dom}(\mathcal{A})$ by $\operatorname{dom}(\mathcal{A}_t)$) that under Hypothesis 3.1, the norms in $\mathcal{D}$ and $\mathcal{H}_+$ are equivalent on $\operatorname{dom}(\mathcal{A}_t)$ for each

$t \in [0,1]$, cf. (3.1), but with the constant c that might depend of t. We will need a uniform for t near t_0 version of this assertion: In addition to Hypothesis 3.4, we will often assume that, for a given $t_0 \in [0,1]$, there are constants $C, c > 0$ such that

$$c\|u\|_{\mathcal{H}_+} \leqslant \|u\|_{\mathcal{D}} \leqslant C\|u\|_{\mathcal{H}_+} \text{ for all } u \in \operatorname{dom}(\mathcal{A}_t) \text{ and } t \text{ near } t_0. \tag{3.10}$$

These inequalities are equivalent to uniform with respect to the parameter t boundedness of the norms of resolvents of $\mathcal{A}_t$ as operators from $\mathcal{H}$ to $\mathcal{D}$, see Proposition 3.15 below. We stress that (3.10) does *not* mean that the norms $\|\cdot\|_{\mathcal{H}_+}$ and $\|\cdot\|_{\mathcal{D}}$ are equivalent on $\mathcal{D}$; they are equivalent only on the domains of the extensions $\mathcal{A}_t$ of A but uniformly for t near t_0.

Hypothesis 3.13. In addition to Hypotheses 3.1 and 3.4, we assume, for a given $t_0 \in [0,1]$, that

$$\|(\mathcal{A}_t - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} = \mathcal{O}(1) \text{ as } t \to t_0. \tag{3.11}$$

Remark 3.14. Suppose that V_t form Hypothesis 3.4 satisfies $V_t = \mathcal{O}(1)$, $t \to t_0$ and that $\zeta \in \mathbb{C}\setminus\mathbb{R}$. Then (3.11) is equivalent to

$$\|(\mathcal{A}_t + V_t - \zeta)^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} = \mathcal{O}(1) \text{ as } t \to t_0.$$

Indeed, we have

$$(\mathcal{A}_t + V_t - \zeta)^{-1} = (\mathcal{A}_t - \mathbf{i})^{-1} + (\mathcal{A}_t - \mathbf{i})^{-1}(\mathbf{i} - \zeta + V_t)(\mathcal{A}_t + V_t - \zeta)^{-1}.$$

Considering $(\mathcal{A}_t - \mathbf{i})^{-1}$ as a mapping from $\mathcal{H}$ to $\mathcal{D}$, $(\mathcal{A}_t + V_t - \zeta)^{-1}$ as a mapping from $\mathcal{H}$ to itself, and using the bound $\|(\mathcal{A}_t + V_t - \zeta)^{-1}\|_{\mathcal{B}(\mathcal{H})} \leqslant (|\operatorname{Im}\zeta|)^{-1}$, we infer the claim.

The equivalence of Hypothesis 3.13 and assertion (3.10) is proven next.

Proposition 3.15. *Assume Hypothesis 3.1. Then, (3.10) is equivalent to (3.11).*

Proof. If (3.11) holds, then for any $u \in \operatorname{dom}(\mathcal{A}_t)$ and t near t_0, one has

$$\begin{aligned}\|u\|_{\mathcal{D}} &= \|(\mathcal{A}_t - \mathbf{i})^{-1}(\mathcal{A}_t - \mathbf{i})u\|_{\mathcal{D}} \leqslant c\|(\mathcal{A}_t - \mathbf{i})u\|_{\mathcal{H}} \\ &\leqslant c(\|\mathcal{A}_t u\|_{\mathcal{H}} + \|u\|_{\mathcal{H}}) \leqslant \sqrt{2}c\|u\|_{\mathcal{H}_+},\end{aligned}$$

thus proving (3.10), as $\|u\|_{\mathcal{H}_+} \leqslant c\|u\|_{\mathcal{D}}$ by Hypothesis 3.1.

Conversely, using (3.10), for all t near t_0 and any $v \in \mathcal{H}$, one has

$$\begin{aligned}\|(\mathcal{A}_t - \mathbf{i})^{-1}v\|_{\mathcal{D}} &\leqslant C\|(\mathcal{A}_t - \mathbf{i})^{-1}v\|_{\mathcal{H}_+} \\ &= C\big(\|(\mathcal{A}_t - \mathbf{i})^{-1}v\|^2_{\mathcal{H}} + \|\mathcal{A}_t(\mathcal{A}_t - \mathbf{i})^{-1}v\|^2_{\mathcal{H}}\big)^{1/2} \\ &\leqslant C\big(\|(\mathcal{A}_t - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H})}\|v\|^2_{\mathcal{H}} + (\|v\|_{\mathcal{H}} + \|(\mathcal{A}_t - \mathbf{i})^{-1}v\|_{\mathcal{H}})^2\big)^{1/2} \\ &\leqslant \sqrt{5}C\|v\|_{\mathcal{H}},\end{aligned}$$

since $\mathcal{A}_t$ is self-adjoint, thus proving (3.11). ∎

Assuming that the families Q_t, T_t are continuous at $t = t_0$, under Hypothesis 3.13 the resolvent difference formula (3.9) with $V_t = 0$ shows (as in the proof of Theorem 3.18 (1) below) that

$$\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H})} \underset{t\to t_0}{=} o(1),$$

$$\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)} \underset{t\to t_0}{=} o(1).$$

In the proof of differentiability of the resolvent of H_t, we will need, however, a somewhat stronger continuity assumption, given next, regarding the resolvents of $\mathcal{A}_t$ considered as operators from $\mathcal{H}$ to $\mathcal{D}$. As we will demonstrate in Sections 4 and 5 below, the stronger assumption does hold in the case of boundary triplets and for Robin-type elliptic partial differential operators on bounded domains.

Hypothesis 3.16. In addition to Hypotheses 3.1 and 3.4, we assume that for a given $t_0 \in [0,1]$, one has

$$\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} = o(1),\ t \to t_0. \tag{3.12}$$

Remark 3.17. Suppose that V_t from Hypothesis 3.4 satisfies $(V_t - V_{t_0}) = o(1)$, $t \to t_0$ and that $\zeta \in \mathbb{C} \setminus \mathbb{R}$. Then (3.12) is equivalent to

$$\|(\mathcal{A}_t + V_t - \zeta)^{-1} - (\mathcal{A}_{t_0} + V_{t_0} - \zeta)^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} = o(1) \text{ as } t \to t_0.$$

The proof is similar to the proof of Remark 3.14. We also note that (3.12) implies (3.11).

After these preliminaries, we are ready to present the main result of this subsection.

Theorem 3.18. *We fix $t_0 \in [0,1]$, $\zeta_0 \notin \operatorname{Spec}(H_{t_0})$ and define*

$$\mathcal{U}_\varepsilon = \{(t,\zeta) \in [0,1]\times\mathbb{C} : |t - t_0| \leqslant \varepsilon, |\zeta - \zeta_0| \leqslant \varepsilon\} \textit{ for } \varepsilon > 0.$$

(1) *Assume Hypothesis 3.13 and suppose that the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are continuous at t_0. Then there exists an $\varepsilon > 0$ such that if $(t,\zeta) \in \mathcal{U}_\varepsilon$, then $\zeta \notin \operatorname{Spec}(H_t)$ and the operator-valued function $t \mapsto R_t(\zeta) = (H_t - \zeta)^{-1}$ is continuous at t_0 uniformly for $|\zeta - \zeta_0| < \varepsilon$.*
(2) *Assume Hypothesis 3.13 and suppose that the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are Lipschitz continuous at t_0. Then, there exists a constant $c > 0$ such that for all $(t,\zeta) \in \mathcal{U}_\varepsilon$, one has*

$$\|R_t(\zeta) - R_{t_0}(\zeta)\|_{\mathcal{B}(\mathcal{H})} \leqslant c|t - t_0|. \tag{3.13}$$

(3) *Assume Hypothesis 3.16 and suppose that the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are differentiable at t_0. Then, for some $\varepsilon > 0$, the following asymptotic expansion holds uniformly for $|\zeta - \zeta_0| < \varepsilon$:*

$$\begin{aligned} R_t(\zeta) \underset{t\to t_0}{=} R_{t_0}(\zeta) + \Big(&-R_{t_0}(\zeta)\dot{V}_{t_0}R_{t_0}(\zeta) + (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}R_{t_0}(\zeta) \\ &+(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta)\Big)(t - t_0) + o(t - t_0), \ \textit{in } \mathcal{B}(\mathcal{H}). \end{aligned} \tag{3.14}$$

In particular, the function $t \mapsto R_t(\zeta_0) = (H_t - \zeta_0)^{-1}$ is differentiable at $t = t_0$ and satisfies the following Riccati equation:

$$\begin{aligned} \dot{R}_{t_0}(\zeta_0) = -R_{t_0}(\zeta_0)\dot{V}_{t_0}R_{t_0}(\zeta_0) + (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}R_{t_0}(\zeta_0) \\ + (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^*J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta_0). \end{aligned} \tag{3.15}$$

The operators whose adjoints enter (3.14), (3.15) are considered as elements of $\mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H})$, cf. Proposition 3.2, and their adjoints are elements of $\mathcal{B}(\mathfrak{H} \times \mathfrak{H}, \mathcal{H})$, the dot denotes the derivative with respect to t evaluated at t_0. We emphasize the generality of formulas (3.14)–(3.15) where all three objects may vary: the domain of the extension, the trace operator, and the "lower order terms" of the operator itself. In Theorem 3.26, we will give analogous results using a slightly different description of the domains of the self-adjoint extensions. Also, see Theorem 4.16 for the case when the trace operator is t-independent. We refer to Remark 3.19 below for somewhat more symmetric versions of the RHS of (3.14) and (3.15) and to Remark 3.20 for a comment on the continuity and differentiability conditions in the theorem.

Proof. First, we prove that the mapping $t \mapsto R_t(\mathbf{i}) \in \mathcal{B}(\mathcal{H})$ is continuous at t_0. Hypothesis 3.13 by Remark 3.14 yields

$$\|R_t(\mathbf{i})\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} = \mathcal{O}(1), t \to t_0. \tag{3.16}$$

Using (3.9) with $\zeta = \mathbf{i}$, $s = t_0$, and (3.16), we get

$$\begin{aligned} R_t(\mathbf{i}) - R_{t_0}(\mathbf{i}) = R_t(\mathbf{i})(V_{t_0} - V_t)R_{t_0}(\mathbf{i}) \\ + (\mathrm{T}_tR_t(-\mathbf{i}))^*(Q_t - Q_{t_0})JQ_{t_0}\mathrm{T}_{t_0}R_{t_0}(\mathbf{i}) \\ + (\mathrm{T}_tR_t(-\mathbf{i}))^*J(\mathrm{T}_t - \mathrm{T}_{t_0})R_{t_0}(\mathbf{i}) \underset{t\to t_0}{=} o(1). \end{aligned} \tag{3.17}$$

Proof of (1),(2). Fix $\varepsilon_0 > 0$ such that $\mathbb{B}_{\varepsilon_0}(\zeta_0) \subset \mathbb{C} \setminus \operatorname{Spec}(H_{t_0})$. Then, by (3.17) and [110, Theorem VIII.23], we have $\mathbb{B}_{\varepsilon_0}(\zeta_0) \cap \operatorname{Spec}(H_t) = \emptyset$ for t sufficiently close to t_0. Hence,

$$\sup\{\|R_t(\zeta)\|_{\mathcal{B}(\mathcal{H})} : (t, \zeta) \in \mathcal{U}_\varepsilon\} < \infty \tag{3.18}$$

for a sufficiently small $\varepsilon > 0$. We claim that yet a smaller choice of $\varepsilon > 0$ gives

$$\sup\{\|R_t(\zeta)\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} : (t, \zeta) \in \mathcal{U}_\varepsilon\} < \infty. \tag{3.19}$$

Indeed, by the resolvent identity, one has

$$R_t(\zeta) = R_t(\mathbf{i}) - (\mathbf{i} - \zeta)R_t(\mathbf{i})R_t(\zeta).$$

Using this and (3.16), we see that (3.18) yields (3.19). Next, by (3.9) and (3.19), we infer

$$
\begin{aligned}
R_t(\zeta) - R_{t_0}(\zeta) = R_t(\zeta)(V_{t_0} - V_t)R_{t_0}(\zeta)& \\
+ (\mathrm{T}_t R_t(\overline{\zeta}))^*(Q_t - Q_{t_0})JQ_{t_0}\mathrm{T}_{t_0}R_{t_0}(\zeta)& \\
+ (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_{t_0})R_{t_0}(\zeta)& \\
\leqslant c\max\{\|Q_t - Q_{t_0}\|_{\mathcal{B}(\mathfrak{H}\times\mathfrak{H})}, \|\mathrm{T}_t - \mathrm{T}_{t_0}\|_{\mathcal{B}(\mathcal{H}_+,\mathfrak{H}\times\mathfrak{H})}, \|V_t - V_{t_0}\|_{\mathcal{B}(\mathcal{H})}\}&
\end{aligned}
\tag{3.20}
$$

for some $c > 0$ and all $(t, \zeta) \in \mathcal{U}_\varepsilon$; here, we used the inequality

$$
\|\mathrm{T}_t R_t(\overline{\zeta})\|_{\mathcal{B}(\mathcal{H},\mathfrak{H}\times\mathfrak{H})} \leqslant \|\mathrm{T}_t\|_{\mathcal{B}(\mathcal{D},\mathfrak{H}\times\mathfrak{H})}\|R_t(\overline{\zeta})\|_{\mathcal{B}(\mathcal{H},\mathcal{D})},
\tag{3.21}
$$

see Proposition 3.2 and Remark 3.3. Now both assertions *(1),(2)* follow from (3.20).

Proof of (3). First, we notice that (3.12) and the resolvent identity give

$$
\|R_t(\zeta) - R_{t_0}(\zeta)\|_{\mathcal{B}(\mathcal{H},\mathcal{D})} \to 0,\ t \to 0,
\tag{3.22}
$$

uniformly for $|\zeta - \zeta_0| < \varepsilon$, with $\varepsilon > 0$ as above. Next, by assumptions, we have

$$
\begin{aligned}
Q_t &\underset{t\to t_0}{=} Q_{t_0} + \dot{Q}_{t_0}(t - t_0) + o(t - t_0),\\
V_t &\underset{t\to t_0}{=} V_{t_0} + \dot{V}_{t_0}(t - t_0) + o(t - t_0),\\
\mathrm{T}_t &\underset{t\to t_0}{=} \mathrm{T}_{t_0} + \dot{\mathrm{T}}_{t_0}(t - t_0) + o(t - t_0).
\end{aligned}
$$

Combining these expansions, (3.9), (3.13), and (3.22), we see that

$$
\begin{aligned}
R_t(\zeta) - R_{t_0}(\zeta) &\underset{t\to t_0}{=} (R_{t_0}(\zeta) + \mathcal{O}(t - t_0))(-\dot{V}_{t_0}(t - t_0) + o(t - t_0))R_{t_0}(\zeta)\\
&+ \Big((\mathrm{T}_{t_0} + \mathcal{O}(t - t_0))(R_{t_0}(\overline{\zeta}) + O_{\|\cdot\|_{\mathcal{B}(\mathcal{H},\mathcal{D})}}(1))\Big)^* \times\\
&\qquad \times (\dot{Q}_{t_0}(t - t_0) + o(t - t_0))JQ_{t_0}\mathrm{T}_{t_0}R_{t_0}(\zeta)\\
&+ \Big((\mathrm{T}_{t_0} + \mathcal{O}(t - t_0))(R_{t_0}(\overline{\zeta}) + O_{\|\cdot\|_{\mathcal{B}(\mathcal{H},\mathcal{D})}}(1))\Big)^* \times\\
&\qquad \times J(\dot{\mathrm{T}}_{t_0}(t - t_0) + o(t - t_0))R_{t_0}(\zeta)\\
&\underset{t\to t_0}{=} \Big(-R_{t_0}(\zeta)\dot{V}_{t_0}R_{t_0}(\zeta) + (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta}))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}R_{t_0}(\zeta)\\
&\qquad + (\mathrm{T}_{t_0}R_{t_0})^*J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta)\Big)(t - t_0) + o(t - t_0),
\end{aligned}
$$

in $\mathcal{B}(\mathcal{H})$ uniformly for $|\zeta - \zeta_0| < \varepsilon$. This shows (3.14) that implies (3.15). □

Remark 3.19. The operator $\dot{Q}_{t_0}J \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H})$ in (3.14), (3.15) is self-adjoint. Indeed, since $\operatorname{ran}(Q_t)$ is Lagrangian, we have $J = JQ_t + Q_tJ$ that implies the assertion upon differentiating with respect to t. Since $\dot{Q}_tJ = -J\dot{Q}$, we can rewrite the term $\dot{Q}_{t_0}J$ in (3.14) and (3.15) in a more symmetric fashion as

$$\dot{Q}_{t_0}J = \frac{1}{2}(\dot{Q}_{t_0}J - J\dot{Q}_{t_0}).$$

Furthermore, the identity $Q_tJQ_t = 0$ yields

$$\left(\mathrm{T}_tR_{t_0}(\overline{\zeta})\right)^* J\mathrm{T}_tR_{t_0}(\zeta) = \left(Q_t\mathrm{T}_tR_{t_0}(\overline{\zeta})\right)^* JQ_t\mathrm{T}_tR_{t_0}(\zeta) = 0.$$

Differentiating this identity at $t = t_0$ shows that the respective terms in the RHS of (3.14) and (3.15) could also be rewritten as

$$\begin{aligned}(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^* J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta_0) = \frac{1}{2}\Big(&(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^* J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta_0)\\ &- (\dot{\mathrm{T}}_{t_0}R_{t_0}(\overline{\zeta_0}))^* J\mathrm{T}_{t_0}R_{t_0}(\zeta_0)\Big).\end{aligned}$$

Remark 3.20. The assumptions of continuity and differentiability of the families T, V and Q are imposed at a fixed point $t_0 \in [0,1]$. For many interesting examples, these assumptions hold for all $t_0 \in [0,1]$; a typical situation of this type is described in Example 4.7. However, these assumptions might fail for some points in [0,1]. A typical example of the latter situation is furnished by the classical Hadamard formula setting for star-shaped domains described in Section 5.4 where the trace operator is singular at $t_0 = 0$ but is differentiable for each $t_0 \in (0,1]$.

Remark 3.21. Discontinuities of the path $t \mapsto Q_t$ in general result in discontinuities of the eigenvalues curves. To give an example, let $\mathcal{A}_t = -\Delta$ be the realization of the Laplacian on a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n, n \geqslant 2$, subject to the boundary conditions $\chi_{[0,1/2]}(t)\gamma_{_D}u + \chi_{(1/2,1]}(t)\gamma_{_N}u = 0$; here $\gamma_{_D}, \gamma_{_N}$ are Dirichlet and Neumann traces and χ is the characteristic function. That is, $\mathcal{A}_t$ is the Dirichlet Laplacian for $t \in [0,1/2]$ and the Neumann Laplacian for $t \in (1/2,1]$. The corresponding path of Lagrangian planes is piece-wise constant with a jump at $t = 1/2$. At this point, the boundary conditions change from Dirichlet to Neumann and, due to the celebrated inequality of L. Friedlander [62], this produces a nontrivial shift in the spectrum, which, in turn, shows the discontinuities of the eigenvalues. We revisit Friedlander's Inequality in Example 5.5 below and provide a symplectic proof thereof, cf. [46].

3.3 | Hadamard-type variational formulas

In this section, we derive the first-order expansion formula for the mapping $t \mapsto P(t)H_tP(t)$ near $t = t_0$. Here, the operator $H_t = \mathcal{A}_t + V_t$ is as in Hypothesis 3.16 and $P(t)$ is a spectral projection of H_t that corresponds to the λ-group, cf. [83, Section II.5.1], consisting of m isolated eigenvalues of H_t bifurcating from the eigenvalue $\lambda = \lambda_{t_0}$ of multiplicity m of the operator H_{t_0}, see Hypothesis 3.22 below. A subtlety is presented by the fact that the operators $P(t)H_tP(t)$ act in varying finite-dimensional spaces $\mathrm{ran}(P(t))$; we rectify this by means of a unitary mapping $U : \mathrm{ran}(P(t_0)) \to \mathrm{ran}(P_t)$, as in, for example, [83, Section I.4.6]. After this, we use the first-order perturbation theory for finite-dimensional operators, cf. [83, Section II.5.4], to deduce a formula for the derivative of the eigenvalue curves which we call the *Hadamard-type variational formula*, see (3.38). This terminology stems from a classical Rayleigh–Hadamard–Rellich formulas for derivatives of the eigenvalues of Laplacian posted on a parameter-dependent family of domains, cf.

Section 5.4 below for details of this particular situation. We note that the approach adopted in this section was originally carried out in [96] for a specific PDE situation of the one-parameter family of Schrödinger operators with Robin boundary conditions on star-shaped domains mentioned in Example 3.5.

Hypothesis 3.22. For a given $t_0 \in [0,1]$, we assume that $\lambda = \lambda(t_0)$ is an isolated eigenvalue of H_{t_0} with finite multiplicity $m \in \mathbb{N}$. Let

$$\gamma := \{z \in \mathbb{C} : 2|z-\lambda| = \operatorname{dist}(\lambda, \operatorname{Spec}(H_{t_0}) \setminus \{\lambda\})\},$$

and let $B \subset \mathbb{C}$ denote the disc enclosed by γ such that $\operatorname{Spec}(H_{t_0}) \cap B = \{\lambda\}$.

Throughout this section, we assume Hypothesis 3.13, and that the maps $t \mapsto \mathrm{T}_t, V_t, Q_t$ are continuous at a given $t_0 \in [0,1]$. By Theorem 3.18, there exists $\varepsilon > 0$ such that γ encloses m eigenvalues (not necessarily distinct) of the operator H_t whenever $|t - t_0| < \varepsilon$ and $\varepsilon > 0$ is sufficiently small. For such t, we let $P(t)$ denote the Riesz projection

$$P(t) := \frac{-1}{2\pi\mathbf{i}} \int_\gamma R_t(\zeta)d\zeta, R_t(\zeta) = (H_t - \zeta)^{-1} \tag{3.23}$$

and recall the reduced resolvent given by

$$S := \frac{1}{2\pi\mathbf{i}} \int_\gamma (\zeta-\lambda)^{-1} R_{t_0}(\zeta)d\zeta \tag{3.24}$$

and the identity $P(t_0)R_{t_0}(\zeta) = (\lambda - \zeta)^{-1}P(t_0)$.

Remark 3.23. The Riemann sums defining integrals in (3.23), (3.24) converge not only in $\mathcal{B}(\mathcal{H})$ but also in $\mathcal{B}(\mathcal{H}, \mathcal{D})$. Consequently, $P(t), S \in \mathcal{B}(\mathcal{H}, \mathcal{D})$. In addition, one has

$$\frac{1}{2\pi\mathbf{i}} \int_\gamma \mathrm{T}_t\big((\zeta-\lambda)^{-1}R_t(\zeta)\big)d\zeta = \mathrm{T}_t \frac{1}{2\pi\mathbf{i}} \int_\gamma \big((\zeta-\lambda)^{-1}R_t(\zeta)\big)d\zeta = \mathrm{T}_t S, \tag{3.25}$$
$$(\mathrm{T}_t P(t)) \in \mathcal{B}(\mathcal{H}, \mathfrak{H} \times \mathfrak{H}).$$

This follows from continuity of the mapping $\mathbb{C} \ni \zeta \mapsto R_t(\zeta) \in \mathcal{B}(\mathcal{H}, \mathcal{D})$ for every $t \in [0,1]$ that can be inferred from $R_t(\zeta) - R_t(\zeta_0) = (\zeta - \zeta_0)R_t(\zeta)R_t(\zeta_0)$, (cf. (3.18), (3.19)), and $\mathrm{T}_t \in \mathcal{B}(\mathcal{D}, \mathfrak{H} \times \mathfrak{H})$.

Next, we derive an asymptotic expansion of $P(t)H_tP(t)$ for t near t_0. To that end, we introduce the operator $D(t) := P(t) - P(t_0)$ satisfying $\|D(t)\|_{\mathcal{B}(\mathcal{H})} \underset{t\to t_0}{=} o(1)$, which follows from (3.13) and (3.23). In particular, for t near t_0, the following operators are well defined:

$$\begin{aligned} U(t) &:= (I - D^2(t))^{-1/2}((I-P(t))(I-P(t_0)) + P(t)P(t_0)),\\ U(t)^{-1} &= ((I-P(t_0))(I-P(t)) + P(t_0)P(t))(I-D^2(t))^{-1/2}, \end{aligned} \tag{3.26}$$

moreover, as in [83, Section I.4.6], [63, Proposition 2.18], we note that

$$U(t)P(t_0) = P(t)U(t), \tag{3.27}$$

and that $U(t)$ maps $\operatorname{ran}(P(t_0))$ onto $\operatorname{ran}(P(t))$ unitarily (for t near t_0). Given this auxiliary operators, we are ready to expand $P(t)H_tP(t)$, which is an m-dimensional operator, for t near t_0.

Lemma 3.24. *For a given $t_0 \in [0,1]$, we assume that the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are differentiable at t_0 and that Hypotheses 3.16 and 3.22 hold. Then, one has*

$$\begin{aligned} P(t_0)U(t)^{-1}H_tP(t)U(t)P(t_0) \underset{t\to t_0}{=} \lambda P(t_0) + \Big(P(t_0)\dot{V}_{t_0}P(t_0) \\ -(\mathrm{T}P(t_0))^*\dot{Q}_{t_0}J\mathrm{T}P(t_0) - (\mathrm{T}_{t_0}P(t_0))^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)(t-t_0) + o(t-t_0). \end{aligned} \tag{3.28}$$

Proof. Our strategy is to expand the left-hand side of (3.28) using (3.14). Multiplying (3.14) by $P(t_0)$ from the right and using identity

$$R_{t_0}(\zeta)P(t_0) = P(t_0)R_{t_0}(\zeta) = (\lambda-\zeta)^{-1}P(t_0), \tag{3.29}$$

where $R_t(\zeta) = (H_t - \zeta)^{-1}$, we get

$$\begin{aligned} R_t(\zeta)P(t_0) \underset{t\to t_0}{=} (\lambda-\zeta)^{-1}P(t_0) + (\lambda-\zeta)^{-1}\Big(-R_{t_0}(\zeta)\dot{V}_{t_0}P(t_0) \\ +\Big(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta})\Big)^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) + \Big(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta})\Big)^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)(t-t_0) \\ + o(t-t_0). \end{aligned} \tag{3.30}$$

The proof is split in several steps.

Step 1. One has

$$P(t_0)P(t)P(t_0) \underset{t\to t_0}{=} P(t_0) + o(t-t_0). \tag{3.31}$$

Proof. For any continuous $F : \gamma \to \mathcal{B}(\mathfrak{H}\times\mathfrak{H}, \mathcal{H})$, we have

$$\Big(\int_\gamma F(\zeta)\,d\zeta\Big)^* = -\int_\gamma (F(\overline{\zeta}))^*\,d\zeta.$$

Applying this to $F(\zeta) = \frac{1}{2\pi\mathbf{i}}(\lambda-\zeta)^{-1}\mathrm{T}_{t_0}R_{t_0}(\zeta)$ and using (3.24), (3.25) yields

$$\int_\gamma \Big(\frac{1}{2\pi\mathbf{i}}(\lambda-\overline{\zeta})^{-1}\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta})\Big)^* d\zeta = \Big(-\int_\gamma \frac{1}{2\pi\mathbf{i}}(\lambda-\zeta)^{-1}\mathrm{T}_{t_0}R_{t_0}(\zeta)\,d\zeta\Big)^* = (\mathrm{T}_{t_0}S)^*.$$

We use this, multiply both sides of (3.30) by $-\frac{1}{2\pi\mathbf{i}}$ and integrate over γ to obtain the following:

$$\begin{aligned} P(t)P(t_0) \underset{t\to t_0}{=} P(t_0) + \Big(-S\dot{V}_{t_0}P(t_0) + \Big(\mathrm{T}_{t_0}S\Big)^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) \\ +\Big(\mathrm{T}_{t_0}S\Big)^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)(t-t_0) + o(t-t_0). \end{aligned} \tag{3.32}$$

Taking adjoints, we get

$$P(t_0)P(t) \underset{t\to t_0}{=} P(t_0) + \Big(-P(t_0)\dot{V}_{t_0}S + (\mathrm{T}_{t_0}P(t_0))^*\,\dot{Q}_{t_0}J\mathrm{T}_{t_0}S$$
$$+\Big(\dot{\mathrm{T}}_{t_0}P(t_0)\Big)^*J\mathrm{T}_{t_0}S\Big)(t-t_0) + o(t-t_0).$$

Multiplying this by $P(t_0)$ from the right and using $SP(t_0) = 0$, we arrive at (3.31). □

Step 2. One has

$$P(t_0)U(t)P(t_0) = (P(t_0)U^{-1}(t)P(t_0))^* \underset{t\to t_0}{=} P(t_0) + o(t-t_0), \tag{3.33}$$

$$\begin{aligned}(I-P(t_0))U(t)P(t_0) &= (P(t_0)U(t)^{-1}(I-P(t_0)))^* \\ &\underset{t\to t_0}{=} (I-P(t_0))\Big(-S\dot{V}_{t_0}P(t_0) + \Big(\mathrm{T}_{t_0}S\Big)^*\,\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) \\ &\quad +\Big(\mathrm{T}_{t_0}S\Big)^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)(t-t_0) + o(t-t_0).\end{aligned} \tag{3.34}$$

Proof. First, we note an auxiliary expansion $D(t) \underset{t\to t_0}{=} \mathcal{O}(t-t_0)$ that follows from (3.13), (3.23) and formula $D(t) = P(t) - P(t_0)$. Thus,

$$(I - D^2(t))^{-1/2} \underset{t\to t_0}{=} I + \mathcal{O}(|t-t_0|^2)$$

and then,

$$\begin{aligned}U(t) &= (I-D^2(t))^{-1/2}((I-P(t))(I-P(t_0)) + P(t)P(t_0)) \\ &\underset{t\to t_0}{=} ((I-P(t))(I-P(t_0)) + P(t)P(t_0)) + o(t-t_0).\end{aligned} \tag{3.35}$$

Using this and (3.31), we obtain

$$P(t_0)U(t)P(t_0) \underset{t\to t_0}{=} P(t_0)P(t)P(t_0) + o(t-t_0) \underset{t\to t_0}{=} P(t_0) + o(t-t_0).$$

Similarly, employing (3.35), one infers

$$(I-P(t_0))U(t)P(t_0) \underset{t\to t_0}{=} (I-P(t_0))P(t)P(t_0) + o(t-t_0),$$

and thus, (3.34) follows by multiplying (3.32) by $I - P(t_0)$ from the left. □

Step 3. One has

$$\begin{aligned}P(t_0)U^{-1}(t)R_t(\zeta)U(t)P(t_0) &\underset{t\to t_0}{=} (\lambda-\zeta)^{-1}P(t_0) \\ &+ (\lambda-\zeta)^{-2}\Big(-P(t_0)\dot{V}_{t_0}P(t_0) + \Big(\mathrm{T}_{t_0}P(t_0)\Big)^*\,\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) \\ &+\Big(\mathrm{T}_{t_0}P(t_0)\Big)^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)(t-t_0) + o(t-t_0).\end{aligned} \tag{3.36}$$

Proof. First, we sandwich the middle term in the left-hand side, $R_t(\zeta)$, by $P(t_0) + (I - P(t_0))$ and write

$$P(t_0)U^{-1}(t)R_t(\zeta)U(t)P(t_0) = I + II + III + IV.$$

Let us treat each term individually, starting with

$$\begin{aligned} I \ :=\ & P(t_0)U^{-1}(t)(I - P(t_0)) \times (I - P(t_0))R_t(\zeta)P(t_0) \\ & \times P(t_0)U(t)P(t_0) \underset{t \to t_0}{=} o(t - t_0), \end{aligned}$$

by (3.30), (3.33), and (3.34) as the main terms in the RHS of (3.30) and (3.34), both contain the factor $(t - t_0)$. Similarly, we infer

$$\begin{aligned} II \ :=\ & P(t_0)U^{-1}(t)P(t_0) \times P(t_0)R_t(\zeta)(I - P(t_0)) \\ & \times (I - P(t_0))U(t)P(t_0) \underset{t \to t_0}{=} o(t - t_0), \end{aligned}$$

by (3.30), (3.33), and (3.34), and

$$\begin{aligned} III \ :=\ & P(t_0)U^{-1}(t)(I - P(t_0)) \times R_t(\zeta) \\ & \times (I - P(t_0))U(t)P(t_0) \underset{t \to t_0}{=} o(t - t_0), \end{aligned}$$

by (3.34). The last term admits the required in (3.36) expansion because

$$IV \ := P(t_0)U^{-1}(t)P(t_0) \times P(t_0)R_t(\zeta)P(t_0) \times P(t_0)U(t)P(t_0)$$

and we can use (3.30), identity (3.29), and (twice)(3.33). □

Step 4. Recalling the identities

$$H_t P(t) := \frac{-1}{2\pi\mathbf{i}} \int_\gamma \zeta R_t(\zeta) d\zeta, \quad \frac{1}{2\pi\mathbf{i}} \int_\gamma \zeta(\lambda - \zeta)^{-2} d\zeta = 1,$$

multiplying (3.36) by $-\zeta/2\pi\mathbf{i}$ and then integrating over γ, we arrive at (3.28) □

We are ready to present the main result of this section that gives a formula for the slopes of the appropriately chosen branches of the eigenvalues curves bifurcating from an isolated eigenvalue of finite multiplicity. We recall that our assumptions on differentiability of T, V, and Q are imposed at a particular point t_0 where $\lambda = \lambda(t_0)$ is the isolated eigenvalue, cf. Remark 3.20. To avoid confusions, we also refer to the classical Rellich's example [83, Example V.4.14] recalled as Example 4.8 below to emphasize that we are not claiming global differentiability of all eigenvalue curves. Indeed, in this example, there is a point t_0 where one eigenvalue curve has a singularity, and so, our assumptions do not hold while all others curves are differentiable as claimed in the theorem.

Theorem 3.25. *Assume Hypotheses 3.16 and 3.22 and suppose that the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are differentiable at t_0. We introduce the operator*

$$T^{(1)} := P(t_0)\dot{V}_{t_0}P(t_0) - (\mathrm{T}_{t_0}P(t_0))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) - (\mathrm{T}_{t_0}P(t_0))^*J\dot{\mathrm{T}}_{t_0}P(t_0),$$

and denote the eigenvalues and the orthonormal eigenvectors of this m-dimensional operator by $\{\lambda_j^{(1)}\}_{j=1}^m$ and $\{u_j\}_{j=1}^m \subset \operatorname{ran}(P(t_0)) = \ker(H_{t_0} - \lambda)$ correspondingly.[†] *Then there exists a labeling of the eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of H_t, for t near t_0, satisfying the asymptotic formula*

$$\lambda_j(t) \underset{t\to t_0}{=} \lambda + \lambda_j^{(1)}(t-t_0) + o(t-t_0), \tag{3.37}$$

moreover, one has

$$\dot{\lambda}_j(t_0) = \langle \dot{V}_{t_0}u_j, u_j\rangle_{\mathcal{H}} + \omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j) + \omega(\mathrm{T}_{t_0}u_j, \dot{\mathrm{T}}_{t_0}u_j), \tag{3.38}$$

for each $1 \leqslant j \leqslant m$.

Proof. Recalling that $U(t)$ is a unitary map between $\operatorname{ran}(P(t_0))$ and $\operatorname{ran}(P(t))$, see [83, Section I.4.6] and [63, Proposition 2.18], we note that $H_t \restriction_{\operatorname{ran}(P(t))}$ is similar to

$$P(t_0)U(t)^{-1}H_tP(t)U(t)P(t_0) \restriction_{\operatorname{ran}(P(t_0))}$$

for t near t_0. In particular, the eigenvalues of these operators coincide and it is sufficient to expand the eigenvalues of the latter. To that end, we utilize the expansion (3.28) together with the finite-dimensional first-order perturbation theory, specifically, [83, Theorem II.5.11], to deduce (3.37). Next, we have

$$\begin{aligned}
\dot{\lambda}_j(t_0) &= \lambda_j^{(1)} = \langle T^{(1)}u_j, u_j\rangle_{\mathcal{H}}\\
&= \langle \Big(P(t_0)\dot{V}_{t_0}P(t_0) - (\mathrm{T}_{t_0}P(t_0))^*\dot{Q}_{t_0}J\mathrm{T}_{t_0}P(t_0) - (\mathrm{T}_{t_0}P(t_0))^*J\dot{\mathrm{T}}_{t_0}P(t_0)\Big)u_j, u_j\rangle_{\mathcal{H}}\\
&= \langle \dot{V}_{t_0}u_j, u_j\rangle_{\mathcal{H}} - \omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j) - \omega(\dot{\mathrm{T}}_{t_0}u_j, \mathrm{T}_{t_0}u_j)\\
&= \langle \dot{V}_{t_0}u_j, u_j\rangle_{\mathcal{H}} + \omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j) + \omega(\mathrm{T}_{t_0}u_j, \dot{\mathrm{T}}_{t_0}u_j),
\end{aligned}$$

which gives (3.38). In the last step, we used the inclusions

$$\omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j) \in \mathbb{R} \text{ and } \omega(\mathrm{T}_{t_0}u_j, \dot{\mathrm{T}}_{t_0}u_j) \in \mathbb{R}.$$

The latter inclusion follows from $\omega(\mathrm{T}_tu_j, \mathrm{T}_tu_j) = 0$ after differentiating at $t = t_0$. To prove the former inclusion, we use $JQ_t + Q_tJ = J$ to get $J\dot{Q}_{t_0} = -\dot{Q}_{t_0}J$ and write

$$\begin{aligned}
\omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j) &= \langle J\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j\rangle_{\mathfrak{H}\times\mathfrak{H}}\\
&= -\langle J\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j\rangle_{\mathfrak{H}\times\mathfrak{H}}\\
&= -\omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j) = \overline{\omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j)},
\end{aligned} \tag{3.39}$$

as claimed. □

[†] We stress that u_j are eigenvectors of H_{t_0} corresponding to its eigenvalue $\lambda = \lambda(t_0)$.

In PDE and quantum graph settings, the Lagrangian planes are often defined by operators $[X, Y]$ as in (2.7)–(2.9) rather than by orthogonal projections onto these planes. It is therefore natural to restate (3.14), (3.38) in these terms which we do next. Given families $t \mapsto X_t, Y_t \in \mathcal{B}(\mathfrak{H})$, we will now denote by $\mathcal{A}_t$ the self-adjoint extension of A with $\operatorname{dom}(\mathcal{A}_t) := \{u \in \mathcal{D} : [X_t, Y_t]\mathrm{T}_t u = 0\}$, that is, we augment (3.3) by requiring that

$$\begin{aligned} &\overline{\mathrm{T}_t(\operatorname{dom}(\mathcal{A}_t))} = \operatorname{ran}(Q_t) = \ker([X_t, Y_t]),\\ &X_t, Y_t \in \mathcal{B}(\mathfrak{H}); X_t Y_t^* = Y_t X_t^*, 0 \notin \operatorname{Spec}(M^{X_t, Y_t}), \end{aligned} \tag{3.40}$$

where M^{X_t,Y_t} is defined in (2.9). We recall formula (2.10) for the projection Q_t onto $\ker([X_t.Y_t])$. A typical example of X_t, Y_t are given by $X_t = I$ and $Y_t = -\Theta_t$ where Θ_t is an operator (in general, not local) entering the Robbin boundary condition.

Theorem 3.26. *Under Hypothesis 3.4, if $\mathcal{A}_t$ satisfies (3.40), then the following symplectic resolvent difference formula holds for the resolvent $R_t(\zeta) = (H_t - \zeta)^{-1}$ of the operator $H_t = \mathcal{A}_t + V_t$,*

$$\begin{aligned} R_t(\zeta) - R_s(\zeta) = R_t(\zeta)(V_s - V_t)R_s(\zeta) + (\mathrm{T}_t R_t(\overline{\zeta}))^* Z_{t,s}\mathrm{T}_s R_s(\zeta)\\ + (\mathrm{T}_t R_t(\overline{\zeta}))^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta), \end{aligned} \tag{3.41}$$

where $\zeta \notin (\operatorname{Spec}(H_t) \cup \operatorname{Spec}(H_s))$, $s, t \in [0,1]$, *and the operator* $Z_{t,s} \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H})$ *is given by formula (2.11),*

$$Z_{t,s} := (W(X_t, Y_t))^*(X_t Y_s^* - Y_t X_s^*)(W(X_s, Y_s)). \tag{3.42}$$

Moreover, under Hypothesis 3.13, if the mappings $t \mapsto \mathrm{T}_t, V_t, X_t, Y_t$ are continuous at $t_0 \in [0,1]$ in the respective spaces of operators, then the function $t \mapsto R_t(\zeta_0)$ is continuous at $t = t_0$ for any $\zeta_0 \notin$ $\operatorname{Spec}(H_{t_0})$. *Further, assume Hypothesis 3.16 and suppose that the mappings $t \mapsto \mathrm{T}_t, V_t, X_t, Y_t$ are differentiable at $t_0 \in [0,1]$. Then, the function $t \mapsto R_t(\zeta_0) = (H_t - \zeta_0)^{-1}$ is differentiable at $t = t_0$ and satisfies the following Riccati equation:*

$$\begin{aligned} &\dot{R}_{t_0}(\zeta_0) = -R_{t_0}(\zeta_0)\dot{V}_{t_0}R_{t_0}(\zeta_0)\\ &+ (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^* \Big(W(X_{t_0}, Y_{t_0})\Big)^* (\dot{X}_{t_0}Y_{t_0}^* - \dot{Y}_{t_0}X_{t_0}^*)\Big(W(X_{t_0}, Y_{t_0})\Big)\times\\ &\qquad\qquad \times \mathrm{T}_{t_0}R_{t_0}(\zeta_0)\\ &+ (\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^* J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta_0), \quad \zeta_0 \notin \operatorname{Spec}(H_{t_0}). \end{aligned} \tag{3.43}$$

Furthermore, if $\lambda(t_0) \in \operatorname{Spec}(H_{t_0})$ is an isolated eigenvalue of multiplicity $m \geqslant 1$, then there exists a choice of orthonormal eigenfunctions $\{u_j\}_{j=1}^m \subset \ker(H_{t_0} - \lambda(t_0))$ and a labeling of the eigenvalues

$\{\lambda_j(t)\}_{j=1}^m$ of H_t, for t near t_0, such that the following Hadamard-type formula holds:

$$\dot{\lambda}_j(t_0) = \langle \dot{V}_{t_0} u_j, u_j \rangle_{\mathcal{H}} + \left\langle (X_{t_0} \dot{Y}^*_{t_0} - Y_{t_0} \dot{X}^*_{t_0}) \phi_j, \phi_j \right\rangle_{\mathfrak{H}} + \omega(\mathrm{T}_{t_0} u_j, \dot{\mathrm{T}}_{t_0} u_j), \tag{3.44}$$

where we denote $\phi_j = W(X_{t_0}, Y_{t_0}) \mathrm{T}_{t_0} u_j$, $1 \leqslant j \leqslant m$, with the operator W defined in (2.11), or, equivalently, ϕ_j is a unique vector in $\mathfrak{H}$ satisfying

$$\Gamma_0 u_j = -Y^*_{t_0} \phi_j \text{ and } \Gamma_1 u_j = X^*_{t_0} \phi_j. \tag{3.45}$$

Proof. The resolvent difference formula (3.41) follows from (3.9) and the computation

$$\begin{aligned}(\mathrm{T}_t R_t(\overline{\zeta}))^* (Q_t - Q_s) J \mathrm{T}_s R_s(\zeta) &= (\mathrm{T}_t R_t(\overline{\zeta}))^* Q_t J Q_s \mathrm{T}_s R_s(\zeta) \\ &= (\mathrm{T}_t R_t(\overline{\zeta}))^* \, Z_{t,s} \mathrm{T}_s \, R_s(\zeta).\end{aligned}$$

Hypothesis 3.13 and (3.41) imply continuity of $t \mapsto R_t(\zeta)$ as in the proof of Theorem 3.18. To prove (3.43), we remark that $X_t Y^*_s - Y_t X^*_s = (X_t - X_s) Y^*_s - (Y_t - Y_s) X^*_s$ by (2.8). Plugging this in (3.42), using (3.41) at $s = t_0$, dividing by $(t - t_0)$ and passing to the limit as $t \to t_0$ yields (3.43). Next, we turn to (3.44). We recall that u_j in Theorem 3.25 are the eigenvectors in $\operatorname{ran}(P(t_0))$ such that $T^{(1)} u_j = \lambda^{(1)}_j u_j$. But since $\operatorname{ran}(P(t_0)) = \ker(H_{t_0} - \lambda(t_0))$, the vectors u_j are also eigenvectors of H_{t_0} such that $H_{t_0} u_j = \lambda(t_0) u_j$. By (3.38), we only need to show

$$\omega(\dot{Q}_{t_0} \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j) = \left\langle (X_{t_0} \dot{Y}^*_{t_0} - Y_{t_0} \dot{X}^*_{t_0}) \phi_j, \phi_j \right\rangle_{\mathfrak{H}}. \tag{3.46}$$

Using (2.10) and differentiating Q_t, we infer

$$\begin{aligned}
&\omega(\dot{Q}_{t_0} \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j) \\
&\quad = \omega\Big([-Y^*_{t_0}, X^*_{t_0}]^\top \Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} W(X_t, Y_t) \Big) \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j \Big) \\
&\qquad + \omega\Big(\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} [-Y^*_{t_0}, X^*_{t_0}]^\top \Big) W(X_{t_0}, Y_{t_0}) \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j \Big) \\
&\quad = \Big\langle \Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} W(X_t, Y_t) \Big) \mathrm{T}_{t_0} u_j, [X_{t_0}, Y_{t_0}] \mathrm{T}_{t_0} u_j \Big\rangle_{\mathfrak{H}} \\
&\qquad + \omega\Big(\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} [-Y^*_{t_0}, X^*_{t_0}]^\top \Big) W(X_{t_0}, Y_{t_0}) \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j \Big) \\
&\quad = \omega\Big(\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} [-Y^*_{t_0}, X^*_{t_0}]^\top \Big) W(X_{t_0}, Y_{t_0}) \mathrm{T}_{t_0} u_j, \mathrm{T}_{t_0} u_j \Big),
\end{aligned}$$

where we used $[X_{t_0}, Y_{t_0}] \mathrm{T}_{t_0} u_j = 0$. Finally, employing (2.10) and

$$\mathrm{T}_{t_0} u_j = Q_{t_0} \mathrm{T}_{t_0} u_j = [-Y^*_{t_0}, X^*_{t_0}]^\top \phi_j, \ \phi_j := W(X_{t_0}, Y_{t_0}) \mathrm{T}_{t_0} u_j, \tag{3.47}$$

we obtain

$$\omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j) = \left\langle [\dot{X}^*_{t_0}, \dot{Y}^*_{t_0}]^\top \phi_j, [-Y^*_{t_0}, X^*_{t_0}]^\top \phi_j \right\rangle_{\mathfrak{H}}$$

$$= \left\langle (X_{t_0}\dot{Y}^*_{t_0} - Y_{t_0}\dot{X}^*_{t_0})\phi_j, \phi_j \right\rangle_{\mathfrak{H}},$$

thus completing the proof of (3.44), while (3.45) follows from (3.47). □

Remark 3.27. We close with a remark that assertions proved in Theorem 3.26 allow one to make conclusions regarding the behavior of the spectra of the operators H_t as a function of t, see, for example, [110, Theorem VIII.23]. Also, the results of this section can be used to study various properties of strongly continuous semigroups generated by the operators $-H_t$. For instance, the Trotter–Kato Approximation Theorem, see, for example, [58, Theorem III.4.8], implies that the semigroups are continuous with respect to the parameter t as soon as the continuity of the resolvent of H_t in Theorem 3.26 is established, see Section 5.3 for an example.

4 | ORDINARY BOUNDARY TRIPLETS

Ordinary boundary triplets have been intensively studied since probably [34, 71], see the vast bibliography in [13, 55, 57, 120] and related papers [15, 33, 53, 54, 56, 79, 86, 126] and the bibliography therein. In this section, we revisit main results of Sections 2 and 3 in the context of ordinary boundary triplets and present several applications. The case of boundary triplets is the one that is widely considered in the literature, and in this section, we will see that for this case, one may impose fewer assumptions to prove the same set of general results. Also, we will demonstrate that this case is sufficient to cover many interesting applications. In particular, we show that conclusions of Theorems 3.18, 3.25, and 3.26 hold under a mere assumption that the mappings $t \mapsto Q_t$, $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$ are continuous (differentiable) with respect to t and that $(\mathfrak{H}, \Gamma_{0,t}, \Gamma_{1,t})$ is an ordinary boundary triplet. Utilizing this, we derive Hadamard-type formulas for quantum graphs, Schrödinger operators with singular potentials, and Robin realizations of the Laplace operator on bounded domains.

We recall the following widely used definition, cf. [13, Section 2.1], [57, 71], and [120, Section 14.2].

Definition 4.1. Given a symmetric densely defined closed operator A on a Hilbert space $\mathcal{H}$ with equal deficiency indices, we equip $\mathcal{H}_+ = \mathrm{dom}(A^*)$ with the graph scalar product and consider linear operators Γ_0 and Γ_1 acting from $\mathcal{H}_+$ to a (boundary) Hilbert space $\mathfrak{H}$. We say that $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is a *ordinary boundary triplet* if the operator $\mathrm{T} := (\Gamma_0, \Gamma_1) : \mathcal{H}_+ \to \mathfrak{H} \times \mathfrak{H}$ is surjective and the following abstract Green identity holds:

$$\langle A^*u, v\rangle_{\mathcal{H}} - \langle u, A^*v\rangle_{\mathcal{H}} = \langle \Gamma_1 u, \Gamma_0 v\rangle_{\mathfrak{H}} - \langle \Gamma_0 u, \Gamma_1 v\rangle_{\mathfrak{H}} \text{ for all } u, v \in \mathcal{H}_+. \tag{4.1}$$

In other words, $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is an ordinary boundary triplet, provided that Hypothesis 2.1 holds with $\mathcal{D} = \mathcal{H}_+$ and surjective T. In this case, we have $\mathrm{T} \in \mathcal{B}(\mathcal{H}_+, \mathfrak{H} \times \mathfrak{H})$ by Lemma 2.3 (2).

Remark 4.2. The setting of ordinary boundary triplets gives a particularly simple illustration of Corollary A.5. Specifically, if $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is a ordinary boundary triplet associated with A, then $\mathcal{F} \subset \mathfrak{H} \times \mathfrak{H}$ is Lagrangian if and only if $\mathcal{A} := A^*|_{\mathrm{T}^{-1}(\mathcal{F})}$ is self-adjoint. In other words, the Lagrangian plane $\mathcal{F}$ and the self-adjoint operator $\mathcal{A} := A^*|_{\mathrm{T}^{-1}(\mathcal{F})}$ are automatically aligned in the sense of Definition A.4 as long as $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is a ordinary boundary triplet. In particular, if $\mathcal{A}$ is a self-adjoint extension of A, then the subspace $\mathrm{T}(\mathrm{dom}(\mathcal{A}))$ is closed, cf. [120, Lemma 14.6(iii)].

4.1 | Main results for the case of boundary triplets

In this section, we discuss our main results, Theorems 3.18, 3.26, in the context of boundary triplets. In Proposition 4.5, we verify that Hypothesis 3.16 (and, hence, Hypothesis 3.13) holds automatically for boundary triplets. This allows us to obtain the central result of the current section, Theorem 4.5. The latter, in turn, gives a plethora of applications discussed in Sections 4.2–4.5.

In the setting of boundary triplets, Hypothesis 3.4 should be naturally replaced by the following assumption.

Hypothesis 4.3. Let

$$\mathrm{T} : [0,1] \to \mathcal{B}(\mathcal{H}_+, \mathfrak{H}\times\mathfrak{H}) : t \mapsto \mathrm{T}_t := [\Gamma_{0t}, \Gamma_{1t}]^\top$$

be a one-parameter family of trace operators. Suppose that $(\mathfrak{H}, \Gamma_{0t}, \Gamma_{1t})$ is an ordinary boundary triplet for each $t \in [0,1]$. Let $Q : [0,1] \to \mathcal{B}(\mathfrak{H}\times\mathfrak{H}), t \mapsto Q_t$ be a one-parameter family of orthogonal projections. Suppose that $\mathrm{ran}(Q_t) \in \Lambda(\mathfrak{H}\times\mathfrak{H})$ is a Lagrangian plane for each $t \in [0,1]$. Let $\mathcal{A}_t$ be a family of self-adjoint extensions of A satisfying

$$\mathrm{T}_t(\mathrm{dom}(\mathcal{A}_t)) = \mathrm{ran}(Q_t).$$

Let $V : [0,1] \to \mathcal{B}(\mathcal{H}) : t \mapsto V_t$ be a one-parameter family of self-adjoint bounded operators. We denote $H_t := \mathcal{A}_t + V_t$ and $R_t(\zeta) := (H_t - \zeta)^{-1} \in \mathcal{B}(\mathcal{H})$ for $\zeta \notin \mathrm{Spec}(H_t)$ and $t \in [0,1]$.

Proposition 4.4. *Suppose that Hypothesis 4.3 holds for the ordinary boundary triplet $(\mathfrak{H}, \Gamma_{0t}, \Gamma_{1t})$. If Q and T are continuous at a given $t_0 \in [0,1]$, then*

$$\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)} = o(1),\ t \to t_0. \tag{4.2}$$

In other words, Hypothesis 3.16 is automatically satisfied for the boundary triplets.

Proof. We claim that

$$\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)} \leqslant \sqrt{2}\|(\mathcal{A}_t - \mathbf{i})^{-1} - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H})}. \tag{4.3}$$

Indeed, using $\mathcal{A}_t \subset A^*$, $\mathcal{A}_{t_0} \subset A^*$, we get

$$\begin{aligned}\|(\mathcal{A}_t - \mathbf{i})^{-1}h - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}h\|^2_{\mathcal{H}_+} &= \|(\mathcal{A}_t - \mathbf{i})^{-1}h - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}h\|^2_{\mathcal{H}}\\ &+ \|A^*(\mathcal{A}_t - \mathbf{i})^{-1}h - A^*(\mathcal{A}_{t_0} - \mathbf{i})^{-1}h\|^2_{\mathcal{H}} = 2\|(\mathcal{A}_t - \mathbf{i})^{-1}h - (\mathcal{A}_{t_0} - \mathbf{i})^{-1}h\|^2_{\mathcal{H}}.\end{aligned}$$

Thus, it is enough to prove that the right-hand side of (4.3) is $o(1)$ as $t \to t_0$. To this end, we first note that, given $\mathcal{A}_t u + \mathbf{i}u = f, u \in \mathrm{dom}(\mathcal{A}_t)$, we have

$$\begin{aligned}\|(\mathcal{A}_t + \mathbf{i})^{-1}f\|^2_{\mathcal{H}_+} &= \|u\|^2_{\mathcal{H}_+} = \|A^*u\|^2_{\mathcal{H}} + \|u\|^2_{\mathcal{H}}\\ &= \|\mathcal{A}_t u\|^2_{\mathcal{H}} + \|u\|^2_{\mathcal{H}} = \|\mathcal{A}_t u + \mathbf{i}u\|^2_{\mathcal{H}} = \|f\|^2_{\mathcal{H}};\end{aligned}$$

hence,

$$\|(\mathcal{A}_t + \mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)} \leqslant 1. \tag{4.4}$$

By resolvent difference formula (2.14), we infer

$$
\begin{aligned}
&\|(\mathcal{A}_t-\mathbf{i})^{-1}-(\mathcal{A}_{t_0}-\mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H})}\\
&\quad=\|(\mathrm{T}_t(\mathcal{A}_t+\mathbf{i})^{-1})^{*}(Q_t-Q_{t_0})J\mathrm{T}_t(\mathcal{A}_{t_0}+\mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H})}\\
&\quad\leqslant\|\mathrm{T}_t\|_{\mathcal{B}(\mathcal{H}_+,\mathfrak{H}\times\mathfrak{H})}\|(\mathcal{A}_t+\mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)}\|(Q_t-Q_{t_0})\|_{\mathcal{B}(\mathfrak{H}\times\mathfrak{H})}\times\\
&\quad\times\|\mathrm{T}_t\|_{\mathcal{B}(\mathcal{H}_+,\mathfrak{H}\times\mathfrak{H})}\|(\mathcal{A}_{t_0}+\mathbf{i})^{-1}\|_{\mathcal{B}(\mathcal{H},\mathcal{H}_+)}\\
&\quad\leqslant c\|Q_t-Q_{t_0}\|_{\mathcal{B}(\mathfrak{H}\times\mathfrak{H})}\underset{t\to t_0}{=}o(1), c>0,
\end{aligned}
\tag{4.5}
$$

where we used (4.4), and continuity of Q and T at t_0. Then (4.3) and (4.5) yield (4.2) and so Equation (3.12) in Hypothesis 3.16 holds. □

We summarize our main results for the case of boundary triplets as follows.

Theorem 4.5. *Assume Hypothesis 4.3. If $\mathcal{A}_t$ is defined as in (3.40) and $H_t=\mathcal{A}_t+V_t$, then for $R_t(\zeta)=(H_t-\zeta)^{-1}$, the following resolvent difference formula holds:*

$$
\begin{aligned}
R_t(\zeta)-R_s(\zeta)=R_t(\zeta)(V_s-V_t)R_s(\zeta)+(\mathrm{T}_tR_t(\overline{\zeta}))^{*}Z_{t,s}\mathrm{T}_sR_s(\zeta)\\
+(\mathrm{T}_tR_t(\overline{\zeta}))^{*}J(\mathrm{T}_t-\mathrm{T}_s)R_s(\zeta),
\end{aligned}
\tag{4.6}
$$

where $\zeta\notin(\operatorname{Spec}(H_t)\cup\operatorname{Spec}(H_s))$, $s,t\in[0,1]$ and

$$
Z_{t,s}:=(W(X_t,Y_t))^{*}(X_tY_s^{*}-Y_tX_s^{*})(W(X_s,Y_s)),
$$

with the operator W defined in (2.11). Moreover, if the mappings $t\mapsto\mathrm{T}_t,V_t,X_t,Y_t$ are continuous at $t_0\in[0,1]$ in the respective spaces of operators, then the function $t\mapsto R_t(\zeta_0)$ is continuous at $t=t_0$ for any $\zeta_0\notin\operatorname{Spec}(H_{t_0})$. Further, if the mappings $t\mapsto\mathrm{T}_t,V_t,X_t,Y_t$ are differentiable at $t_0\in[0,1]$, then the function $t\mapsto R_t(\zeta_0)=(H_t-\zeta_0)^{-1}$ is differentiable. In this case, the following two assertions hold.

(1) *The resolvent operators satisfy the following differential equation:*

$$
\begin{aligned}
&\dot{R}_{t_0}(\zeta_0)=-R_{t_0}(\zeta_0)\dot{V}_{t_0}R_{t_0}(\zeta_0)\\
&+(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^{*}\Big(W(X_{t_0},Y_{t_0})\Big)^{*}(\dot{X}_{t_0}Y_{t_0}^{*}-\dot{Y}_{t_0}X_{t_0}^{*})\Big(W(X_{t_0},Y_{t_0})\Big)\mathrm{T}_{t_0}R_{t_0}(\zeta_0)\\
&+(\mathrm{T}_{t_0}R_{t_0}(\overline{\zeta_0}))^{*}J\dot{\mathrm{T}}_{t_0}R_{t_0}(\zeta_0),\quad \zeta_0\notin\operatorname{Spec}(H_{t_0}).
\end{aligned}
\tag{4.7}
$$

(2) *If $\lambda(t_0)\in\operatorname{Spec}(H_{t_0})$ is an isolated eigenvalue of multiplicity $m\geqslant1$, then there exists a choice of orthonormal eigenfunctions $\{u_j\}_{j=1}^m\subset\ker(H_{t_0}-\lambda(t_0))$ and a labeling of the eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of H_t, for t near t_0, such that*

$$
\dot{\lambda}_j(t_0)=\langle\dot{V}_{t_0}u_j,u_j\rangle_{\mathcal{H}}+\Big\langle(X_{t_0}\dot{Y}_{t_0}^{*}-Y_{t_0}\dot{X}_{t_0}^{*})\phi_j,\phi_j\Big\rangle_{\mathfrak{H}}+\omega(\mathrm{T}_{t_0}u_j,\dot{\mathrm{T}}_{t_0}u_j),
\tag{4.8}
$$

where $\phi_j = W(X_{t_0}, Y_{t_0})\mathrm{T}_{t_0} u_j$, $1 \leqslant j \leqslant m$, or, equivalently, ϕ_j is a unique vector in $\mathfrak{H}$ satisfying

$$\Gamma_0 u_j = -Y^*_{t_0}\phi_j \text{ and } \Gamma_1 u_j = X^*_{t_0}\phi_j. \tag{4.9}$$

Proof. The resolvent difference formula (4.6) follows directly from (3.41). The continuity of $t \mapsto R_t(\zeta_0)$ at t_0 follows from Theorem 3.26 upon noticing that Hypothesis 3.13 holds in the setting of boundary triplets by Proposition 4.4. Similarly, Proposition 4.4 combined with (3.43) and (3.44) yields (4.7) and (4.8). □

Remark 4.6.

(1) In the setting of Theorem 4.5, the resolvent difference formula (4.6) can also be rewritten as

$$\begin{aligned} R_t(\zeta) - R_s(\zeta) = \mathcal{R}_t(\zeta)(V_s - V_t)R_s(\zeta) + \mathcal{R}_t(\zeta)\mathrm{T}_t^* Z_{t,s}\mathrm{T}_s R_s(\zeta) \\ + \mathcal{R}_t(\zeta)\mathrm{T}_t^* J(\mathrm{T}_t - \mathrm{T}_s)R_s(\zeta), \end{aligned} \tag{4.10}$$

where in the RHS, we have $\mathcal{R}_t(\zeta) \in \mathcal{B}(\mathcal{H}_-, \mathcal{H})$, that is, as in Proposition 2.12 and Corollary 2.13, we view $\mathcal{R}_t(\zeta) \in \mathcal{B}(\mathcal{H}_-, \mathcal{H})$ as a unique extension of $R_t(\zeta) \in \mathcal{B}(\mathcal{H})$ to an element of $\mathcal{B}(\mathcal{H}_-, \mathcal{H})$, while $\mathrm{T}_t \in \mathcal{B}(\mathcal{H}_+, \mathfrak{H} \times \mathfrak{H})$, $\mathrm{T}_t^* \in \mathcal{B}(\mathfrak{H} \times \mathfrak{H}, \mathcal{H}_-)$. We note that, in a more general setting of Theorem 3.26, the trace operator T_t is unbounded and one only has the inclusion $(\mathrm{T}_t R_t(\overline{\zeta}))^* \supseteq R_t(\zeta)(\mathrm{T}_t)^*$. In this case, (4.10) holds provided $\operatorname{ran}(Z_{t,s}\mathrm{T}_s R_s(\zeta)) \subseteq J\mathrm{T}(\mathcal{D})$.

(2) The resolvent difference formula derived in Theorem 4.5 yields continuity of the mapping $\mathcal{B}(\mathfrak{H}) \times \mathcal{B}(\mathfrak{H}) \ni (X, Y) \mapsto (\mathcal{A}_{X,Y} - \mathbf{i})^{-1} \in \mathcal{B}(\mathcal{H})$; here, for an ordinary boundary triplet $(\mathfrak{H}, \Gamma_0, \Gamma_1)$, we denote by $\mathcal{A}_{X,Y}$ the self-adjoint extension of A such that $\mathrm{T}(\operatorname{dom}(\mathcal{A}_{X,Y})) = \ker([X, Y])$, cf. (3.40).

In Sections 4.2–4.5 below, we will give applications of Theorem 4.5 for several important classes of problems that fit the framework of the boundary triplets. To give the simplest possible illustration of the setup described in Hypothesis 4.3 and of Theorem 4.5, we now consider the following two ODE examples where the conclusions of the theorem are probably well known, see, for example, [10, 40, 41, 83] and the vast bibliography therein.

Example 4.7. Let $Au = -u''$ be the minimal symmetric operator on $\mathcal{H} = L^2(0,1)$ with domain $\operatorname{dom}(A) = H^2_0(0,1)$ so that $A^*u = -u''$ with $\operatorname{dom}(A^*) = \mathcal{H}_+ = H^2(0,1)$, set $\mathfrak{H} = \mathbb{C}^2$ and introduce the surjective trace operator $\mathrm{T} = (\Gamma_0, \Gamma_1) \in \mathcal{B}(\mathcal{H}_+, \mathfrak{H} \times \mathfrak{H})$ using the Dirichlet and (inward) Neumann traces $\Gamma_0 u = [u(0), u(1)]^\top$ and $\Gamma_1 u = [u'(0), -u'(1)]^\top$. Integration by parts yields (4.1), and thus, $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is an ordinary boundary triplet, cf. [120, Section 14.4]. For $t \in [0,1]$, we let $\mathcal{A}_t$ denote the self-adjoint extension of A with the domain

$$\operatorname{dom}(\mathcal{A}_t) = \{u \in H^2(0,1) : \cos(\pi t/2)\Gamma_0 u - \sin(\pi t/2)\Gamma_1 u = 0\} = \ker([X_t, Y_t]), \tag{4.11}$$

where, cf. (3.40),

$$X_t = \cos(\pi t/2) I_2,\ Y_t = -\sin(\pi t/2) I_2,\ Q_t = \begin{bmatrix} \sin^2(\pi t/2) & \frac{1}{2}\sin(\pi t) \\ \frac{1}{2}\sin(\pi t) & \cos^2(\pi t/2) \end{bmatrix}.$$

Given a bounded real-valued potential V, we let $H_t u = -u'' + Vu$, $t \in [0,1]$, be the family of scalar Schrödinger operators on $L^2(0,1)$ equipped with the boundary conditions specified in (4.11) so that Hypothesis 4.3 holds. In particular, H_0 is the Dirichlet and H_1 is the Neumann

Schrödinger operator. To apply Theorem 4.5, we first perform a standard calculation of the resolvent $R_t(\zeta) = (H_t - \zeta)^{-1}$, cf. for example, [123, Lemma 9.7]: For $t \in [0,1]$ and $\zeta \in \mathbb{C}$, we let $v_t(\cdot\,;\zeta)$, $w_t(\cdot\,;\zeta)$ denote the solutions to the equation $-u'' + Vu = \zeta u$ that satisfy the initial conditions

$$\begin{aligned}(v_t(0;\zeta), v_t'(0,\zeta)) &= (\sin(\pi t/2), \cos(\pi t/2)),\\ (w_t(1;\zeta), w_t'(1,\zeta)) &= (\sin(\pi t/2), -\cos(\pi t/2)),\end{aligned}$$

and let $\mathcal{W}_t(\zeta) = v_t(x;\zeta)w_t'(x;\zeta) - v_t'(x;\zeta)w_t(x;\zeta)$ denote their Wronskian. Then, for each $u \in L^2(0,1)$, the function $R_t(\zeta)u$ is given by the formula

$$(R_t(\zeta)u)(x) = (\mathcal{W}_t(\zeta))^{-1}\left(w_t(x;\zeta)\int_0^x v_t(y;\zeta)u(y)\mathrm{d}y + v_t(x;\zeta)\int_x^1 w_t(y;\zeta)u(y)\mathrm{d}y\right),$$

$x \in [0,1]$. Using this, it is convenient to write $\mathrm{T}R_t(\zeta) = K_t(\zeta)L_t(\zeta)$ where we temporarily introduced the (4×2) matrix $K_t(\zeta)$ and the operator $L_t(\zeta)$ by the formulas

$$\begin{aligned}K_t(\zeta) &= (\mathcal{W}_t(\zeta))^{-1}[\sin(\pi t/2)I_2, \cos(\pi t/2)I_2]^\top,\\ L_t(\zeta)u &= \left[\langle w_t(\cdot;\zeta), \overline{u}\rangle_{L^2}, \langle v_t(\cdot;\zeta), \overline{u}\rangle_{L^2}\right]^\top, L_t(\zeta) \in \mathcal{B}(L^2(0,1), \mathbb{C}^2)\end{aligned}$$

so that $(L_t(\zeta))^*$ maps $(z_1, z_2) \in \mathbb{C}^2$ into $w_t(\cdot\,;\overline{\zeta})z_1 + v_t(\cdot\,;\overline{\zeta})z_2 \in L^2(0,1)$. Theorem 4.5 and a short calculation now yield

$$\begin{aligned}(R_t(\zeta) - R_s(\zeta))u &= (\mathcal{W}_t(\zeta)\mathcal{W}_s(\zeta))^{-1}\sin(\pi(t-s)/2)\\ &\times \big(\langle w_s(\cdot;\zeta), \overline{u}\rangle_{L^2} w_t(\cdot;\zeta) + \langle v_s(\cdot;\zeta), \overline{u}\rangle_{L^2} v_t(\cdot;\zeta)\big),\ \zeta \notin \mathrm{Spec}(H_t) \cup \mathrm{Spec}(H_s),\end{aligned}$$

$$\dot{R}_t(\zeta)u = \frac{\pi}{2}(\mathcal{W}_t(\zeta))^{-2}\big(\langle w_t(\cdot;\zeta), \overline{u}\rangle_{L^2} w_t(\cdot;\zeta) + \langle v_t(\cdot;\zeta), \overline{u}\rangle_{L^2} v_t(\cdot;\zeta)\big),\quad \zeta \notin \mathrm{Spec}(H_t),$$

$$\dot{\lambda}(t_0) = -\frac{\pi}{2}\|\sin(\pi t_0/2)\Gamma_0 u_0 + \cos(\pi t_0/2)\Gamma_1 u_0\|^2_{\mathbb{C}^2},\ t_0 \in [0,1],$$

where u_0 is the normalized eigenfunction corresponding to the eigenvalue $\lambda(t_0) \in \mathrm{Spec}(H_{t_0})$.

Example 4.8. As promised prior to Theorem 3.25, we now recall the classical Rellich's example, cf., for example, [83, Example V.4.14] which shows the singularity at $t_0 = 0$ of the smallest eigenvalue $\lambda^{(0)}(t)$ of the operator $\mathcal{A}_t = -\partial^2_{xx}$ in $L^2(0,1)$ equipped with the boundary conditions $u(0) = 0$, $tu'(1) = u(1)$ for real t; meanwhile, the resolvent $t \mapsto (\mathcal{A}_t - \mathbf{i})^{-1}$ is continuous and all other eigenvalues $\lambda^{(k)}(t)$, $k = 1, 2, \ldots$, are differentiable for each t including $t = 0$, see [83, Fig. 1, p.292]. Indeed, letting $\Gamma_0 u = (u(0), u(1))^\top$, $\Gamma_1 u = (u'(0), -u'(1))^\top$ for $u \in \mathcal{H}_+ := H^2(0,1)$, $\mathfrak{H} = \mathbb{C}^2$ and

$$X_t = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},\ Y_t = \begin{bmatrix}0 & 0\\ 0 & -t\end{bmatrix},\ Q_t = \begin{bmatrix}0 & 0 & 0 & 0\\ 0 & t^2(1+t^2)^{-1} & 0 & -t(1+t^2)^{-1}\\ 0 & 0 & 1 & 0\\ 0 & -t(1+t^2)^{-1} & 0 & (1+t^2)^{-1}\end{bmatrix}, \tag{4.12}$$

we notice that $\operatorname{dom}(\mathcal{A}_t) = \ker([X_t\, Y_t]) = \operatorname{ran}Q_t$. The maps $t \mapsto X_t, Y_t, Q_t$ are all differentiable at each $t \in \mathbb{R}$, and so, Theorem 4.5 (or Theorem 3.26) applies. In particular, the resolvent operators of $\mathcal{A}_t$ are differentiable at each t, and a short calculation using (4.8), (4.9), and (4.12) shows that if u denotes the norm one eigenfunction with the eigenvalue $\lambda(t) \in \operatorname{Spec}(\mathcal{A}_t)$ then $\dot{\lambda}(t) = |u'(1)|^2$, provided that we know that $\lambda(t)$ is an eigenvalue of $\mathcal{A}_t$ for a given $t \in \mathbb{R}$. Thus, each of the branches $\lambda^{(k)}(\cdot)$, $k \in \{0\} \cup \mathbb{N}$, of the eigenvalues is monotone for all t where it is defined.

We proceed with finding the actual location of $\lambda \in \operatorname{Spec}(\mathcal{A}_t)$ and formulas for u dealing with the two possible cases: (i) $\lambda = \varkappa^2 > 0$, respectively, and (ii) $\lambda = -\varkappa^2 < 0$ for $\varkappa = \varkappa(t) \in \mathbb{R}$. Solving the equation $u'' = 0$ with the boundary conditions, we note that $\lambda = 0 \in \operatorname{Spec}(\mathcal{A}_1)$ with $u = x$, and that $0 \notin \operatorname{Spec}(\mathcal{A}_t)$ for all $t \neq 1$. Plugging a linear combination of (i) $\cos(\varkappa x)$ and $\sin(\varkappa x)$, respectively, (ii) $\sinh(\varkappa x)$ and $\cosh(\varkappa x)$ into the boundary value problem $-u'' = \lambda u$, $u(0) = 0$, $tu'(1) = u(1)$ shows that nonzero $\varkappa = \varkappa(t)$ are the solutions to the equation (i) $t\varkappa = \tan\varkappa$ with $u = a\sin(\varkappa x)$, $a^{-2} = (1 - t\cos^2\varkappa)/2$, respectively, equation (ii) $t\varkappa = \tanh\varkappa$ with $u = a\sinh(\varkappa x)$, $a^{-2} = (t\cosh^2\varkappa - 1)/2$. By inspection of the graphs in the equations, in case (i), for each $t \in \mathbb{R}$ and $n \in \mathbb{Z} \setminus \{0\}$, there is a unique solution $\varkappa \in (-\pi/2 + \pi n, \pi/2 + \pi n)$, for each $t > 1$, there is a unique solution $\varkappa = \varkappa(t) \in (-\pi/2, \pi/2)$ with $\varkappa(t) \to 0^+$ as $t \to 1^+$, and for any $t < 1$, there are no solutions $\varkappa \in (-\pi/2, \pi/2)$. In case (ii), for any $t \leqslant 0$ or $t > 1$, there are no solutions $\varkappa \in \mathbb{R}$, while for each $t \in (0, 1]$, there exists a unique solution $\varkappa = \varkappa(t) \in \mathbb{R}$ such that $\varkappa(t) \to 0$ as $t \to 1^-$ and $\varkappa(t) \to +\infty$ as $t \to 0^+$. By squaring $\varkappa$, we obtain the branches $\lambda^{(0)}(t) < \lambda^{(1)}(t) < \dots$ of the eigenvalues of $\mathcal{A}_t$ such that $\lambda^{(0)}(t)$ are defined for $t > 0$ with $\lambda^{(0)}(t) \to -\infty$ as $t \to 0^+$, is negative for $t \in (0, 1)$ and positive for $t > 1$, while $\lambda^{(k)}(t)$ for $k \in \mathbb{N}$ is defined and positive for all $t \in \mathbb{R}$, cf. [83, Fig. 1, p. 292]. Using $\dot{\lambda}(t) = |u'(1)|^2$ and the expressions for u just given, one obtains very particular formulas for $\dot{\lambda}^{(k)}(t)$ for all t and k except when $k = 0$ and $t \leqslant 0$.

4.2 | Laplace operator on bounded domains via boundary triplets

The main result of this section is Theorem 4.13 in which we derive the resolvent difference formula, Riccati equation, and Hadamard-type formula for a family of Robin-type Laplacians. To that end, we employ abstract results of Theorem 4.5 with an ordinary boundary triplet specifically defined for the Laplace operator. The construction of such triplet for second-order elliptic operators goes back to the work of M.I. Višik [124, 125] who proposed the regularization of the Neumann trace by means of the Dirichlet-to-Neumann map, G. Grubb [73] who investigated the case of higher order operators building upon the trace theory of J. L. Lions and E. Magenes [98]. We also note that the work of M. Malamud [100] provides boundary triplets with dual parity in $L^2(\partial\Omega) \times L^2(\partial\Omega)$ as well as important relation between the Weyl function and the Dirichlet-to-Neumann map. Another relevant construction of trace maps is offered in [17] where a B-regularized boundary triplet was originally proposed.

Throughout this section, we assume the following.

Hypothesis 4.9. Let $n \in \mathbb{N}, n \geqslant 2$, and $\Omega \subset \mathbb{R}^n$ be a bounded domain with $C^{1,r}$, $r > 1/2$, boundary.

Remark 4.10. The construction of trace maps, which we briefly recall below, is of paramount importance to this paper. We stress that the material discussed up to Theorem 4.13 is well known and presented here only for the sake of a smoother exposition of the subsequent results. The full credit for original discoveries in this direction belongs to M.I. Višik, J. L. Lions, E. Magenes, and G. Grubb, see [73, 75, 98, 100, 124, 125].

Let us briefly recall trace maps that will be used below. The Dirichlet trace operator

$$\gamma_{_D} : H^s(\Omega) \to H^{s-1/2}(\partial\Omega) \hookrightarrow L^2(\partial\Omega), \quad 1/2 < s < 3/2. \tag{4.13}$$

is a bounded and surjective extension of the mapping $\gamma_{_D}^0 : C^0(\overline{\Omega}) \to C^0(\partial\Omega), \quad \gamma_{_D}^0 u = u|_{\partial\Omega}$, see [122, Proposition 4.4.5]. The operator $\gamma_{_N} : \{u \in H^1(\Omega) \,|\, \Delta u \in L^2(\Omega)\} \to H^{-1/2}(\partial\Omega)$ is the weak extension of the usual Neumann trace operator, still denoted by $\gamma_{_N}$,

$$\gamma_{_N} = \nu \cdot \gamma_{_D} \nabla : H^{s+1}(\Omega) \to L^2(\partial\Omega), \quad 1/2 < s < 3/2. \tag{4.14}$$

As shown in [69, Corollary 6.6, Corollary 6.11],[†] there exist unique linear bounded operators

$$\begin{aligned} \widehat{\gamma}_{_D} &: \{u \in L^2(\Omega) \,|\, \Delta u \in L^2(\Omega)\} \to H^{-1/2}(\partial\Omega), \\ \widehat{\gamma}_{_N} &: \{u \in L^2(\Omega) \,|\, \Delta u \in L^2(\Omega)\} \to H^{-3/2}(\partial\Omega), \end{aligned} \tag{4.15}$$

which are compatible with the Dirichlet and Neumann trace introduced in (4.13) and (4.14), respectively. We note that both $\widehat{\gamma}_{_D}, \widehat{\gamma}_{_N}$ have dense ranges. These trace maps give rise to the Dirichet-to-Neumann map $M_{D,N}$ associated with $-\Delta$ on Ω via $M_{D,N} : H^{-1/2}(\partial\Omega) \to H^{-3/2}(\partial\Omega) : g \mapsto -\widehat{\gamma}_{_N}(u_D)$, where u_D is the unique solution of the boundary value problem

$$-\Delta u = 0,\; u \in L^2(\Omega), \quad \widehat{\gamma}_{_D} u = g \text{ on } \partial\Omega. \tag{4.16}$$

As was shown in [69, Theorem 12.1], the map

$$\tau_{_N} : \{u \in L^2(\Omega) | \Delta u \in L^2(\Omega)\} \to H^{1/2}(\partial\Omega),\; \tau_{_N} u := \widehat{\gamma}_{_N} u + M_{D,N}(\widehat{\gamma}_{_D} u), \tag{4.17}$$

is bounded when the space $\{u \in L^2(\Omega) | \Delta u \in L^2(\Omega)\} = \mathrm{dom}(-\Delta_{\max})$ is equipped with the natural graph norm $(\|u\|^2_{L^2(\Omega)} + \|\Delta u\|^2_{L^2(\Omega)})^{1/2}$. Moreover, this operator is onto. In fact,

$$\tau_{_N}(H^2(\Omega) \cap H^1_0(\Omega)) = H^{1/2}(\partial\Omega). \tag{4.18}$$

Also, the null space of the map $\tau_{_N}$ is given by

$$\ker(\tau_{_N}) = H^2_0(\Omega) \dot{+} \{u \in L^2(\Omega),\; -\Delta u = 0\}. \tag{4.19}$$

Let us note that the following Green formula holds for every $u, v \in \mathrm{dom}(-\Delta_{\max})$,

$$\begin{aligned} &(-\Delta u, v)_{L^2(\Omega)} - (u, -\Delta v)_{L^2(\Omega)} \\ &= -{}_{H^{1/2}(\partial\Omega)}\langle \tau_{_N} u, \widehat{\gamma}_{_D} v\rangle_{H^{-1/2}(\partial\Omega)} + \overline{{}_{H^{1/2}(\partial\Omega)}\langle \tau_{_N} v, \widehat{\gamma}_{_D} u\rangle_{H^{-1/2}(\partial\Omega)}}. \end{aligned} \tag{4.20}$$

[†] In the context of Remark 4.10, we note that the series of papers [67–69] provides an extension of the classical results to the setting of domains with $C^{1,r}$ boundaries.

In the sequel, we use the Reisz isomorphism given by

$$\begin{aligned}
&\Phi : H^{-1/2}(\partial\Omega) \to H^{1/2}(\partial\Omega),\\
&H^{-1/2}(\partial\Omega) \ni \psi \mapsto \Phi_\psi \in H^{1/2}(\partial\Omega), \qquad (4.21)\\
&\langle f, \psi\rangle_{-1/2} := \psi(f) = \langle f, \Phi_\psi\rangle_{1/2}, f \in H^{1/2}(\partial\Omega), \psi \in H^{-1/2}(\partial\Omega),
\end{aligned}$$

in particular, for $f, \psi \in H^{1/2}(\partial\Omega) \hookrightarrow L^2(\partial\Omega) \hookrightarrow H^{-1/2}(\partial\Omega)$, we have

$$\langle f, \psi\rangle_{-1/2} = \langle f, \psi\rangle_{L^2(\partial\Omega)}.$$

We also note that Φ is a conjugate linear mapping.

Having recalled the trace maps above, we are ready to define the maximal and minimal Laplace operators as follows:

$$\begin{aligned}
-\Delta_{\max} &: \operatorname{dom}(-\Delta_{\max}) \subset L^2(\Omega) \to L^2(\Omega),\\
\operatorname{dom}(-\Delta_{\max}) &= \big\{u \in L^2(\Omega) \big|\, \Delta u \in L^2(\Omega)\big\},\\
-\Delta_{\max} u &= -\Delta u \ \text{ (in the sense of distributions)},\\
\operatorname{dom}(-\Delta_{\min}) &= H_0^2(\Omega),\ -\Delta_{\min} u = -\Delta u,
\end{aligned}$$

and remark that by [69, Theorem 8.14],[†] one has

$$\begin{aligned}
&\operatorname{dom}(-\Delta_{\min}) = H_0^2(\Omega) = \{u \in L^2(\Omega) |\ \Delta u \in L^2(\Omega),\ \widehat{\gamma}_D(u) = 0,\ \widehat{\gamma}_N(u) = 0\},\\
&-\Delta_{\min} = (-\Delta_{\max})^*,\ -\Delta_{\max} = (-\Delta_{\min})^*.
\end{aligned} \qquad (4.22)$$

The next lemma is a well-known fact that goes back to [73, 124, 125].

Lemma 4.11. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded domain with $C^{1,r}$-boundary, $r > 1/2$, and the boundary traces $\widehat{\gamma}_D$, τ_N are as in (4.15), (4.17). Then*

$$(\mathfrak{H}, \Gamma_0, \Gamma_1) := (H^{1/2}(\partial\Omega), \tau_N, \Phi\widehat{\gamma}_D) \qquad (4.23)$$

is an ordinary boundary triplet for $A = -\Delta_{\min}$.

Proof. The trace operator $\mathrm{T} := [\tau_N, \Phi\widehat{\gamma}_D]^\top$ is defined on the space

$$\mathcal{H}_+ := \{u \in L^2(\Omega) : \Delta u \in L^2(\Omega)\}$$

with the norm

$$\|u\|_{\mathcal{H}_+} = (\|u\|^2_{L^2(\Omega)} + \|\Delta u\|^2_{L^2(\Omega)})^{1/2}.$$

Recalling the Green identity (4.20)

$$(-\Delta u, v)_{L^2(\Omega)} - (u, -\Delta v)_{L^2(\Omega)}$$

[†] The description of the minimal domain in the case of C^2 boundary $\partial\Omega$ is a classical result, cf. [75, 98].

$$= -{}_{H^{1/2}(\partial\Omega)}\langle \tau_{_N} u, \widehat{\gamma}_{_D} v\rangle_{H^{-1/2}(\partial\Omega)} + \overline{{}_{H^{1/2}(\partial\Omega)}\langle \tau_{_N} v, \widehat{\gamma}_{_D} u\rangle_{H^{-1/2}(\partial\Omega)}},$$

we rewrite it as

$$\begin{aligned}\langle A^* u, v\rangle_{\mathcal{H}} - \langle u, A^* v\rangle_{\mathcal{H}} &= -\langle \Gamma_0 u, \Gamma_1 v\rangle_{\mathfrak{H}} + \overline{\langle \Gamma_0 v, \Gamma_1 u\rangle_{\mathfrak{H}}},\\ &= \langle \Gamma_1 u, \Gamma_0 v\rangle_{\mathfrak{H}} - \langle \Gamma_0 u, \Gamma_1 v\rangle_{\mathfrak{H}},\end{aligned}$$

and thus check that (4.23) satisfies the abstract Green identity. It remains to show that the map $\mathrm{T} : \mathcal{H}_+ \to H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$ is onto. We fix a vector $(f, g) \in H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$. By (4.18), there exists $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$ such that $\tau_{_N} u_0 = f$. By [69, Theorem 10.4], the boundary value problem (4.16) has a unique solution that we denote by v_0 (we note that zero is outside of the spectrum of the Dirichlet Laplacian). Employing (4.19) and $v_0 \in \ker(\tau_{_N})$ yields

$$\mathrm{T}(u_0 + v_0) = (\tau_{_N}(u_0 + v_0), \Phi\widehat{\gamma}_{_D}(u_0 + v_0)) = (\tau_{_N} u_0, \Phi\widehat{\gamma}_{_D} v_0) = (f, \Phi g)$$

since $\widehat{\gamma}_{_D} u_0 = \gamma_{_D} u_0 = 0$. □

Remark 4.12. In PDE literature, boundary value problems are often formulated in terms of the Dirichlet and Neumann traces defined by

$$\begin{aligned}&\gamma_{_D} : \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\} \to H^{1/2}(\partial\Omega), \gamma_{_D} := \widehat{\gamma}_{_D} \restriction_{\{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\}},\\ &\gamma_{_N} : \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\} \to H^{-1/2}(\partial\Omega), \gamma_{_N} := \widehat{\gamma}_{_N} \restriction_{\{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\}}.\end{aligned}$$

We note that $(-\Delta_{\max}, \gamma_{_D}, \gamma_{_N})$ is not an ordinary boundary triplet. First, $\mathrm{T} := (\gamma_{_D}, \gamma_{_N})$ is not defined on the entire space $\mathrm{dom}(-\Delta_{\max})$. Second, T is not onto, see [93, Proposition 2.11]. However, Hypothesis 2.1 is still satisfied with $\mathcal{D} := \{u \in H^1(\Omega) : \Delta u \in L^2(\Omega)\}$ and equipped with the norm $(\|u\|^2_{H^1(\Omega)} + \|\Delta u\|^2_{L^2(\Omega)})^{1/2}$. In fact, Hypothesis 3.1 is also satisfied for this choice of $\mathrm{T}, \mathcal{D}$. These facts serve as our main motivation for introducing Hypotheses 2.1 and 3.1. We elaborate on this further in Section 5.

Having constructed the ordinary boundary triplet for the Laplacian, we can now apply the abstract results from Theorem 4.5.

Theorem 4.13. *Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with $C^{1,r}$-boundary, $r > 1/2$, and let $t \mapsto \Xi_t \in \mathcal{B}(H^{1/2}(\partial\Omega))$, $t \in [0, 1]$, be a differentiable family of self-adjoint operators. Then, for $t \in [0, 1]$, the linear operator*

$$\begin{aligned}&-\Delta_t : \mathrm{dom}(-\Delta_t) \subset L^2(\Omega) \to L^2(\Omega), -\Delta_t u = -\Delta u,\\ &u \in \mathrm{dom}(-\Delta_t) := \{u \in \mathrm{dom}(\Delta_{\max}) : \Phi\widehat{\gamma}_{_D} u + \Xi_t \tau_{_N} u = 0\},\end{aligned}$$

is self-adjoint. The following resolvent difference formula holds:

$$\begin{aligned}&(-\Delta_t - \zeta)^{-1} - (-\Delta_s - \zeta)^{-1}\\ &\qquad = \Big(\tau_{_N}(-\Delta_t - \overline{\zeta})^{-1}\Big)^* (\Xi_t - \Xi_s)\Big(\tau_{_N}(-\Delta_s - \zeta)^{-1}\Big),\end{aligned} \tag{4.24}$$

for $t, s \in [0,1]$, $\zeta \notin (\mathrm{Spec}(-\Delta_t) \cup \mathrm{Spec}(-\Delta_s))$. *Moreover, for a fixed* $t_0 \in [0,1]$, *the mapping*

$$t \mapsto (-\Delta_t - \zeta)^{-1} \in \mathcal{B}(L^2(\Omega)) \tag{4.25}$$

is well defined for t *near* t_0 *as long as* $\zeta \notin \mathrm{Spec}(-\Delta_{t_0})$. *This mapping is differentiable at* t_0 *and satisfies the following Riccati equation:*

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0}\big((-\Delta_t - \zeta)^{-1}\big)\\ &\quad= \Big(\tau_{_N}(-\Delta_{t_0} - \overline{\zeta})^{-1}\Big)^*\Big(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0}\Xi_t\Big)\Big(\tau_{_N}(-\Delta_{t_0} - \zeta)^{-1}\Big).\end{aligned} \tag{4.26}$$

Finally, if $\lambda(t_0)$ *is an eigenvalue of* $-\Delta_{t_0}$ *of multiplicity* $m \geqslant 1$, *then there exists a choice of orthonormal eigenfunctions* $\{u_j\}_{j=1}^m \subset \ker(-\Delta_{t_0} - \lambda(t_0))$ *and a labeling of eigenvalues* $\{\lambda_j(t)\}_{j=1}^m$ *of* $-\Delta_t$, *for* t *near* t_0, *such that*

$$\dot{\lambda}_j(t_0) = -\langle \dot{\Xi}_{t_0}\tau_{_N}u_j, \tau_{_N}u_j\rangle_{L^2(\partial\Omega)}, 1 \leqslant j \leqslant m. \tag{4.27}$$

Proof. By Lemma 4.11, $(H^{1/2}(\partial\Omega), \tau_{_N}, \Phi\widehat{\gamma}_{_D})$ is an ordinary boundary triplet. In order to check that $-\Delta_t$ is self-adjoint, it suffices to check conditions (2.8) and (2.9) with $X := \Xi_t$, $Y := I$. Indeed, (2.8) holds since Ξ_t is self-adjoint, and (2.9) holds since the operator $XX^* + YY^*$ given by $I + \Xi_t^2 > 0$ is invertible. The fact that (4.25) is well defined for t near t_0 follows from continuity of Ξ_t and Theorems 4.5 and 3.18 upon setting $\mathcal{A}_t := -\Delta_t$, $V_t := 0$, $\mathrm{T}_t := [\tau_{_N}, \Phi\widehat{\gamma}_{_D}]^\top$. In order to prove (4.24), (4.26), and (4.27), we use (3.41), (3.43), and (3.44), respectively, with

$$\begin{aligned}(W(\Xi_t, I))\mathrm{T}R_t(\zeta) &= (I + \Xi_t^2)^{-1}(-\Gamma_0 R_t(\zeta) + \Xi_t\Gamma_1 R_t(\zeta))\\ &= (I + \Xi_t^2)^{-1}(-\Gamma_0 R_t(\zeta) - \Xi_t^2\Gamma_0 R_t(\zeta)) = -\Gamma_0 R_t(\zeta) = -\tau_N R_t(\zeta)\end{aligned}$$

and $\phi_j = -\tau_{_N}u_j$. □

Remark 4.14. The assumption $\partial\Omega$ being $C^{1,r}$, $r > 1/2$, imposed in this section could be replaced by $\partial\Omega$ being Lipschitz and Ω quasi-convex, see [69, Section 8] for the definition. As proved in [69], these weaker assumptions are sufficient for the domains of the Dirichlet and Neumann Laplacians to belong to $H^2(\Omega)$, which, in turn, is equivalent to (4.22) to hold. Also, for the case of Lipschitz domains Lemma 4.11 as well as the discussion of trace maps prior to Lemma 4.11 hold with the Sobolev spaces $H^{1/2}(\partial\Omega)$ and $H^{-1/2}(\partial\Omega)$ replaced by $N^{1/2}(\partial\Omega)$ and its adjoint $\big(N^{1/2}(\partial\Omega)\big)^*$, respectively, where the space $N^{1/2}(\partial\Omega)$ is defined as $\{f \in L^2(\partial\Omega) : f\nu_j \in H^{1/2}(\partial\Omega)\}$, $\nu = (\nu_j)_{j=1}^n$, and is equal to $H^{1/2}(\partial\Omega)$ provided $\partial\Omega$ is $C^{1,r}$, $r > 1/2$, see [69]. In the context of Lipschitz domains, we also mention an important paper [18].

Remark 4.15. Our motivation to consider the boundary condition in Theorem 4.13 stems from [44, 67, 96]. More generally, the boundary condition described in Theorem 4.13 can be replaced by $X_t\widehat{\gamma}_{_N}u + Y_t\tau_{_N}u = 0$ for $X_t, Y_t \in \mathcal{B}(H^{1/2}(\partial\Omega))$ satisfying (2.8) and (2.9). In this case, as in Theorem 4.13, continuity of the mappings $t \mapsto X_t$, $t \mapsto Y_t$ yields continuity of the resolvent operator with respect to t. Moreover, differentiability of the mappings $t \mapsto X_t$, $t \mapsto Y_t$ yields differentiability of the resolvent operator with respect to t as well as the Reccati equation and the formula for the slopes of the eigenvalue curves (both obtained by dropping the potential terms V_t in (4.7) and (4.8), respectively).

4.3 Quantum graphs

The main result of this section is Theorem 4.16 in which we derive the resolvent difference formula, Riccati equation, and Hadamard-type formula for Schrödinger operators on metric graphs. To that end, we employ the abstract results discussed in Theorem 4.5 with an ordinary boundary triplet specifically defined for quantum graphs. Examples 4.17 and 4.18 give two applications of Theorem 4.16. Both examples concern monotonicity of eigenvalue curves of Schrödinger operators with respect to some natural parameter present in the boundary conditions.

We begin by discussing differential operators on metric graphs. To set the stage, let us fix a discrete graph $(\mathcal{V}, \mathcal{E})$ where $\mathcal{V}$ and $\mathcal{E}$ denote the set of vertices and edges, respectively. We assume that $(\mathcal{V}, \mathcal{E})$ consists of a finite number of vertices, $|\mathcal{V}|$, and a finite number of edges, $|\mathcal{E}|$. We assign to each edge $e \in \mathcal{E}$ a positive and finite length $\ell_e \in (0, \infty)$. The corresponding metric graph is denoted by $\mathcal{G}$. The boundary $\partial\mathcal{G}$ of the metric graph is defined by

$$\partial\mathcal{G} := \cup_{e\in\mathcal{E}}\{a_e, b_e\},$$

where a_e, b_e denote the end points of the edge e. It is convenient to treat $2|\mathcal{E}|$-dimensional vectors as functions on the boundary $\partial\mathcal{G}$, in particular, $L^2(\partial\mathcal{G}) \cong \mathbb{C}^{2|\mathcal{E}|}$, where the space $L^2(\partial\mathcal{G}) = \bigoplus_{e\in\mathcal{E}} \left(L^2(\{a_e\}) \times L^2(\{b_e\})\right)$ corresponds to the discrete Dirac measure with support $\cup_{e\in\mathcal{E}}\{a_e, b_e\}$. In addition to the space of functions on the boundary, we consider the Sobolev spaces of functions on the graph $\mathcal{G}$,

$$L^2(\mathcal{G}) := \bigoplus_{e\in\mathcal{E}} L^2(e),\ \widehat{H}^2(\mathcal{G}) := \bigoplus_{e\in\mathcal{E}} H^2(e),$$

where $H^2(e)$ is the standard L^2 based Sobolev space. As in the setting of Laplace operators on bounded domains, the spaces $L^2(\mathcal{G})$ and $L^2(\partial\mathcal{G})$ are related via the trace maps. We define the trace operators (Γ_0, Γ_1) by the formulas

$$\Gamma_0 : \widehat{H}^2(\mathcal{G}) \to L^2(\partial\mathcal{G}),\ \Gamma_0 u := u|_{\partial\mathcal{G}}, u \in \widehat{H}^2(\mathcal{G}),$$

$$\Gamma_1 : \widehat{H}^2(\mathcal{G}) \to L^2(\partial\mathcal{G}),\ \Gamma_1 u := \partial_n u|_{\partial\mathcal{G}}, u \in \widehat{H}^2(\mathcal{G}),$$

where $\partial_n u$ denotes the derivative of u taken in the *inward* direction. The trace operator is a bounded, linear operator given by

$$\mathrm{T} := [\Gamma_0, \Gamma_1]^\top,\ \mathrm{T} : \widehat{H}^2(\mathcal{G}) \to L^2(\partial\mathcal{G}) \times L^2(\partial\mathcal{G}) \cong \mathbb{C}^{4|\mathcal{E}|}.$$

The Sobolev space of functions vanishing on the boundary $\partial\mathcal{G}$ together with their derivatives is denoted by

$$H_0^2(\mathcal{G}) := \left\{u \in \widehat{H}^2(\mathcal{G}) : \mathrm{T}u = 0\right\}.$$

Using our notation for the trace maps, the Green identity can be written as follows:

$$\begin{aligned}\int_{\mathcal{G}}(-u'')\overline{v} - u\overline{(-v'')} &= \int_{\partial\mathcal{G}} \partial_n u\overline{v} - u\overline{\partial_n v}\\ &= \langle [J\otimes I_{2|\mathcal{E}|}]\mathrm{T}u, \mathrm{T}v\rangle_{\mathbb{C}^{4|\mathcal{E}|}},\ u,v\in \widehat{H}^2(\mathcal{G}).\end{aligned}$$

The right-hand side of the Green identity defines a symplectic form

$$\begin{aligned}&\omega:\ {}^dL^2(\partial\mathcal{G})\times {}^dL^2(\partial\mathcal{G})\to\mathbb{C},\\ &\omega((f_1,f_2),(g_1,g_2)) := \int_{\partial\mathcal{G}} f_2\overline{g_1} - f_1\overline{g_2},\\ &(f_1,f_2),(g_1,g_2)\in {}^dL^2(\partial\mathcal{G}),\end{aligned}$$

where ${}^dL^2(\partial\mathcal{G}) := L^2(\partial\mathcal{G})\times L^2(\partial\mathcal{G})$.

Next, we introduce the minimal Laplace operator $A_{\min}$ and its adjoint $A_{\max}$. The operator

$$A_{\min} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2},\quad \mathrm{dom}(A_{\min}) = \widehat{H}^2_0(\mathcal{G}),$$

is symmetric in $L^2(\mathcal{G})$. Its adjoint $A_{\max} := A^*_{\min}$ is given by

$$A_{\max} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2},\quad \mathrm{dom}(A_{\max}) = \widehat{H}^2(\mathcal{G}).$$

The deficiency indices of $A_{\min}$ are finite and equal, that is,

$$0<\dim\ker(A_{\max}-\mathbf{i}) = \dim\ker(A_{\max}+\mathbf{i})<\infty.$$

Theorem 4.16. *Assume that*

$$\begin{aligned}&t\mapsto V_t \textit{ is in } C^1([0,1],L^\infty(\mathcal{G})),\\ &t\mapsto X_t,Y_t \textit{ is in } C^1([0,1],\mathbb{C}^{2|\mathcal{E}|\times 2|\mathcal{E}|}),\ \det(X_tX_t^*+Y_tY_t^*)\neq 0, X_tY_t^* = Y_t^*Y_t.\end{aligned}$$

Then, the operator

$$\begin{aligned}&\mathcal{A}_t : L^2(\mathcal{G})\to L^2(\mathcal{G}), \mathrm{dom}(\mathcal{A}_t) := \{u\in H^2(\mathcal{G}) : [X_t,Y_t]\mathrm{T}u = 0\},\\ &\mathcal{A}_t u = -u'', u\in\mathrm{dom}(\mathcal{A}_t),\end{aligned}$$

is a self-adjoint extension of A_{min}. The operator-valued function

$$t\mapsto R_t(\zeta_0) := (\mathcal{A}_t+V_t-\zeta_0)^{-1} \textit{ for all } \zeta_0\notin \mathrm{Spec}(\mathcal{A}_t)$$

is in $C^1([0,1],\mathcal{B}(L^2(\mathcal{G})))$ and for any $t_0\in[0,1]$ one has

$$\begin{aligned}&\dot R_{t_0}(\zeta_0) = -R_{t_0}(\zeta_0)\dot V_{t_0}R_{t_0}(\zeta_0)\\ &+(\mathrm{T}R_{t_0}(\overline{\zeta_0}))^*\Big(W(X_{t_0},Y_{t_0})\Big)^*(\dot X_{t_0}Y^*_{t_0}-\dot Y_{t_0}X^*_{t_0})\Big(W(X_{t_0},Y_{t_0})\Big)\mathrm{T}R_{t_0}(\zeta_0),\end{aligned}\tag{4.28}$$

where $W(X_{t_0}, Y_{t_0})$ is as in (2.11). Furthermore, if $\lambda(t_0)$ is an eigenvalue of $\mathcal{A}_{t_0} + V_{t_0}$ of multiplicity $m \geqslant 1$, then there exist a choice of orthonormal eigenfunctions

$$\{u_j\}_{j=1}^m \subset \ker(\mathcal{A}_{t_0} + V_{t_0} - \lambda(t_0))$$

and a labeling of eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of $\mathcal{A}_t + V_t$, for t near t_0, such that

$$\dot{\lambda}_j(t_0) = \langle \dot{V}_{t_0} u_j, u_j \rangle_{L^2(\mathcal{G})} + \left\langle (X_{t_0} \dot{Y}_{t_0}^* - Y_{t_0} \dot{X}_{t_0}^*) \phi_j, \phi_j \right\rangle_{L^2(\partial\mathcal{G})}, \tag{4.29}$$

where $\phi_j = W(X_{t_0}, Y_{t_0}) \mathrm{T} u_j$ is a unique $2|\mathcal{E}|$-dimensional vector satisfying $\Gamma_0 u_j = -Y_{t_0}^* \phi_j$ and $\Gamma_1 u_j = X_{t_0}^* \phi_j$, $1 \leqslant j \leqslant m$.

Proof. Since $(L^2(\partial\mathcal{G}), \Gamma_0, \Gamma_1)$ is an ordinary boundary triplet, Equations (4.7) and (4.8) in Theorem 4.5 give (4.28) and (4.29), respectively. $\square$

Example 4.17. Consider the Schrödinger operator $H_t = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ on a compact star graph $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ with a bounded real-valued potential V subject to arbitrary self-adjoint vertex conditions at the vertices of degree one and the following δ-type condition at the center $\mathrm{v_c} \in \mathcal{V}$,

$$\sum_{e \sim \mathrm{v_c}} \partial_n u_e(\mathrm{v_c}) = t u(\mathrm{v_c}), \; t \in \mathbb{R}.$$

We recall that the spectrum of H_t can be described via secular equations [21]. In this example, we will derive an Hadamard-type formula (4.30) for the derivative of the eigenvalues of H_t. Such a formula is discussed in [21, Proposition 3.1.6] for simple eigenvalues. The general case can be treated using (4.29) as follows. The boundary matrices describing the vertex conditions are given by $\widetilde{X} \times X_t$ and $\widetilde{Y} \times Y$ where

$$X_t = \begin{bmatrix} 1 & -1 & & \cdots & 0 \\ 0 & 1 & -1 & \cdots & 0 \\ & & \ddots & & \\ 0 & & & 1 & -1 \\ -t & 0 & \cdots & & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & & \cdots & 0 \\ 0 & & \cdots & 0 \\ & & \ddots & \\ 0 & & \cdots & 0 \\ 1 & 1 & \cdots & 1 \end{bmatrix},$$

and the matrices $\widetilde{X}$ and $\widetilde{Y}$ correspond to the vertex conditions at $\mathcal{V} \setminus \{\mathrm{v_c}\}$. A direct computation gives

$$X_t^* Y = Y^* X_t = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ & & \ddots & \\ 0 & 0 & \cdots & -t \end{bmatrix}.$$

For the eigenvalue $\lambda(t_0)$ of H_{t_0} of multiplicity $m \in \mathbb{N}$, we use (4.29) to get

$$\dot{\lambda}_j(t_0) = \left\langle (X_{t_0} \dot{Y}_{t_0}^* - Y_{t_0} \dot{X}_{t_0}^*) \phi_j, \phi_j \right\rangle_{L^2(\partial\mathcal{G})} = |\phi_j(\mathrm{v_c})|^2,$$

where $1 \leqslant j \leqslant m$, $\phi_j = W(X_{t_0}, Y_{t_0})\mathrm{T}u_j$, and $\{u_j\}_{j=1}^m$ are the eigenfunctions of H_{t_0} corresponding to $\lambda(t_0)$. Furthermore, using (3.45), we obtain $\phi_j(\mathrm{v_c}) = -u_j(\mathrm{v_c})$, and hence,

$$\dot{\lambda}_j(t_0) = |u_j(\mathrm{v_c})|^2,\ 1 \leqslant j \leqslant m. \tag{4.30}$$

Example 4.18. This example concerns monotonicity of eigenvalue curves of a class of Schrödinger operators on a compact interval arising in the spectral theory of periodic Hamiltonians. Specifically, we consider the Schrödinger operators H_ϑ with a real-valued potential $V \in L^\infty(0,1)$ which are parameterized by $\vartheta \in [0, 2\pi)$ and defined as follows:

$$\begin{aligned} &H_\vartheta = \mathcal{A}_\vartheta + V,\ \mathcal{A}_\vartheta : L^2(0,1) \to L^2(0,1), \mathcal{A}_\vartheta u = -u'', u \in \operatorname{dom}(\mathcal{A}_\vartheta), \\ &\operatorname{dom}(\mathcal{A}_\vartheta) := \{u \in H^2(0,1) : e^{\mathbf{i}\vartheta}u(0) = u(1), e^{\mathbf{i}\vartheta}u'(0) = u'(1)\}. \end{aligned} \tag{4.31}$$

Such operators are of interest, in particular, because their eigenvalues fill up the spectral bands of the Schrödinger operator in $L^2(\mathbb{R})$ with the potential given by the periodic extension of V, see [111, Theorems XIII.89, XIII.90]. We claim that the eigenvalue curves satisfy

$$\dot{\lambda}_j(\vartheta_0) = 2\,\mathrm{Im}(u_j'(0)\overline{u_j(0)}) \text{ for all } \vartheta_0 \in (0, 2\pi), \tag{4.32}$$

where, as usual, $u_j \in \ker(\mathcal{A}_{\vartheta_0} - \lambda_j(\vartheta_0))$, $j = 1, 2$ (in fact, all but, possibly, periodic and antiperiodic operators have simple spectra). We derive this formula from (4.8) by defining trace operators appropriately. It is well known that ordinary differential operators fit well into the scheme of boundary triplets, cf. for example [71, Chapter 3]; however, for completeness, we recall the setting. We set

$$\begin{aligned} &\mathcal{H} := L^2(0,1), \mathcal{H}_+ := H^2(0,1), A = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \operatorname{dom}(A) = H_0^2(0,1) \\ &\mathrm{T} : H^2(0,1) \to \mathbb{C}^4, \Gamma_0 u := (u(0), u(1))^\top, \Gamma_1 u := (u'(0), -u'(1))^\top. \end{aligned}$$

Next, to utilize (4.8), we first rewrite the boundary conditions in (4.31) as follows:

$$X_\vartheta \Gamma_0 u + Y_\vartheta \Gamma_1 u = 0, \text{ where } X_\vartheta := \begin{bmatrix} -\mathrm{e}^{\mathbf{i}\vartheta} & 1 \\ 0 & 0 \end{bmatrix}, Y_\vartheta := \begin{bmatrix} 0 & 0 \\ \mathrm{e}^{\mathbf{i}\vartheta} & 1 \end{bmatrix},$$

and compute

$$\begin{aligned} &\phi_j = W(X_\vartheta, Y_\vartheta)\mathrm{T}u_j = \frac{1}{2}(-Y_{\vartheta_0}\Gamma_0 u_j + X_{\vartheta_0}\Gamma_1 u_j) = -e^{\mathbf{i}\vartheta_0}(u_j'(0), u_j(0))^\top, \\ &X_{\vartheta_0}\dot{Y}^*_{\vartheta_0} - Y_{\vartheta_0}X^*_{\vartheta_0} = \begin{bmatrix} 0 & \mathbf{i} \\ -\mathbf{i} & 0 \end{bmatrix}. \end{aligned}$$

Plugging this in (4.29) yields (4.32). Monotonicity of the eigenvalues follows from linear independence of $u_j, \overline{u_j}$ and the formula

$$2|\,\mathrm{Im}(u_j'(0)\overline{u_j(0)})| = |\mathcal{W}(u_j, \overline{u_j})(0)| \neq 0, \vartheta_0 \in (0, 2\pi).$$

involving the Wronskian.

4.4 | Periodic Kronig–Penney model

† In this section, we give yet another application of Theorem 4.5 proving a version of B. Simon's theorem [121] that states that a certain open gap property (described below) of periodic Schrödinger operators is generic in the class of periodic $C^\infty(\mathbb{R})$ potentials. The main result of this section, Theorem 4.19, states this assertion for singular δ-type potentials. Its proof is based on a perturbative argument inspired by [121] and technically made available by Theorem 4.5.

The spectrum of the Schrödinger operator with periodic potential on the line has a bandgap structure, that is, in general, it consists of closed segments, called *bands*, such that two adjacent bands can either have a common endpoint or be separated by an open interval, a *gap*, of the resolvent set; in the latter case, we say that the gap is open. We will now use Theorem 4.5 to prove that *all gaps* of a generic periodic Kronig–Penney model are open. The operators in question are the Schrödinger operators with δ-type potentials that in physics literature are written as follows:

$$H_\alpha := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{k\in\mathbb{Z}} \alpha_k \delta(x-k),$$

and mathematically are defined by

$$H_\alpha u := -u'', u \in \mathrm{dom}(H_\alpha), H_\alpha : \mathrm{dom}(H_\alpha) \subset L^2(\mathbb{R}) \to L^2(\mathbb{R}),$$

$$\mathrm{dom}(H_\alpha) = \{u \in \widehat{H}^2(\mathbb{R}\setminus\mathbb{Z}) : u \text{ satisfies (4.33) for all } k \in \mathbb{Z}\},$$

$$u(k^+) = u(k^-),\ u'(k^+) - u'(k^-) = \alpha_k u(k), \tag{4.33}$$

where $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \in \ell^\infty(\mathbb{Z};\mathbb{R})$, $u(k^\pm)$ are the one-sided limits, and $\widehat{H}^2$ denotes the direct sum of the Sobolev spaces on respective intervals. The spectrum of H_α for the case of periodic sequence α has a bandgap structure, see [3, Theorem 2.3.3]. This was originally proved for 1-periodic sequences but can be directly extended to any p-periodic ones. Specifically, given a p-periodic sequence $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \in \ell^\infty(\mathbb{Z};\mathbb{R})$, the operator H_α is unitary equivalent to the direct integral

$$\int_{[0,2\pi)}^{\oplus} H_{\alpha^{(p)},\vartheta} \frac{\mathrm{d}\vartheta}{2\pi}, \text{ where we denote } \alpha^{(p)} := \{\alpha_0, \dots, \alpha_{p-1}\} \in \mathbb{R}^p,$$

and $H_{\alpha^{(p)},\vartheta}$ for $\vartheta \in [0,2\pi)$ is the operator defined in $L^2(I_p)$ with $I_p := (-1/2, p-1/2)$ by

$$H_{\alpha^{(p)},\vartheta} u := -u'',\ H_{\alpha^{(p)},\vartheta} : \mathrm{dom}(H_{\alpha^{(p)},\vartheta}) \subset L^2(I_p) \to L^2(I_p),$$

$$\mathrm{dom}(H_{\alpha^{(p)},\vartheta}) = \left\{u \in \widehat{H}^2(I_p\setminus\mathbb{Z}) : u \text{ satisfies (4.33) for } k \in I_p \cap \mathbb{Z} \text{ and (4.34)}\right\},$$

$$u(-1/2^+) = e^{\mathrm{i}\vartheta} u((p-1/2)^-),\ u'(-1/2^+) = e^{\mathrm{i}\vartheta} u'((p-1/2)^-), \tag{4.34}$$

where

$$\widehat{H}^2(I_p\setminus\mathbb{Z}) := H^2(-1/2,0) \oplus H^2(0,1) \oplus \dots \oplus H^2(p-2,p-1) \oplus H^2(p-1,p-1/2).$$

† An alternative approach applicable to a very broad class of second-order operators is discussed in the upcoming work of D. Damanik, J. Fillman, and the second author. See also [24].

Denoting the eigenvalues of $H_{\alpha^{(p)},\vartheta}$ (ordered in nondecreasing order) by

$$\lambda_j(\alpha^{(p)},\vartheta),\ j=1,2,\dots,$$

we have

$$\begin{aligned}\lambda_1(\alpha^{(p)},0)&\leqslant\lambda_1(\alpha^{(p)},\vartheta)\leqslant\lambda_1(\alpha^{(p)},\pi)\leqslant\lambda_2(\alpha^{(p)},\pi)\leqslant\lambda_2(\alpha^{(p)},\vartheta)\leqslant\lambda_2(\alpha^{(p)},0)\\&\leqslant\lambda_3(\alpha^{(p)},0)\leqslant\lambda_3(\alpha^{(p)},\vartheta)\leqslant\lambda_3(\alpha^{(p)},\pi)\leqslant\dots\ \text{for}\ \vartheta\in[0,\pi].\end{aligned}$$

Then, the spectrum of H_α is given by

$$\begin{aligned}\operatorname{Spec}(H_\alpha)&=\bigcup_{\vartheta\in[0,\pi]}\operatorname{Spec}(H_{\alpha^{(p)},\vartheta})\\&=[\lambda_1(\alpha^{(p)},0),\lambda_1(\alpha^{(p)},\pi)]\cup[\lambda_2(\alpha^{(p)},\pi),\lambda_2(\alpha^{(p)},0)]\cup\dots.\end{aligned}$$

The intervals $[\lambda_1(\alpha^{(p)},0),\lambda_1(\alpha^{(p)},\pi)]$, $[\lambda_2(\alpha^{(p)},\pi),\lambda_2(\alpha^{(p)},0)]$, ... are called *bands*. The endpoints of two adjacent bands may coincide. In this case, we say that the respective gap is closed; otherwise the respective *gap*, $\big(\lambda_1(\alpha^{(p)},\pi),\lambda_2(\alpha^{(p)},\pi)\big)$, $\big(\lambda_2(\alpha^{(p)},0),\lambda_3(\alpha^{(p)},0)\big)$, ... is said to be open. In the following theorem, we show that all gaps are open for a generic periodic sequence α.

Theorem 4.19. *There is a dense G_δ-set $\mathcal{S}\subset\ell^\infty(\mathbb{Z};\mathbb{R})$ of sequences α such that for each $\alpha\in\mathcal{S}$, all gaps in the spectrum of H_α are open.*

Proof. We let

$$\mathcal{S}_n:=\{\alpha\in\ell^\infty(\mathbb{Z};\mathbb{R}) : \alpha \text{ is } p\text{-periodic and the } n\text{th gap of } H_\alpha \text{ is open}\}.$$

It is enough to prove that each $\mathcal{S}_n$ is open and dense (then $\bigcap_{n\in\mathbb{N}}\mathcal{S}_n$ gives the required dense G_δ-set of potentials). To begin, let us rewrite $\operatorname{dom}(H_{\alpha^{(p)},\vartheta})$ in terms of Lagrangian planes in $\Lambda(\mathbb{C}^{4(p+1)})$. For $u\in\widehat{H}^2(I_p\setminus\mathbb{Z})$, we introduce the traces $\Gamma_0u,\Gamma_1u\in\mathbb{C}^{2(p+1)}$ by

$$\begin{aligned}\Gamma_0u&:=\{u(-1/2^+),u((p-1/2)^-),u(0^-),u(0^+),\dots,u(k^-),u(k^+),\dots,\\&\qquad u((p-1)^-),u((p-1)^+)\}\in\mathbb{C}^{2(p+1)},\\\Gamma_1u&:=\{u'(-1/2^+),-u'((p-1/2)^-),-u'(0^-),u'(0^+),\dots,-u'(k^-),u'(k^+),\dots,\\&\qquad -u'((p-1)^-),u'((p-1)^+)\}\in\mathbb{C}^{2(p+1)}.\end{aligned}$$

Also, let us introduce $2(p+1)\times2(p+1)$ matrices

$$\begin{aligned}X_{\alpha^{(p)},\vartheta}&:=\begin{bmatrix}-e^{\mathbf{i}\vartheta}&1\\0&0\end{bmatrix}\oplus\begin{bmatrix}1&-1\\-\alpha_0&0\end{bmatrix}\oplus\dots\oplus\begin{bmatrix}1&-1\\-\alpha_{p-1}&0\end{bmatrix},\\Y_{\alpha^{(p)},\vartheta}&:=\begin{bmatrix}0&0\\e^{\mathbf{i}\vartheta}&1\end{bmatrix}\oplus\begin{bmatrix}0&0\\1&1\end{bmatrix}\oplus\dots\oplus\begin{bmatrix}0&0\\1&1\end{bmatrix}.\end{aligned}$$

Then, one has

$$\operatorname{dom}(H_{\alpha^{(p)},\vartheta})=\{u\in\widehat{H}^2(I_p\setminus\mathbb{Z}) : X_{\alpha^{(p)},\vartheta}\Gamma_0u+Y_{\alpha^{(p)},\vartheta}\Gamma_1u=0\}.$$

That is, the Lagrangian plane corresponding to $H_{\alpha^{(p)},\vartheta}$ is given by

$$\ker[X_{\alpha^{(p)},\vartheta}, Y_{\alpha^{(p)},\vartheta}].$$

In order to prove that $\mathcal{S}_n$ is open, let us recall that the edges of the spectral gaps are given by consecutive eigenvalues of the periodic, $H_{\alpha^{(p)},0}$, or antiperiodic, $H_{\alpha^{(p)},\pi}$, operators. Suppose that $\alpha \in \mathcal{S}_n$ and that the edges of the nth gap satisfy $\lambda_n(\alpha^{(p)},\vartheta) < \lambda_{n+1}(\alpha^{(p)},\vartheta)$ with either $\vartheta = 0$ or $\vartheta = \pi$. We claim that this strict inequality holds for all $\widetilde{\alpha}^{(p)} \in \mathbb{R}^p$ near $\alpha^{(p)}$, that is, that the gap is open under small perturbations of $\alpha^{(p)}$. Indeed, since the mapping

$$\mathbb{R}^p \ni \alpha^{(p)} \mapsto [X_{\alpha^{(p)},\vartheta}, Y_{\alpha^{(p)},\vartheta}] \text{ for } \vartheta = 0 \text{ or } \vartheta = \pi$$

is continuous, Theorem 4.5 yields continuity of the mapping

$$\mathbb{R}^p \ni \alpha^{(p)} \mapsto (H_{\alpha^{(p)},\vartheta} - \mathbf{i})^{-1} \in \mathcal{B}(L^2(I_p)) \text{ for } \vartheta = 0 \text{ or } \vartheta = \pi;$$

hence, the mappings

$$\alpha^{(p)} \mapsto \lambda_j(\alpha^{(p)},\vartheta), \alpha^{(p)} \mapsto \lambda_{j+1}(\alpha^{(p)},\vartheta), \text{ for } \vartheta = 0 \text{ or } \vartheta = \pi$$

are also continuous, which implies the asserted strict inequality

$$\lambda_n(\widetilde{\alpha}^{(p)},\vartheta) < \lambda_{n+1}(\widetilde{\alpha}^{(p)},\vartheta)$$

for all $\widetilde{\alpha}^{(p)}$ near $\alpha^{(p)}$.

In order to prove that $\mathcal{S}_n$ is dense, we need to show that for both cases $\vartheta = 0$ and $\vartheta = \pi$, the equality $\lambda_n(\alpha^{(p)},\vartheta) = \lambda_{n+1}(\alpha^{(p)},\vartheta)$ will not hold if $\alpha^{(p)}$ is replaced by its small perturbation. We will consider the case $\vartheta = 0$, that is, we will assume that $\lambda_n(\alpha^{(p)},0) = \lambda_{n+1}(\alpha^{(p)},0)$; the case $\vartheta = \pi$ is treated analogously. For $t \in \mathbb{R}$, let us introduce the perturbation $\alpha^{(p)}(t) := \{t + \alpha_0, \alpha_1, \dots, \alpha_{p-1}\}$. We claim that for every $\varepsilon > 0$, there is a $t_0 \in (0,\varepsilon)$ with

$$\lambda_n(\alpha^{(p)}(t_0),0) < \lambda_{n+1}(\alpha^{(p)}(t_0),0). \tag{4.35}$$

When proven, this inequality shows that there exist arbitrarily close to $\alpha^{(p)}$ perturbations that open the closed gap. To prove the claim, we utilize the Hadamard-type formula (4.29) for the boundary matrices $X_{\alpha^{(p)}(t),0}$, $Y_{\alpha^{(p)}(t),0}$. We recall that $\lambda := \lambda_n(\alpha^{(p)},0) = \lambda_{n+1}(\alpha^{(p)},0)$ is an eigenvalue of $H_{\alpha^{(p)},0}$ of multiplicity two. By Theorem 4.16, there is a basis $\{u_1,u_2\}$ in $\ker(H_{\alpha^{(p)},0} - \lambda)$ such that

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}\lambda_n(\alpha^{(p)}(t),0) = |u_1(0)|^2, \tag{4.36}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}\lambda_{n+1}(\alpha^{(p)}(t),0) = |u_2(0)|^2. \tag{4.37}$$

Next, we will prove that the values of the derivatives in (4.36) and (4.37) are not equal to each other. This fact implies that the eigenvalue curves $t \mapsto \lambda_n(\alpha^{(p)}(t),0)$ and $t \mapsto \lambda_{n+1}(\alpha^{(p)}(t),0)$ do not coincide for t near $t = 0$, which, in turn, yields (4.35) as needed. Starting the proof of the fact, we first remark that the eigenfunctions u_1 and u_2 are real-valued because the boundary conditions for $\vartheta = 0$ are real. Upon multiplying the eigenfunctions by appropriate constants, we may and will assume that $u_1(0)$ and $u_2(0)$ are nonnegative. If $u_1(0) \neq u_2(0)$, then the left-hand sides of (4.36) and (4.37) are not equal as required. If $u_1(0) = u_2(0)$, then for any $t \in \mathbb{R}$, the function $u_1 - u_2$ satisfies the boundary condition at $x = 0$ with α_0 replaced by $t + \alpha_0$. Therefore, $u_1 - u_2 \in \ker(H_{\alpha^{(p)}(t),0} - \lambda) \setminus \{0\}$ and thus λ is an eigenvalue of $H_{\alpha^{(p)}(t),0}$ for all $t \in \mathbb{R}$. That is, either $\lambda_n(\alpha^{(p)}(t), 0)$ or $\lambda_{n+1}(\alpha^{(p)}(t), 0)$ should be identically equal to λ for all t near 0. Hence, one of the derivatives in (4.36) and (4.37) vanishes, say, the first one. Then $u_1(0) = 0$. But in this case, $u_2(0) \neq 0$ for otherwise u_1 and u_2 would be linearly dependent. Thus, the value of the derivative in (4.36) is equal to zero, while the value of the derivative in (4.37) is not, as required. □

4.5 | Maslov crossing form for abstract boundary triplets

In this section, we discuss an infinitesimal version of the formula equating the Maslov index and the spectral flow for the family of operators $H_t = \mathcal{A}_t + V_t$ satisfying Hypothesis 4.3, which is assumed throughout this section. Formulas relating these two quantities are quite classical, and we refer the reader to the papers [26–29, 35, 44, 45, 63, 93, 95, 96, 114] and the literature therein. Employing the abstract Hadamard-type formula obtained in Theorem 3.25, we prove in Theorem 4.22 that the signature of the Maslov crossing form defined in (4.41) at an eigenvalue λ of the operator H_{t_0} is equal to the difference between the number of monotonically decreasing and the number of monotonically increasing eigenvalue curves for H_t bifurcating from λ.

For $\lambda \in \mathbb{R}$ and $t \in [0, 1]$, we introduce the following subspaces:

$$\begin{aligned}
\mathbb{K}_{\lambda,t} &:= \mathrm{T}_t(\ker(A^* + V_t - \lambda)) \subset \mathfrak{H} \times \mathfrak{H},\\
\mathcal{F}_t &:= \mathrm{ran}(Q_t) \subset \mathfrak{H} \times \mathfrak{H},\\
\mathrm{Y}_{\lambda,t} &:= \mathbb{K}_{\lambda,t} \oplus \mathcal{F}_t \subset ((\mathfrak{H} \times \mathfrak{H}) \oplus (\mathfrak{H} \times \mathfrak{H})),\\
\mathfrak{D} &:= \{\mathbf{p} = (p, p)^\top \,:\, p \in \mathfrak{H} \times \mathfrak{H}\} \subset ((\mathfrak{H} \times \mathfrak{H}) \oplus (\mathfrak{H} \times \mathfrak{H})).
\end{aligned} \tag{4.38}$$

Since $\mathrm{T}_t(\mathrm{dom}(\mathcal{A}_t)) = \mathrm{ran}(Q_t)$ by Hypothesis 4.3, the following assertions are equivalent:

$$(i)\ \ker(H_t - \lambda) \neq \{0\}, \quad (ii)\ \mathbb{K}_{\lambda,t} \cap \mathcal{F}_t \neq \{0\}, \quad (iii)\ \mathrm{Y}_{\lambda,t} \cap \mathfrak{D} \neq \{0\} \tag{4.39}$$

since $\mathfrak{D}$ is the diagonal subspace in $(\mathfrak{H} \times \mathfrak{H}) \oplus (\mathfrak{H} \times \mathfrak{H})$. In fact, using a fundamental [26, Proposition 3.5], one can deduce deeper connections between the spectral information for H_t and the behavior of Lagrangian planes under the following hypotheses.

Hypothesis 4.20. Given $\lambda \in \mathbb{R}$ and $t_0 \in [0, 1]$, we assume that

(i) $\lambda \notin \mathrm{Spec}_{\mathrm{ess}}(H_{t_0})$.

Moreover, there exists an interval $\mathcal{J} \subset [0, 1]$ centered at t_0 such that

(ii) the mappings $t \mapsto \mathrm{T}_t$, $t \mapsto V_t$, $t \mapsto Q_t$ are C^1 on $\mathcal{J}$,
(iii) $\ker(A^* + V_t - \lambda) \cap \mathrm{dom}(A) = \{0\}$ for all $t \in \mathcal{J}$.

Hypothesis 4.20 will be assumed through this section. Part (iii) of this hypothesis is an abstract version of the unique continuation principle for PDEs, and we refer to [93, Theorems 3.2 and Hypothesis 5.9] for a discussion of this connection. Part (i) implies that the operator $H_{t_0} - \lambda$ is Fredholm. Since $\ker(\mathrm{T}) = \mathrm{dom}(A)$ by Lemma 2.3(1), parts (i) and (iii) of Hypothesis 4.20 imply that $\mathrm{T}|_{\ker(H_{t_0} - \lambda)}$ is an isomorphism between $\ker(H_{t_0} - \lambda)$ and $\mathbb{K}_{\lambda,t} \cap \mathcal{F}_t$, cf. (4.39). Moreover, the subspaces $\mathbb{K}_{\lambda,t_0}$ and $\mathcal{F}_{t_0}$ form a Fredholm pair (i.e., their intersection is finite dimensional and their sum is closed and has finite codimension). The latter fact has been established in [26, Proposition 3.5] in the setting of Lagrangian planes in $\operatorname{dom}(A^*)/\operatorname{dom}(A)$; using this one can readily deduce the Fredholm property of the pair in the present setting via the symplectomorphism introduced in [93, Proposition 5.3]. The subspace $\mathcal{F}_t$ is Lagrangian by Hypothesis 4.3. The subspace $\mathbb{K}_{\lambda,t}$ is also Lagrangian again by [26, Proposition 3.5]. Furthermore, part (ii) of Hypothesis 4.20 yields continuity in t of the resolvent operators for H_t by Theorem 3.18. This, together with part (i), shows that $\lambda \notin \operatorname{Spec}_{\rm ess}(H_t)$ for t near t_0; hence, the subspaces $\mathbb{K}_{\lambda,t}, \mathcal{F}_t$ form a Fredholm pair of Lagrangian subspaces for each t near t_0. Hence, $\big(\Upsilon_{\lambda,t}, \mathfrak{D}\big)$ is a Fredholm pair of Lagrangian subspaces for each t near t_0.

Let $\Pi_{\lambda,t}$ be the orthogonal projection onto $\Upsilon_{\lambda,t}$ from (4.38) so that the mapping $t \mapsto \Pi_{\lambda,t}$ is continuously differentiable on [0,1] for each $\lambda \in \mathbb{R}$, see [93, pp.480–481]. Furthermore, for $\lambda \in \mathbb{R}$ and $t_0 \in [0,1]$ satisfying Hypothesis 4.20, there is an interval $\mathcal{I} \subseteq \mathcal{J} \subset [0,1]$ centered at t_0 and a family of operators $t \mapsto \mathcal{M}_{\lambda,t}$, $t \in \mathcal{I}$, which is in $C^1\big(\mathcal{I}, \mathcal{B}(\Upsilon_{\lambda,t_0}, (\Upsilon_{\lambda,t_0})^{\perp})\big)$ with $\mathcal{M}_{\lambda,t_0} = 0$ such that

$$\Upsilon_{\lambda,t} = \big\{\mathbf{q} + \mathcal{M}_{\lambda,t}\mathbf{q} \,\big|\, \mathbf{q} \in \Upsilon_{\lambda,t_0}\big\}, t \in \mathcal{I}, \tag{4.40}$$

see, for example, [44, Lemma 3.8]. We call (λ, t_0) a conjugate point if $\ker(H_{t_0} - \lambda) \neq \{0\}$, or equivalently, if assertions (ii) and (iii) in (4.39) hold for $t = t_0$. The Maslov crossing form $\mathfrak{m}_{t_0}$ for $\Upsilon_{\lambda,t}$ relative to $\mathfrak{D}$ at the conjugate point (λ, t_0) is defined on the finite-dimensional intersection $\Upsilon_{\lambda,t_0} \cap \mathfrak{D}$ of the Lagrangian subspaces by the formula

$$\mathfrak{m}_{t_0}(\mathbf{q}, \mathbf{p}) := \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} \widehat{\omega}(\mathbf{q}, \mathcal{M}_{\lambda,t}\mathbf{p}) = \widehat{\omega}(\mathbf{q}, \dot{\mathcal{M}}_{\lambda,t_0}\mathbf{p}),\ \mathbf{p}, \mathbf{q} \in \Upsilon_{\lambda,t_0} \cap \mathfrak{D}, \tag{4.41}$$

where $\widehat{\omega} = \omega \oplus (-\omega)$ is a symplectic form on $(\mathfrak{H} \times \mathfrak{H}) \oplus (\mathfrak{H} \times \mathfrak{H})$ and, as usual, we abbreviate $\dot{\mathcal{M}}_{\lambda,t_0} = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{M}_{\lambda,t}\big|_{t=t_0}$.

Lemma 4.21. *Let (λ, t_0) be a conjugate point satisfying Hypothesis 4.20 and let $u \in \ker(H_{t_0} - \lambda)$. Then there exist an open interval $\mathcal{I} \subseteq \mathcal{J}$ centered at t_0, a family $t \mapsto w_t$ in $C^1(\mathcal{I}, \mathcal{H}_+)$, and a family $t \mapsto g_t \in \operatorname{ran}(Q_t)$ in $C^1(\mathcal{I}, \mathfrak{H} \times \mathfrak{H})$ such that*

$$\begin{aligned} w_{t_0} &= u, \quad g_{t_0} = \mathrm{T}_{t_0}u, \\ w_t &\in \ker(A^* + V_t - \lambda), \end{aligned} \tag{4.42}$$

$$(\mathrm{T}_t w_t, g_t)^\top = \Big(\mathrm{T}_{t_0}u, \mathrm{T}_{t_0}u\Big)^\top + \mathcal{M}_{\lambda,t}\Big(\mathrm{T}_{t_0}u, \mathrm{T}_{t_0}u\Big)^\top,\ t \in \mathcal{I}, \tag{4.43}$$

where $\mathcal{M}_{\lambda,t}$ is as in (4.40).

Proof. The proof is similar to that of [95, Lemma 2.6, p. 355]. For brevity, we denote $N_t := \ker(A^* + V_t - \lambda)$, $q := \mathrm{T}_{t_0}u$, $\mathbf{q} := (q, q)$ and let P_t be the orthogonal projections onto $\mathbb{K}_{\lambda,t}$. Then $P_t \in C^1\big(\mathcal{I}, \mathcal{B}(\mathfrak{H} \times \mathfrak{H})\big)$ for some open interval $\mathcal{I} \subseteq \mathcal{J}$ centered at t_0 (see, e.g., [26, Theorem 3.9], [93, Theorem 5.10]). We now consider the projections in $(\mathfrak{H} \times \mathfrak{H}) \times (\mathfrak{H} \times \mathfrak{H})$ given by

$$\widehat{P}_t := \begin{bmatrix} P_t & 0 \\ 0 & 0 \end{bmatrix}, \ \widehat{Q}_t := \begin{bmatrix} 0 & 0 \\ 0 & Q_t \end{bmatrix},$$

so that $\widehat{P}_t + \widehat{Q}_t = \Pi_{\lambda,t}$, $\operatorname{ran}(\Pi_{\lambda,t}) = \mathrm{Y}_{\lambda,t} = \mathbb{K}_{\lambda,t} \oplus \mathcal{F}_t$. Using the definition of $\mathrm{Y}_{\lambda,t}$ and $\mathcal{M}_{\lambda,t}$, see (4.38) and (4.40), we define

$$h_t \in \operatorname{ran}(P_t) \subset \mathfrak{H} \times \mathfrak{H},\ g_t \in \operatorname{ran}(Q_t) \subset \mathfrak{H} \times \mathfrak{H},$$

such that

$$(h_t, 0)^\top = \widehat{P}_t(\mathbf{q} + \mathcal{M}_{\lambda,t}\mathbf{q}) \text{ and } (0, g_t)^\top = \widehat{Q}_t(\mathbf{q} + \mathcal{M}_{\lambda,t}\mathbf{q}), \tag{4.44}$$

and so $h_{t_0} = g_{t_0} = q$. Since $t \mapsto \mathcal{M}_{\lambda,t}$, $t \mapsto P_t$ and $t \mapsto Q_t$ are C^1, we know that the maps $t \mapsto h_t$ and $t \mapsto g_t$ are C^1. As above, employing Hypothesis 4.20 and $\ker \mathrm{T}_t = \operatorname{dom}(A)$, see Lemma 2.3 (1), we conclude that the restriction

$$\mathrm{T}_t \restriction_{N_t} : N_t \to \operatorname{ran}(P_t) \subset \mathfrak{H} \times \mathfrak{H},$$

of T_t to N_t is a bijection. Therefore, there is a unique vector $w_t \in N_t$ satisfying $\mathrm{T}_t w_t = h_t$. Assertions (4.42) and (4.43) hold with this choice of w_t and g_t.

It remains to show that the function $t \mapsto w_t$ is in $C^1(\mathcal{I}, \mathcal{H}_+)$. Let U_t denote the C^1 family of boundedly invertible transformation operators in $\mathcal{H}_+$ that split the projections $\mathcal{P}_{N_t}$ onto N_t and $\mathcal{P}_{N_{t_0}}$ onto N_{t_0} so that the identity $U_t\mathcal{P}_{N_{t_0}} = \mathcal{P}_{N_t}U_t$ holds, and $U_t : N_{t_0} \mapsto N_t$ are bijections for t near t_0, cf. [95, Remark 2.4], [44, Remark 3.5], [47, Section IV.1], [63, Remark 6.11]. We temporarily introduce $v_t \in N_{t_0}$ by $v_t = U_t^{-1}w_t$ so that $\mathrm{T}_t w_t = h_t$ yields $(\mathrm{T}_t \circ U_t)v_t = h_t$. The map $\mathrm{T}_t \circ U_t|_{N_{t_0}} : N_{t_0} \to \operatorname{ran}(P_t)$ is a bijection and $t \mapsto \mathrm{T}_t \circ U_t|_{N_{t_0}}$ is in $C^1\big(\mathcal{I}, \mathcal{B}(N_{t_0}, \mathfrak{H} \times \mathfrak{H})\big)$ by the assumptions in the lemma. Since $w_t = U_t \circ \big(\mathrm{T}_t \circ U_t\big)^{-1} h_t$, the function $t \mapsto w_t$ is C^1 because each of the three terms in the composition is C^1. $\square$

Theorem 4.22. *Under Hypothesis 4.3, let (λ, t_0) be a conjugate point satisfying Hypothesis 4.20. Let $\{\lambda_j(t)\}_{j=1}^m$, with $\lambda = \lambda(t_0)$, $\{u_j\}_{j=1}^m$ be as in Theorem 4.5, and let $\mathbf{q}_j := (\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j)^\top \in \mathrm{Y}_{\lambda,t_0} \cap \mathfrak{D}$. Then, the slope of the eigenvalue curves satisfies*

$$\dot{\lambda}_j(t_0) = \mathfrak{m}_{t_0}(\mathbf{q}_j, \mathbf{q}_j),\ 1 \leqslant j \leqslant m, \tag{4.45}$$

where $\mathfrak{m}_{t_0}$ is the Maslov form introduced in (4.41).

Proof. For a fixed j, let (w_t, g_t) be as in Lemma 4.21 with $u := u_j$. Differentiating

$$A^* w_t + V_t w_t - \lambda w_t = 0, \tag{4.46}$$

at t_0 and multiplying the result by $w_{t_0} = u_j$, we get

$$\langle (A^* + V_{t_0} - \lambda)\dot{w}_{t_0}, w_{t_0} \rangle_{\mathcal{H}} + \langle \dot{V}_{t_0} w_{t_0}, w_{t_0} \rangle_{\mathcal{H}} = 0.$$

Using the Green identity (4.1) with $u = \dot{w}_{t_0}$ and $v = w_{t_0}$, we obtain

$$\begin{aligned} \langle (A^* + V_{t_0} - \lambda)\dot{w}_{t_0}, w_{t_0} \rangle_{\mathcal{H}} &= \langle \dot{w}_{t_0}, (A^* + V_{t_0} - \lambda) w_{t_0} \rangle_{\mathcal{H}} \\ &+ \langle \Gamma_{1t_0}\dot{w}_{t_0}, \Gamma_{0t_0} w_{t_0} \rangle_{\mathfrak{H}} - \langle \Gamma_{0t_0}\dot{w}_{t_0}, \Gamma_{1t_0} w_{t_0} \rangle_{\mathfrak{H}}. \end{aligned} \tag{4.47}$$

Combining (4.46) and (4.47) yields

$$\omega\left(\mathrm{T}_{t_0}\dot{w}_{t_0},\, \mathrm{T}_{t_0}u_j\right) + \langle \dot{V}_{t_0}u_j,\, u_j\rangle_{\mathcal{H}} = 0. \tag{4.48}$$

Next, (4.41) and (4.43) yield

$$\mathfrak{m}_{t_0}(\mathbf{q}_j, \mathbf{q}_j) = \omega\left(\mathrm{T}_{t_0}u_j,\, \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0}(\mathrm{T}_t w_t)\right) - \omega(\mathrm{T}_{t_0}u_j,\, \dot{g}_{t_0}). \tag{4.49}$$

Since $g_t = Q_t g_t$, we have

$$\dot{g}_{t_0} = \dot{Q}_{t_0}g_{t_0} + Q_{t_0}\dot{g}_{t_0} = \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j + Q_{t_0}\dot{g}_{t_0}.$$

Utilizing this, the fact that $\mathrm{ran}(Q_{t_0})$ is Lagrangian and $\mathrm{T}u_j \in \mathrm{ran}(Q_{t_0})$, we get

$$\omega(\mathrm{T}_{t_0}u_j,\, \dot{g}_{t_0}) = \omega(\mathrm{T}_{t_0}u_j,\, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j + Q_{t_0}\dot{g}_{t_0}) = \omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j). \tag{4.50}$$

Then, (4.48), (4.49), and (4.50) yield

$$\begin{aligned}
\mathfrak{m}_{t_0}(\mathbf{q}_j, \mathbf{q}_j) &= \omega\left(\mathrm{T}_{t_0}u_j, \dot{\mathrm{T}}_{t_0}u_j\right) + \omega\left(\mathrm{T}_{t_0}u_j,\, \mathrm{T}_{t_0}\dot{w}_{t_0}\right)\\
&\quad - \omega(\mathrm{T}_{t_0}u_j, \dot{Q}_{t_0}\mathrm{T}_{t_0}u_j)\\
&= \omega\left(\mathrm{T}_{t_0}u_j, \dot{\mathrm{T}}_{t_0}u_j\right) + \langle \dot{V}_{t_0}u_j,\, u_j\rangle_{\mathcal{H}}\\
&\quad + \omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j),
\end{aligned} \tag{4.51}$$

where we used $\omega(\dot{Q}_{t_0}\mathrm{T}_{t_0}u_j, \mathrm{T}_{t_0}u_j) \in \mathbb{R}$, see (3.39). Comparing (4.51) and (3.38), one infers (4.45) as required. □

Remark 4.23. Formula (4.45) in Theorem 4.22 yields a fundamental relation between the Maslov index and the spectral flow of the family of operators $H_t = \mathcal{A}_t + V_t$ satisfying the condition $\mathrm{T}_t(\mathrm{dom}(H_t)) = \mathcal{F}_t$ for a given family of Lagrangian subspaces $\mathcal{F}_t$, $t \in [0,1]$. This relation goes back to the celebrated Atiyah–Patodi–Singer theorem and it has been a subject of intensive research ever since, see, for example, [26–29, 35, 44, 114] and many more references therein. We will briefly comment on the equality of the Maslov index and the spectral flow. First, we recall the definition of the Maslov index via crossing forms. For a fixed $\lambda = \lambda_0$ from now on, we assume that Hypothesis 4.20 is satisfied for all $t = t_0 \in [0,1]$. Then, given the subspaces defined in (4.38), and assuming that all conjugate points (λ, t_0) for $t_0 \in [0,1]$ are nondegenerate (in the sense that the quadratic form $\mathfrak{m}_{t_0}$ from (4.41) is nondegenerate), one defines the Maslov index by the formula

$$\mathrm{Mas}\left(\mathrm{Y}_{\lambda_0,t} : t \in [0,1]\right) = -m_-(0) + \sum_{0<t_0<1}\left(m_+(t_0) - m_-(t_0)\right) + m_+(1), \tag{4.52}$$

where the summation is taken over all t_0 such that (λ, t_0) is a conjugate point and we denote by $m_+(t_0)$, respectively, $m_-(t_0)$ the number of positive, respectively, negative squares of the quadratic form $\mathfrak{m}_{t_0}$ at the conjugate point. Next, we recall the definition of the spectral flow: The spectral flow $\mathrm{SpF}_{\lambda_0}(H_t : t \in [0,1])$ for the family of operators H_t is the net count of the eigenvalues of H_t passing through λ_0 as t changes from $t = 0$ to $t = 1$ and is defined as follows, cf., for example, [28, Appendix]. Take a partition $0 = t_0 < t_1 < \cdots < t_N = 1$ and N intervals $[a_\ell, b_\ell]$ such that $a_\ell < \lambda_0 < b_\ell$ and $a_\ell, b_\ell \notin \mathrm{Spec}(H_t)$ for all $t \in [t_{\ell-1}, t_\ell]$, $1 \leqslant \ell \leqslant N$. Then, the spectral flow is defined by

$$\mathrm{SpF}_{\lambda_0}(H_t \,:\, t \in [0,1]) = \sum_{\ell=1}^{N} \sum_{a_\ell \leqslant \lambda < \lambda_0} \Big(\dim\ker(H_{t_{\ell-1}} - \lambda) - \dim\ker(H_{t_\ell} - \lambda)\Big). \tag{4.53}$$

By our assumptions, due to part (i) in Hypothesis 4.20, λ_0 does not belong to the essential spectrum of the operator H_t for all $t \in [0,1]$. Moreover, let us assume, in addition, that for each $t_0 \in [0,1]$ such that $\lambda_0 \in \mathrm{Spec}_{\mathrm{disc}}(H_{t_0})$, the inequality $\dot{\lambda}_j(t_0) \neq 0$ holds for all $j = 1, \dots, m$. Here, $m = m(t_0)$ is the multiplicity of the isolated eigenvalue λ_0 of H_{t_0}, and $\{\lambda_j(t)\}$ are the eigenvalues of H_t as in Theorem 3.26(2) and Theorem 4.5(2) for $t \in [t_0', t_0'']$ near t_0. With no loss of generality, $t = t_0$ could be assumed to be the only point in $[t_0', t_0'']$ such that $\lambda_0 \in \mathrm{Spec}(H_t)$. By our assumptions and formula (4.45) in Theorem 4.22, the quadratic form $\mathfrak{m}_{t_0}$ defined in (4.41) is nondegenerate and $m_+(t_0)$, respectively, $m_-(t_0)$ is equal to the number of j's such that the eigenvalue $\lambda_j(t)$ moves through λ_0 in the positive, respectively, negative direction as t changes from t_0' to t_0''. Formulas (4.52) and (4.53) now show that $\mathrm{Mas}\big(\Upsilon_{\lambda_0,t} \,:\, t \in [t_0', t_0'']\big) = \mathrm{SpF}_{\lambda_0}(H_t \,:\, t \in [t_0', t_0''])$. Passing to a partition of [0,1] then gives

$$\mathrm{Mas}\Big(\Upsilon_{\lambda_0,t} \,:\, t \in [0,1]\Big) = \mathrm{SpF}_{\lambda_0}(H_t \,:\, t \in [0,1]), \tag{4.54}$$

the desired equality of the Maslov index and the spectral flow.

5 | HADAMARD-TYPE FORMULA FOR ELLIPTIC OPERATORS VIA DIRICHLET AND NEUMANN TRACES

In this section, concerns self-adjoint realizations of second-order elliptic operators on bounded domains. We begin by discussing a resolvent difference formula, see Proposition 5.1, an Hadamard-type formula, (5.9), and asymptotic resolvent expansions, Theorem 5.2, for the elliptic operators (5.1) posted on bounded domains with smooth boundary. We deduce all these results from Theorem 3.26 by appropriately choosing the trace maps. The main technical issue is to validate Hypotheses 3.10 and 3.13, which is done in Proposition 5.4. Next, these results are utilized to give simple and unified proofs of Friedlander's theorem [62, Theorem 1.1], see Example 5.5, and Rohleder's theorem [116, Theorem 3.2], see Example 5.6. Furthermore, in Section 5.3, we consider the heat equation with space-dependent diffusion coefficient equipped with Robin boundary conditions so that both the equation and the boundary conditions contain a physically relevant parameter, the thermal conductivity. The results in this section provide, in particular, a new proof of the fact that the temperature of a nonhomogeneous material immersed into a surrounding medium of constant temperature depends continuously on the thermal conductivity of the material.

5.1 | Elliptic operators

On a C^∞-smooth bounded domain Ω, we consider the following differential expression:

$$\begin{aligned}\mathcal{L} :&= -\sum_{j,k=1}^{n} \partial_j \mathrm{a}_{jk} \partial_k + \sum_{j=1}^{n} \mathrm{a}_j \partial_j - \partial_j \mathrm{a}_j + \mathrm{q}, \\ &= -\operatorname{div}(\mathrm{A}\nabla) + \mathrm{a}\cdot\nabla - \nabla\cdot\mathrm{a} + \mathrm{q},\end{aligned} \tag{5.1}$$

with coefficients $\mathrm{A} = \{\mathrm{a}_{ij}\}_{1\leqslant i,j\leqslant n}$, $\mathrm{a} := \{\mathrm{a}_i\}_{1\leqslant i\leqslant n}$ satisfying, for some $c = c(\mathcal{L}) > 0$,

$$\sum_{j,k=1}^{n} \mathrm{a}_{jk}(x)\xi_k\overline{\xi_j} \geqslant c\sum_{j=1}^{n} |\xi_j|^2, x \in \overline{\Omega}, \xi = \{\xi_j\}_{j=1}^n \in \mathbb{C}^n, \tag{5.2}$$

$$\mathrm{a}_{jk}, \mathrm{a}_j \in C^\infty(\overline{\Omega};\mathbb{R}), \mathrm{q} \in L^\infty(\Omega;\mathbb{R}), \mathrm{a}_{jk}(x) = \mathrm{a}_{kj}(x), 1 \leqslant j,k \leqslant n.$$

Associated with $\mathcal{L}$ is the following space of distributions:

$$\mathcal{D}^s(\Omega) := \{u \in H^s(\Omega) : \mathcal{L}u \in L^2(\Omega)\},\ s \geqslant 0,$$

equipped with the norm

$$\|u\|_s := \left(\|u\|^2_{H^s(\Omega)} + \|\mathcal{L}u\|^2_{L^2(\Omega)}\right)^{1/2}, \tag{5.3}$$

where $\mathcal{L}u$ should be understood in the sense of distributions. Let us introduce two operators acting in $L^2(\Omega)$,

$$\begin{aligned}\mathcal{L}_{\min} f &:= \mathcal{L}f,\ f \in \operatorname{dom}(\mathcal{L}_{\min}) := H^2_0(\Omega), \\ \mathcal{L}_{\max} f &:= \mathcal{L}f,\ f \in \operatorname{dom}(\mathcal{L}_{\max}) := \mathcal{D}^0(\Omega).\end{aligned}$$

The operator $\mathcal{L}_{\min}$ is closed, symmetric, and $(\mathcal{L}_{\min})^* = \mathcal{L}_{\max}$. Associated with $\mathcal{L}$ is a first-order trace operator $\gamma_{_{N,\mathcal{L}}} \in \mathcal{B}(\mathcal{D}^1(\Omega), H^{-1/2}(\partial\Omega))$ that is a unique extension of the conormal derivative

$$\gamma_{_{N,\mathcal{L}}} u := \sum_{j,k=1}^{n} \mathrm{a}_{jk}\nu_j\gamma_{_D}(\partial_k u) + \sum_{j=1}^{n} \mathrm{a}_j\nu_j\gamma_{_D} u, u \in H^2(\Omega)$$

to the space $\mathcal{D}^1(\Omega)$ (here, $(\nu_1, \dots, \nu_n)$ is the outward unit normal on $\partial\Omega$). Then, the following Green identity holds:

$$\langle \mathcal{L}u, v\rangle_{L^2(\Omega)} - \langle u, \mathcal{L}v\rangle_{L^2(\Omega)} = \langle \gamma_{_D} u, \gamma_{_{N,\mathcal{L}}} v\rangle_{-1/2} - \overline{\langle \gamma_{_D} v, \gamma_{_{N,\mathcal{L}}} u\rangle_{-1/2}},$$

for all $u, v \in \mathcal{D}^1(\Omega)$. In order to rewrite this identity in a form compatible with (2.3), let Φ denote the Riesz isomorphism $\Phi \in \mathcal{B}(H^{-1/2}(\partial\Omega), H^{1/2}(\partial\Omega))$ as in (4.21) and define

$$\Gamma_0 := \gamma_{_D} \in \mathcal{B}(\mathcal{D}^1(\Omega), H^{1/2}(\partial\Omega)),\ \Gamma_1 := -\Phi\gamma_{N,\mathcal{L}} \in \mathcal{B}(\mathcal{D}^1(\Omega), H^{1/2}(\partial\Omega)). \tag{5.4}$$

Then, we have, for all $u, v \in \mathcal{D}^1(\Omega)$,

$$\begin{aligned}\langle \mathcal{L}_{\max} u, v\rangle_{L^2(\Omega)} - \langle u, \mathcal{L}_{\max} v\rangle_{L^2(\Omega)} \\ = \langle \Gamma_1 u, \Gamma_0 v\rangle_{H^{1/2}(\partial\Omega)} - \langle \Gamma_0 u, \Gamma_1 v\rangle_{H^{1/2}(\partial\Omega)}.\end{aligned} \tag{5.5}$$

We claim that Hypotheses 2.1 and 3.1 are satisfied for

$$A = \mathcal{L}_{\min}, \mathcal{H}_+ = \mathcal{D}^0(\Omega), \mathcal{D} = \mathcal{D}^1(\Omega), \Gamma_0 = \gamma_{_D}, \Gamma_1 = -\Phi\gamma_{N,\mathcal{L}}. \tag{5.6}$$

Since we already checked the Green identity, (5.5), to justify the claim, it remains to show that $\mathrm{T}(\mathcal{D})$ is dense in $H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$ and that $\mathcal{D}^1(\Omega)$ is dense in $\mathcal{D}^0(\Omega)$. By [73, Proposition 2.1] and [18, Section 4.3], one has

$$(\gamma_{_D}, \gamma_{_{N,\mathcal{L}}})(H^2(\Omega)) = H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega),$$

and the right-hand side is dense in $H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$. By [73, Theorem 3.2], $H^2(\Omega)$ is dense in $\mathcal{D}^s(\Omega), s < 2$; hence, $\mathcal{D}^1(\Omega)$ is dense in $\mathcal{D}^0(\Omega)$.

Proposition 5.1. *Under the assumptions on $\mathcal{L}$ imposed in this section, for any two self-adjoint extensions $\mathcal{L}_1, \mathcal{L}_2$ of $\mathcal{L}_{min}$ with domains containing in $\mathcal{D}^1(\Omega)$ and $\zeta \notin (\mathrm{Spec}(\mathcal{L}_1) \cup \mathrm{Spec}(\mathcal{L}_2))$, the following resolvent difference formula holds:*

$$(\mathcal{L}_2 - \zeta)^{-1} - (\mathcal{L}_1 - \zeta)^{-1} = (\mathrm{T}(\mathcal{L}_2 - \bar{\zeta})^{-1})^* J \mathrm{T}(\mathcal{L}_1 - \zeta)^{-1},$$

where $\mathrm{T} = [\Gamma_0, \Gamma_1]^\top$ is defined in (5.4), and

$$(\mathrm{T}(\mathcal{L}_2 - \bar{\zeta})^{-1})^* \in \mathcal{B}(H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega), L^2(\Omega)).$$

Proof. The results follow directly from (2.13). ☐

5.2 | Hadamard-type formulas for Robin elliptic operators, L. Friedlander's and J. Rohleder's inequalities

In this section, we obtain an Hadamard-type formula for a one-parameter family of differential operators $\mathcal{L}_t u = \mathcal{L} u$ as in (5.1) for which the dependence on the parameter t enters through the Robin boundary condition $\gamma_{_{N,\mathcal{L}}} u = \Theta_t \gamma_{_D} u$, see Theorem 5.2. We will utilize Theorem 3.26 by choosing the symmetric operator A, the function spaces $\mathcal{H}, \mathcal{H}_+, \mathfrak{H}$, and the trace operator T as indicated in (5.6). The main challenge is to check Hypothesis 3.16 that in this setting reads as follows:

$$\|(\mathcal{L}_t - \mathbf{i})^{-1} - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}\|_{\mathcal{B}(L^2(\Omega), \mathcal{D}^1(\Omega))} = o(1),\ t \to t_0,$$

and can be reduced to showing that for some constant $c > 0$, one has the inequality

$$\|\nabla u\|^2_{L^2(\Omega)} \leqslant c\Big(\|\mathcal{L} u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)}\Big), u \in \mathrm{dom}(\mathcal{L}_t),$$

for t near t_0. We discuss the reduction and give the proof of this inequality in Proposition 5.4. Throughout this section, we will make use of the continuous embedding $\iota : H^{1/2}(\partial\Omega) \hookrightarrow L^2(\Omega)$ and its adjoint $\iota^* : L^2(\Omega) \hookrightarrow H^{-1/2}(\partial\Omega)$.

Theorem 5.2. *Suppose that, in addition to the assumptions on $\mathcal{L}$ listed in Subsection 5.1, we are given a mapping $t \mapsto \Theta_t$ belonging to $C^1([0,1], L^\infty(\partial\Omega, \mathbb{R}))$. Then, for $t \in [0,1]$, the Robbin elliptic operator $\mathcal{L}_t$ defined by*

$$\mathcal{L}_t : \mathrm{dom}(\mathcal{L}_t) \subset L^2(\Omega) \to L^2(\Omega), \quad \mathcal{L}_t u = \mathcal{L}u,$$
$$u \in \mathrm{dom}(\mathcal{L}_t) = \{u \in \mathcal{D}^1(\Omega) : \gamma_{_{N,\mathcal{L}}} u = \iota^*\Theta_t \iota \gamma_{_D} u\},$$

is self-adjoint, where ι denotes the embedding of $H^{1/2}(\partial\Omega)$ into $L^2(\Omega)$. The following resolvent difference formula holds:

$$(\mathcal{L}_t - \zeta)^{-1} - (\mathcal{L}_s - \zeta)^{-1} = \Big(\gamma_{_D}(\mathcal{L}_t - \overline{\zeta})^{-1}\Big)^*(\Theta_t - \Theta_s)\Big(\gamma_{_D}(\mathcal{L}_s - \zeta)^{-1}\Big), \tag{5.7}$$

for $t, s \in [0,1]$, $\zeta \notin (\mathrm{Spec}(\mathcal{L}_t) \cup \mathrm{Spec}(\mathcal{L}_s))$. Moreover, the mapping

$$t \mapsto (\mathcal{L}_t - \zeta)^{-1} \in \mathcal{B}(L^2(\Omega))$$

is well defined for t near t_0 as long as $\zeta \notin \mathrm{Spec}(\mathcal{L}_{t_0})$. This mapping is differentiable at t_0 and satisfies the following Riccati equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0}\big((\mathcal{L}_t - \zeta)^{-1}\big) = \Big(\gamma_{_D}(\mathcal{L}_{t_0} - \overline{\zeta})^{-1}\Big)^*\left(\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0}\Theta_t\right)\Big(\gamma_{_D}(\mathcal{L}_{t_0} - \zeta)^{-1}\Big). \tag{5.8}$$

Finally, if $\lambda(t_0)$ is an isolated eigenvalue of $\mathcal{L}_{t_0}$ of multiplicity $m \geqslant 1$, then there exists a choice of orthonormal eigenfunctions $\{u_j\}_{j=1}^m \subset \ker(\mathcal{L}_{t_0} - \lambda(t_0))$ and a labeling of eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of $\mathcal{L}_t$, for t near t_0, such that

$$\dot{\lambda}_j(t_0) = -\langle \dot{\Theta}_{t_0}\gamma_{_D} u_j, \gamma_{_D} u_j\rangle_{L^2(\partial\Omega)}, 1 \leqslant j \leqslant m. \tag{5.9}$$

Proof. We will employ Theorem 3.26. The proof consists of two steps. First, we derive (5.7) from (3.41). We can use (3.41) because Hypothesis 3.4 is trivially satisfied. Second, we derive (5.8) and (5.9) from (3.43) and (3.44). To apply (3.43) and (3.44), we need to verify Hypotheses 3.13 and 3.16. They are satisfied by Proposition 5.4 given next; the proof of this proposition uses formula (5.7) proved in the first step.

To proceed, we choose $\mathcal{H}_+, \mathcal{D}, A$ as in (5.6) and rewrite the Robin condition $\gamma_{_{N,\mathcal{L}}} u = \iota^*\Theta_t\iota\gamma_{_D} u$ in the definition of $\mathcal{L}_t$ as $\Phi\gamma_{_{N,\mathcal{L}}} u = \Phi\iota^*\Theta_t\iota\gamma_{_D} u$

$$X_t\Gamma_0 u + Y_t\Gamma_1 u = 0, \text{ where we set } X_t := \Phi\iota^*\Theta_t\iota, Y_t := I.$$

It is worth noting that X_t just defined is self-adjoint in $H^{1/2}(\partial\Omega)$ since for $\phi, \psi \in H^{1/2}(\partial\Omega)$, one has

$$\langle \Phi\iota^*\Theta_t\iota\phi, \psi\rangle_{1/2} = \overline{\langle \psi, \Phi\iota^*\Theta_t\iota\phi, \psi\rangle_{1/2}} = \overline{\langle \psi, \iota^*\Theta_t\iota\phi, \psi\rangle_{-1/2}}$$
$$= \overline{\langle \iota\psi, \Theta_t\iota\phi\rangle_{L^2(\partial\Omega)}} = \langle \iota\phi, \Theta_t\iota\psi\rangle_{L^2(\partial\Omega)}$$

$$= \langle \phi, \iota^*\Theta_t\iota\psi\rangle_{-1/2} = \langle \phi, \Phi\iota^*\Theta_t\iota\psi\rangle_{1/2}.$$

Continuity of Θ_t with respect to t and Theorem 3.18 with $\mathcal{A}_t := \mathcal{L}_t, V_t := 0, \mathrm{T}_t := [\gamma_{_D}, -\Phi\gamma_{N,\mathcal{L}}]^\top$ yield that the map $t \mapsto R_t(\zeta) := (\mathcal{L}_t - \zeta)^{-1}$ is well defined for t near t_0. Next, with W defined in (2.11), we observe that $R_t(\zeta)u \in \mathrm{dom}(\mathcal{A}_t)$ yields

$$(W(X_t, I))\mathrm{T}R_t(\zeta)u = -\Gamma_0 R_t(\zeta)u = -\gamma_{_D} R_t(\zeta)u \text{ for all } u \in L^2(\Omega).$$

This can be checked directly or by noting that $\phi = \big(W(X_t, I)\big)\mathrm{T}R_t(\zeta)u$ is the unique vector satisfying the relations $\Gamma_0 R_t(\zeta)u = -\phi$, $\Gamma_1 R_t(\zeta)u = X_t\phi$, cf. (3.45). This observation together with (3.41) yield (5.7). We can now involve Proposition 5.4 given next and verify Hypotheses 3.13 and 3.16 in the present setting. Thus, Theorem 3.26 applies and therefore (5.8) and (5.9) follow from (3.43) and (3.44) with $\phi_j = -\Gamma_0 u_j$. □

Remark 5.3. It is worth comparing Theorems 4.13 and 5.2 for the case $\mathcal{L} = -\Delta$ where both theorems apply. The major difference is in the type of trace operators utilized in each theorem. In Theorem 4.13, we use $\mathrm{T} = [-\tau_{_N}, \Phi\widehat{\gamma}_{_D}]^\top$ that is defined on the entire space $\mathcal{H}_+ = \mathrm{dom}(-\Delta_{\max})$ and is surjective, while in Theorem 5.2, we have $\mathrm{T} = [\gamma_{_D}, -\Phi\gamma_{_{N,\mathcal{L}}}]^\top$ that is defined only on a dense subset $\mathcal{D} = \mathcal{D}^1(\Omega)$ of $\mathcal{H}_+ = \mathcal{D}^0(\Omega)$. We note that the latter trace operator is local, while the former is not. In addition, these trace maps do not match even on smooth functions on Ω. Another major technical difference is that Hypotheses 3.13 and 3.16 are automatically satisfied in one case but not in the other.

Proposition 5.4. *Under assumptions of Theorem 5.2, one has*

$$\|(\mathcal{L}_t - \mathbf{i})^{-1}\|_{\mathcal{B}(L^2(\Omega), \mathcal{D}^1(\Omega))} = \mathcal{O}(1),\ t \to t_0, \tag{5.10}$$

$$\big\|(\mathcal{L}_t - \mathbf{i})^{-1} - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}\big\|_{\mathcal{B}(L^2(\Omega), \mathcal{D}^1(\Omega))} = o(1),\ t \to t_0, \tag{5.11}$$

for all $t_0 \in [0, 1]$. In other words, Hypotheses 3.13 and 3.16 hold for $\mathcal{A}_t := \mathcal{L}_t$.

Proof. To prove (5.10), it is enough to show that there exists a constant $c > 0$ such that

$$\|u\|^2_{\mathcal{D}^1(\Omega)} \leqslant c\|\mathcal{L}u - \mathbf{i}u\|^2_{L^2(\Omega)}, u \in \mathrm{dom}(\mathcal{L}_t),$$

for all $t \in [0, 1]$. By the definition of $\mathcal{D}^1(\Omega)$-norm, see (5.3), we need to prove that

$$\|\nabla u\|^2_{L^2(\Omega)} \leqslant c(\|\mathcal{L}u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)}), u \in \mathrm{dom}(\mathcal{L}_t). \tag{5.12}$$

To show this, we first notice that for $u \in \mathrm{dom}(\mathcal{L}_t)$, one has

$$\langle \mathtt{A}\nabla u, \nabla u\rangle_{L^2(\Omega)} = \langle \mathcal{L}u, u\rangle_{L^2(\Omega)} - \langle \mathtt{q}u, u\rangle_{L^2(\Omega)} - \langle \Theta_t\gamma_{_D} u, \gamma_{_D} u\rangle_{L^2(\partial\Omega)}.$$

Using the Cauchy–Schwartz inequality and (5.2), we get

$$\|\nabla u\|^2_{L^2(\Omega)} \leqslant c(\|\mathcal{L}u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)} + \|\Theta_t\|_{L^\infty(\partial\Omega)}\|\gamma_{_D} u\|^2_{L^2(\partial\Omega)}), \tag{5.13}$$

for $c > 0$ (which is t- and u-independent). Let us recall from [67, Lemma 2.5] the inequality

$$\|\gamma_{_D} u\|^2_{L^2(\Omega)} \leqslant \varepsilon \|\nabla u\|^2_{L^2(\Omega)} + \beta(\varepsilon)\|u\|^2_{L^2(\Omega)}, \text{ where } \varepsilon > 0 \text{ and } \beta(\varepsilon) \underset{\varepsilon\to 0}{=} \mathcal{O}(\varepsilon^{-1}).$$

Thus, continuing (5.13), we infer

$$\|\nabla u\|^2_{L^2(\Omega)} \leqslant c\Big(\|\mathcal{L}u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)} + \varepsilon\|\Theta_t\|_{L^\infty(\partial\Omega)}\|\nabla u\|^2_{L^2(\Omega)}$$
$$+\beta(\varepsilon)\|\Theta_t\|_{L^\infty(\partial\Omega)}\|u\|_{L^2(\Omega)}\Big)$$

for some $c > 0$. Taking $\varepsilon > 0$ sufficiently small yields (5.12) and thus (5.10).

Starting the proof of (5.11), we first show that

$$\big\|(\mathcal{L}_t - \mathbf{i})^{-1} - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}\big\|_{\mathcal{B}(L^2(\Omega),H^1(\Omega))} = o(1),\ t \to t_0. \tag{5.14}$$

We denote $R(t) := (\mathcal{L}_t - \mathbf{i})^{-1}$ and recall that we may use resolvent difference formula (5.7) already established in the first part of the proof of Theorem 5.2. It yields

$$\langle R(t)u - R(t_0)u, v\rangle_{L^2(\Omega)} = \langle (\Theta_{t_0} - \Theta_t)\gamma_{_D} R(t)u, \gamma_{_D} R(t_0)v\rangle_{L^2(\partial\Omega)} \tag{5.15}$$

for all $u, v \in L^2(\Omega)$. For $v \in (H^1(\Omega))^* = H^{-1}(\Omega)$, we view $w := R(t_0)v \in H^1(\Omega)$ as the solution to the boundary value problem $(\mathcal{L} - \mathbf{i})w = v$, $\gamma_{_{N,\mathcal{L}}} w = \Theta_{t_0}\gamma_{_D} w$. Using a well-known elliptic estimate $\|w\|_{H^1(\Omega)} \leqslant c\|v\|_{H^{-1}(\Omega)}$ from [104, Theorem 4.11(i)], the operator $R(t_0)$ can be extended to an operator in $\mathcal{B}((H^1(\Omega))^*, H^1(\Omega))$. So, (5.15) can be extended as follows:

$${}_{H^1(\Omega))}\langle R(t)u - R(t_0)u, v\rangle_{(H^1(\Omega))^*} = \langle (\Theta_{t_0} - \Theta_t)\gamma_{_D} R(t)u, \gamma_{_D} R(t_0)v\rangle_{L^2(\partial\Omega)},$$

now for all $u \in L^2(\Omega)$ and $v \in (H^1(\Omega))^*$. Hence,

$$|{}_{H^1(\Omega))}\langle R(t)u - R(t_0)u, v\rangle_{(H^1(\Omega))^*}| \leqslant \|\Theta_{t_0} - \Theta_t\|_{L^\infty(\partial\Omega)}\|\gamma_{_D}\|^2_{\mathcal{B}(D^1(\Omega),H^{1/2}(\partial\Omega))}$$
$$\times \|R(t)\|_{\mathcal{B}(L^2(\Omega),D^1(\Omega))}\|u\|_{L^2(\Omega)}\|R(t_0)\|_{\mathcal{B}((H^1(\Omega))^*,H^1(\Omega))}\|v\|_{(H^1(\Omega))^*}.$$

Since $\|R(t)\|_{\mathcal{B}(L^2(\Omega),D^1(\Omega))} = \mathcal{O}(1)$ by (5.10), and $\|\Theta_{t_0} - \Theta_t\|_{L^\infty(\partial\Omega)} = o(1)$, $t \to t_0$, the above inequality gives (5.14). We now combine (5.14) with the estimate

$$\big\|(\mathcal{L}_t - \mathbf{i})^{-1}u - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}u\big\|^2_{D^1(\Omega)} = \big\|(\mathcal{L}_t - \mathbf{i})^{-1}u - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}u\big\|^2_{H^1(\Omega)}$$
$$+ \big\|\mathcal{L}(\mathcal{L}_t - \mathbf{i})^{-1}u - \mathcal{L}(\mathcal{L}_{t_0} - \mathbf{i})^{-1}u\big\|^2_{L^2(\Omega)}$$
$$\leqslant 2\big\|(\mathcal{L}_t - \mathbf{i})^{-1}u - (\mathcal{L}_{t_0} - \mathbf{i})^{-1}u\big\|^2_{H^1(\Omega)}, u \in L^2(\Omega),$$

finishing the proof of (5.11). □

Example 5.5. Theorem 5.2 can be used in proving the celebrated Friedlander inequalities $\lambda_{D,k} \geqslant \lambda_{N,k+1}$, $k = 1, 2, \ldots$, for the eigenvalues of the Dirichlet and Neumann Laplacians, see [62], which was improved in [60] to state that $\lambda_{D,k} > \lambda_{N,k+1}$, see also [19, 61, 68, 117] for further advances, detailed bibliography and a historical account of this beautiful subject. Also, we refer to Example 5.10 for connections to the Maslov index. The proof of the Friedlander inequalities consists of two major steps. First, one proves that the counting functions of the Dirichlet and Neumann boundary problems differ by a number of negative eigenvalues of the Dirichlet-to-Neumann operator, see (5.33) below. Second, one proves the existence of a nonnegative eigenvalue of the latter. The first step involves a one-parameter family of Robin boundary value problems giving a homotopy of the Dirichlet to the Neumann boundary problem. The critical issue here is to show monotonicity of the eigenvalues of the Robin problems with respect to the parameter, and this is where the results of the current paper help. (In fact, monotonicity holds not merely for the Laplacian but for general elliptic operators as described in Subsection 5.1). Indeed, formula (5.9) in Theorem 5.2 with $\mathcal{L} = -\Delta$ and $\Theta_t = -\cot(\frac{\pi}{2}t)$ shows that the eigenvalues $\lambda = \lambda(t)$ of the Robin problem

$$\begin{cases} \mathcal{L}u = \lambda u \text{ in } \ \Omega, \\ \sin(\frac{\pi}{2}t)\gamma_{_N} u + \cos(\frac{\pi}{2}t)\gamma_{_D} u = 0 \text{ on } \partial\Omega \text{ for } t \in [0,1], \end{cases} \tag{5.16}$$

are monotonically decreasing with respect to $t \in [0, 1]$. We note that

$$\lambda_k(0) = \lambda_{D,k} \leqslant \lambda_{D,k+1} = \lambda_{k+1}(0) \text{ and}$$

$$\lambda_k(1) = \lambda_{N,k} \leqslant \lambda_{N,k+1} = \lambda_{k+1}(1), k = 1, 2, \dots,$$

are the Dirichlet and Neumann eigenvalues. From this point on, the arguments given in [62] and [60] are as follows. Monotonicity in t of the Robin eigenvalues $\lambda_k(t)$ just proved, and the standard inequalities $\lambda_{D,k} \geqslant \lambda_{N,k}$ show the strict inequalities $\lambda_{D,k} > \lambda_{N,k+1}$, provided that we know the fact, cf. [62, Lemma 1.3], that for each λ, there is a $t \in [0, 1]$ such that (5.16) has a nontrivial solution. This fact is equivalent to the existence of a positive eigenvalue $\cot(\frac{\pi}{2}t)$ of the Dirichlet-to-Neumann operator when $\lambda \notin \operatorname{Spec}(-\Delta_D)$, and its proof has been carried out in [62] and [60] for the Laplacian using the minimax principle and infinitely many linearly independent explicit functions $e^{i\eta\cdot x}$, with $\eta \in \mathbb{R}^n$ such that $\|\eta\|^2_{\mathbb{R}^n} = \lambda$, which satisfy $-\Delta(e^{i\eta\cdot x}) = \lambda e^{i\eta\cdot x}$.

Example 5.6. We will now derive from Theorem 5.2 an elegant result in [116, Theorem 3.2] regarding monotonicity of Robin eigenvalues. Given $\Theta^{(\ell)} \in L^\infty(\Omega; \mathbb{R})$, $\ell = 0, 1$, we define the Robin operators $\mathcal{L}^{(\ell)}u = \mathcal{L}u$ such that

$$\operatorname{dom}(\mathcal{L}^{(\ell)}) = \{u \in \mathcal{D}^1(\Omega) : \gamma_{_{N,\mathcal{L}}} u = \Theta^{(\ell)}\gamma_{_D} u\}$$

for the elliptic differential expression in (5.1). We let $\lambda_1(\mathcal{L}^{(\ell)}) \leqslant \lambda_2(\mathcal{L}^{(\ell)}) \leqslant \dots$ denote the eigenvalues of $\mathcal{L}^{(\ell)}$ counting multiplicities. Assume that $\Theta^{(0)} \leqslant \Theta^{(1)}$. We will give a new proof of J. Rohleder's result stating that

$$\text{if } \Theta^{(0)} < \Theta^{(1)} \text{ on a set of positive measure then } \lambda_k(\mathcal{L}^{(0)}) > \lambda_k(\mathcal{L}^{(1)}) \tag{5.17}$$

for $k = 1, 2, \dots$. Denote $\Theta_t = \Theta^{(0)} + t(\Theta^{(1)} - \Theta^{(0)})$ for $t \in [0, 1]$ and introduce operators $\mathcal{L}_t$ as in Theorem 5.2 such that $\mathcal{L}_0 = \mathcal{L}^{(0)}$ and $\mathcal{L}_1 = \mathcal{L}^{(1)}$. Denoting by $\lambda_k(t) := \lambda_k(\mathcal{L}_t)$ the eigenvalues of $\mathcal{L}_t$ counting multiplicities and by u_k the respective eigenfunctions, formula (5.9) implies

$$\frac{\mathrm{d}\lambda_k(t)}{\mathrm{d}t} = -\langle(\Theta^{(1)} - \Theta^{(0)})\gamma_{_D} u_k, \gamma_{_D} u_k\rangle_{L^2(\partial\Omega)} < 0, k = 1, 2, \dots, t \in [0, 1] \tag{5.18}$$

because $\Theta^{(0)} < \Theta^{(1)}$ on a set of positive measure, thus proving (5.17). Let us elaborate on some additional consequences of monotonicity of eigenvalues. As the eigenvalue curves $t \mapsto \lambda_k(t)$ are strictly

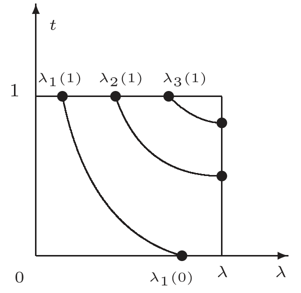

FIGURE 1 Illustration of (5.18), (5.19).

monotone and continuous, we obtain the following count for the eigenvalues, see Figure 1,

$$\begin{aligned}(\#\{k : \lambda_k(\mathcal{L}^{(1)}) < \lambda\}) - (\#\{k : \lambda_k(\mathcal{L}^{(0)}) < \lambda\})\\ = \sum_{t\in[0,1]} \dim\ker(\mathcal{L}_t - \lambda).\end{aligned} \tag{5.19}$$

A weaker version of this counting formula

$$(\#\{k : \lambda_k(\mathcal{L}^{(1)}) < \lambda\}) - (\#\{k : \lambda_k(\mathcal{L}^{(0)}) < \lambda\}) \geqslant \dim\ker(\mathcal{L}^{(0)} - \lambda),$$

was obtained by J. Rohleder [116, (3.4)] by variational methods. This is a key estimate in [116] leading to (5.17) in the original proof. Now, (5.19) can be viewed as a prequel to Section 5.5, where the left-hand side of (5.19) is treated as the spectral flow of the family $\{\mathcal{L}_t\}_{t\in[0,1]}$ through λ and the right-hand side is viewed as the Maslov index of a certain path of Lagrangian planes. The equality between the Maslov index and the spectral flow in a very general setting has been recently investigated in, for example, [44–46, 93, 95] and the vast literature cited therein.

5.3 | Continuous dependence of solutions to heat equation on thermal conductivity

In this section, we apply our general results to give a new proof that solutions to the linear homogeneous heat equation depend continuously on a certain physically relevant parameter present in both the operator and the boundary condition. The assertions of this type have a long and distinguished history, and have been resolved even for quite general Wentzell boundary conditions. We refer the reader to [42, 43] where one can also find further literature. We did not attempt to cover the case of Wentzell boundary conditions anywhere in this paper but remark parenthetically that it is an interesting open area to develop a version of the asymptotic perturbation theory for operators equipped with this type of dynamical boundary conditions. At the moment, as in [70], we consider the following heat equation:

$$\begin{cases} u_{\mathrm{t}}(\mathrm{t},x) = \varkappa\rho(x)\Delta_x u(\mathrm{t},x), x\in\Omega, \mathrm{t}\geqslant 0,\\ -\varkappa\frac{\partial u}{\partial n} = u, \text{ on } \partial\Omega,\end{cases} \tag{5.20}$$

describing the temperature u of a material in the region $\Omega\subset\mathbb{R}^3$ with thermal conductivity $\varkappa$ immersed in a surrounding medium of zero temperature. Here, $1/\rho(x)$ is the product of the density of the material times its heat capacity. The continuous dependence of the temperature u on the thermal conductivity $\varkappa$ with respect to $L^2(\Omega)$ norm follows from Theorem 5.7 proved below, which is a version of Theorem 5.2. To sketch the argument, we consider the self-adjoint operator $\mathcal{L}_\varkappa := -\varkappa\Delta$, $\mathcal{L}_\varkappa : \operatorname{dom}(\mathcal{L}_\varkappa) \subset L^2(\Omega) \to L^2(\Omega)$ with $\operatorname{dom}(\mathcal{L}_\varkappa) = \{u \in \mathcal{D}^1(\Omega) : -\varkappa\gamma_{_N} u = \gamma_{_D} u\}$. Then by Trotter–Kato Approximation Theorem [58, Theorem III.4.8], the family of semigroups $\{e^{-\mathtt{t}\rho\mathcal{L}_\varkappa}\}_{\mathtt{t}\geqslant 0}$ is strongly continuous in $\varkappa$ uniformly for $\mathtt{t}$ from compact subsets whenever $\varkappa \mapsto (\rho\mathcal{L}_\varkappa - \zeta)^{-1}$ is continuous as a mapping from $(0, +\infty)$ to $\mathcal{B}(L^2(\Omega))$ for some $\zeta \notin \operatorname{Spec}(\mathcal{L}_\varkappa)$ (we note that $\rho\mathcal{L}_\varkappa$ is not necessarily self-adjoint). The next theorem gives a rigorous argument for the required continuity of the resolvent in a slightly more general form. (In the next theorem, to keep up with notation used in the rest of the paper, we denote the parameter with respect to which the continuity is established by t, not by $\varkappa$; this is not to be confused with notation $\mathtt{t}$ for time used in (5.20)).

Theorem 5.7. *Let $\Omega \subset \mathbb{R}^d$ be a bounded open set with C^∞-smooth boundary $\partial\Omega$. We assume that $t \mapsto \alpha_t$, $t \mapsto \beta_t$ are mappings in $C([0,1], L^\infty(\partial\Omega;\mathbb{R}))$ such that $\alpha_t^2(x) + \beta_t^2(x) \neq 0$ for $x \in \partial\Omega$, $t \in [0,1]$, and $t \mapsto \rho_t$ is a mapping in $C([0,1], C(\overline{\Omega};\mathbb{R}))$ such that $\inf\{\rho_t(x) : t \in [0,1], x \in \overline{\Omega}\} > 0$. Recall the differential expression $\mathcal{L}$ from (5.1) and define the following operator acting in $L^2(\Omega)$:*

$$\mathcal{L}_{t,\rho} u := \rho_t \mathcal{L} u, u \in \operatorname{dom}(\mathcal{L}_{t,\rho}),$$
$$\operatorname{dom}(\mathcal{L}_{t,\rho}) := \{u \in \mathcal{D}^1(\Omega) : \alpha_t \gamma_{_D} u + \beta_t \gamma_{_{N,\mathcal{L}}} u = 0\}.$$

Then, the operator $\mathcal{L}_{t,\rho}$ is sectorial and the mapping $t \mapsto (\mathcal{L}_{t,\rho} - \zeta)^{-1}$ lies in $C([0,1], \mathcal{B}(L^2(\Omega)))$ for all $\zeta \in \mathbb{C} \setminus \operatorname{Spec}(\mathcal{L}_{t,\rho})$.

Proof. To prove that $\mathcal{L}_{t,\rho}$ is sectorial, we have to show the existence of such $\theta \in (0, \frac{\pi}{2})$ and $M = M(\theta) > 0$ that

$$\zeta \in \mathbb{C} \setminus \operatorname{Spec}(\mathcal{L}_{t,\rho}) \text{ and } \|(\mathcal{L}_{t,\rho} - \zeta)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant M|\zeta|^{-1},$$

provided $\zeta \neq 0$ and $|\arg\zeta| \in (\theta, \pi]$. First, we introduce a self-adjoint operator $\mathcal{L}_t$ acting in $L^2(\Omega)$ and defined by $\mathcal{L}_t u := \mathcal{L} u$ for $u \in \operatorname{dom}(\mathcal{L}_t) := \operatorname{dom}(\mathcal{L}_{t,\rho})$ so that $\mathcal{L}_{t,\rho} = \rho_t \mathcal{L}_t$. Since $\mathcal{L}_t$ is bounded from below, we may assume without loss of generality that $\mathcal{L}_t \geqslant 0$ and, given a $\theta \in (0, \frac{\pi}{2})$, use the estimate

$$\|(\mathcal{L}_t - \xi)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant (|\xi| \sin\theta)^{-1} \text{ for all } \xi \in \mathbb{C} \setminus \{0\} \text{ such that } |\arg\xi| \in (\theta, \pi]. \tag{5.21}$$

Indeed, (5.21) follows from the estimate

$$\|(\mathcal{L}_t - \xi)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant |\operatorname{Im}\xi|^{-1} \leqslant (|\xi| \sin\theta)^{-1}$$

provided $|\arg\xi| \in (\theta, \frac{\pi}{2}]$ and

$$\|(\mathcal{L}_t - \xi)^{-1}\|_{\mathcal{B}(L^2(\Omega))} = (\operatorname{dist}(\xi, \operatorname{Spec}(\mathcal{L}_t)))^{-1} \leqslant |\xi|^{-1} \leqslant (|\xi| \sin\theta)^{-1}$$

provided $|\arg\xi| \in (\frac{\pi}{2}, \pi]$.

Throughout the rest of this proof, we take all inf's and sup's over $(t, x) \in [0,1] \times \overline{\Omega}$. We pick $\theta \in (0, \frac{\pi}{2})$ such that

$$(1 - \sin^2\theta) \sup \rho_t(x) < \inf \rho_t(x) \tag{5.22}$$

and fix any $\zeta \in \mathbb{C} \setminus \{0\}$ such that $|\arg \zeta| \in (\theta, \pi]$. Using (5.22), we can choose $\xi \in \mathbb{C}$ such that $\arg \xi = \arg \zeta$ with $|\xi|$ that satisfies the inequality

$$(1 - \sin^2\theta) \sup \rho_t(x) < |\zeta||\xi|^{-1} < \inf \rho_t(x). \tag{5.23}$$

Dividing this by $\rho_t(x)$, we infer

$$\sup \big|(|\zeta|(|\xi|\rho_t(x))^{-1} - 1)\big| \leqslant \sin^2\theta. \tag{5.24}$$

Since $\xi \in \mathbb{C} \setminus \operatorname{Spec}(\mathcal{L}_t)$, we have

$$\rho_t \mathcal{L}_t - \zeta = \rho_t(\mathcal{L}_t - \xi)\big(I - (\mathcal{L}_t - \xi)^{-1}(\zeta\rho_t^{-1} - \xi)\big). \tag{5.25}$$

Combining (5.21) and (5.24), we infer

$$\begin{aligned}\|(\mathcal{L}_t - \xi)^{-1}(\zeta\rho_t^{-1} - \xi)\|_{\mathcal{B}(L^2(\Omega))} &\leqslant (|\xi|\sin\theta)^{-1} \sup \big|e^{\mathbf{i}\arg\zeta}(|\zeta|\rho_t(x)^{-1} - |\xi|)\big| \\ &\leqslant \sin\theta < 1,\end{aligned}$$

which by (5.25) gives $\lambda \in \mathbb{C} \setminus \operatorname{Spec}(\rho_t\mathcal{L}_t)$ and, using the second inequality in (5.23), the required resolvent estimate $\|(\mathcal{L}_{t,\rho} - \zeta)^{-1}\|_{\mathcal{B}(L^2(\Omega))} \leqslant M|\zeta|^{-1}$. Thus, $\mathcal{L}_{t,\rho}$ is sectorial.

It is enough to prove continuity of the resolvent mapping at any $\zeta \in \mathbb{R}$ in the resolvent set of $\mathcal{L}_{t,\rho}$. We note that if $\zeta \in \mathbb{R} \setminus \operatorname{Spec}(\mathcal{L}_{t,\rho})$, then $0 \in \mathbb{C} \setminus \operatorname{Spec}(\mathcal{L}_t - \rho_t^{-1}\zeta)$ and the identity $(\rho_t\mathcal{L}_t - \zeta)^{-1} = (\mathcal{L}_t - \rho_t^{-1}\zeta)^{-1}\rho_t^{-1}$ holds. Since the map $t \mapsto \rho_t^{-1}$ is continuous, it remains to prove continuity of the map $t \mapsto (\mathcal{L}_t - \rho_t^{-1}\zeta)^{-1}$, that is, of the resolvent of the operator $H_t = \mathcal{L}_t - \rho_t^{-1}\zeta$ at zero. This follows from Theorem 3.26 with $\mathcal{A}_t = \mathcal{L}_t$, $V_t = -\rho_t^{-1}\zeta$, $\mathrm{T} := (\gamma_{{}_D}, \gamma_{{}_{N,\mathcal{L}}}) \in \mathcal{B}(\mathcal{D}^1(\Omega), H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega))$ and

$$Z_{t,s} := [W(\alpha_t, \beta_t)]^*(\alpha_t\beta_s - \beta_t\alpha_s)[W(\alpha_s, \beta_s)] \to 0, s \to t.$$

To justify the use of Theorem 3.26, we note that Hypothesis 3.13 in the theorem is satisfied, that is, $(\mathcal{L}_t - \mathbf{i})^{-1} = \mathcal{O}(1)$ as $t \to s$ in $\mathcal{B}(L^2(\Omega), \mathcal{D}^1(\Omega))$. The proof of this assertion is similar to that of (5.10) (one imposes Robin boundary condition with $\Theta_t(x) := -\alpha_t(x)\beta_t^{-1}(x)$ on the portion of the boundary where $\beta_t^{-1}(x) \neq 0$ and the Dirichlet condition elsewhere). $\square$

5.4 | The Hadamard formula for star-shaped domains

In this section, we show how to use Theorem 3.26 to derive the classical Hadamard formula for the Schrödinger operators subject to the Dirichlet boundary condition on variable star-shaped domains.

Let $\Omega \subset \mathbb{R}^n$ be a smooth star-shaped domain centered at zero and $\Omega_t = \{tx : x \in \Omega\}$ be its variation for $t \in (0,1]$. We consider a smooth $(N \times N)$-matrix potential $V = V(x)$ for $x \in \overline{\Omega}$ taking symmetric values. Suppose that $\mu \in \mathbb{R}$ is such that $\dim\ker(-\Delta_{D,\Omega} + V - \mu) = m \geqslant 1$, where $-\Delta_{D,\Omega}$ denotes the Dirichlet Laplacian acting in $L^2(\Omega)$. We claim that there exists a choice of orthonormal eigenfunctions $\{u_j\}_{j=1}^m \subset (-\Delta_{D,\Omega} + V - \mu)$ and a labeling of the eigenvalues $\{\mu_j(t)\}_{j=1}^m$ of $-\Delta_{D,\Omega_t} + V \restriction_{\Omega_t}$, for t near 1, such that $\mu_j(1) = \mu$ for each j, and that the following classical Rayleigh–Hadamard–Rellich formula holds, cf. [80, Chapter 5],

$$\dot{\mu}_j(1) = -\int_{\partial\Omega} (\nu \cdot x)(\nu \cdot \nabla u_j)^2 \mathrm{d}x, 1 \leqslant j \leqslant m. \tag{5.26}$$

Rescaling $\Omega \ni t \mapsto tx \in \Omega_t$ of the operator $\big(-\Delta_{D,\Omega_t} + V\big)\big|_{\Omega_t}$ back to Ω yields a one-parameter family of self-adjoint operators $H_t = -\Delta_{D,\Omega} + t^2 V(tx)$, $t \in (0,1]$ acting in the fixed space $L^2(\Omega)$. This family of operators fits the framework of Theorem 3.26 with $\mathcal{A}_t \equiv -\Delta_\Omega$, $V_t(x) = t^2 V(tx)$, $\mathrm{T}_t = [\gamma_{_D}, -t^{-1}\Phi\gamma_{_N}]^\top$, cf. (5.4), $t_0 = 1$, $\lambda(t_0) = \mu$ and Q_t given by the t-independent projection onto the Dirichlet subspace $\{(0,g) : g \in H^{1/2}(\partial\Omega)\}$ for all t. All assumptions of Theorem 3.26 are clearly satisfied in the present setting. By the theorem, there exists a choice of orthonormal eigenfunctions $\{u_j\}_{j=1}^m \subset \ker(-\Delta_{D,\Omega} + V - \mu)$ and a labeling of the eigenvalues $\{\lambda_j(t)\}_{j=1}^m$ of H_t, for t near 1, such that

$$\begin{aligned}\dot{\lambda}_j(1) &= \left\langle \frac{\mathrm{d}(t^2V(tx))}{\mathrm{d}t}\Big|_{t=1} u_j, u_j \right\rangle_{L^2(\Omega)} \\ &= 2\langle V u_j, u_j\rangle_{L^2(\Omega)} + \langle (\nabla V \cdot x) u_j, u_j\rangle_{L^2(\Omega)}, 1 \leqslant j \leqslant m.\end{aligned} \tag{5.27}$$

By the same rescaling as above, the eigenvalues $\lambda_j(t)$ uniquely determine the eigenvalues $\mu_j(t)$ for t near 1, and one has $\lambda_j(t) = t^2\mu_j(t)$. Our next objective is to use this identity together with (5.27) to derive (5.26).

We pause to consider the case of the Laplace operator with no potential. If $V \equiv 0$, then the proof is essentially completed as H_t does not depend on t and $0 = \dot{\lambda}_j(1) = 2\mu_j(1) + \dot{\mu}_j(1)$. This yields (5.26) by the celebrated Rellich formula [112] expressing the eigenvalues $\lambda_j(1) = \mu_j(1)$ of the Dirichlet Laplacian via the Neumann boundary values of the respective eigenfunctions (this formula, in turn, easily follows from the Pokhozaev–Rellich identity, see, for example, [12, p. 201], [85, p. 237], and formula (5.30) below).

Returning to the general case of nonzero potential, to derive (5.26) from (5.27), we will follow the strategy of [44, Lemma 5.5]. Let us fix j and denote, for brevity, $u := u_j$ and $\lambda(t) := \lambda_j(t)$, $\mu(t) = \mu_j(t)$. First, integration by parts for $\Omega \subseteq \mathbb{R}^n$ yields

$$\langle (\nabla V \cdot x)u, u\rangle_{L^2(\Omega)} = -\langle Vu, 2(\nabla u \cdot x) + nu\rangle_{L^2(\Omega)} \text{ and } \langle u, \nabla u \cdot x\rangle_{L^2(\Omega)} = -n/2. \tag{5.28}$$

Using $-\Delta u + Vu = \lambda(1)u$ and replacing Vu by $\Delta u + \lambda(1)u$ in (5.27) and (5.28), a short calculation gives

$$\dot{\mu}(1) = \dot{\lambda}(1) - 2\lambda(1) = (2-n)\langle \Delta u, u\rangle_{L^2(\Omega)} - 2\langle \Delta u, \nabla u \cdot x\rangle_{L^2(\Omega)}. \tag{5.29}$$

The standard Rellich's identity, see, for example, [12, p. 201], yields

$$\begin{aligned}\langle \Delta u, \nabla u \cdot x\rangle_{L^2(\Omega)} = \int_{\partial\Omega} \Big((\nu \cdot \nabla u)(x \cdot \nabla u) - \frac{1}{2}(x \cdot \nu)\|\nabla u\|^2\Big)\mathrm{d}x \\ + \frac{n-2}{2}\int_\Omega \|\nabla u\|^2 \mathrm{d}x.\end{aligned} \tag{5.30}$$

Since u satisfies the Dirichlet condition, $\partial\Omega$ is a level curve, and thus, ∇u and ν are parallel, that is, $\nabla u = (\nu \cdot \nabla u)\nu$. Using all this in (5.29) yields (5.26) because

$$\dot{\mu}(1) = \int_{\partial\Omega} \big(-2(\nu \cdot \nabla u)(x \cdot \nabla u) + (x \cdot \nu)\|\nabla u\|^2\big)\mathrm{d}x = -\int_{\partial\Omega} (\nu \cdot \nabla u)^2(\nu \cdot x)\mathrm{d}x.$$

5.5 | Maslov crossing form for elliptic operators

In this section, we continue the discussion began in Section 4.5 on the relation between the Maslov crossing form and the slopes of the eigenvalue curves bifurcating from a multiple eigenvalue of the unperturbed elliptic operator. Here, we assume the setting of Theorem 5.2 and obtain a version of formula (4.45) for the Robin-type elliptic operators $\mathcal{L}_t$, see Proposition 5.8 below. For $\lambda \in \mathbb{R}$, we let

$$\mathcal{K}_\lambda := \mathrm{T}\Bigg(\Bigg\{u \in H^1(\Omega) : \sum_{j,k=1}^n \langle \mathrm{a}_{jk}\partial_k u, \partial_j \varphi\rangle_{L^2(\Omega)} + \sum_{j=1}^n \langle \mathrm{a}_j \partial_j u, \varphi\rangle_{L^2(\Omega)}$$
$$+ \sum_{j=1}^n \langle u, \mathrm{a}_j \partial_j \varphi\rangle_{L^2(\Omega)} + \langle \mathrm{v}u - \lambda u, \varphi\rangle_{L^2(\Omega)} = 0,\ \varphi \in H_0^1(\Omega)\Bigg\}\Bigg),$$

where the trace operator $\mathrm{T} = [\Gamma_0, \Gamma_1]^\top$ is as in (5.6). This is a “weak” version of the set $\mathbb{K}_{\lambda,t}$ from Section 4.5. The mapping $\lambda \mapsto \mathcal{K}_\lambda$ is in $C^1(\mathbb{R}, \Lambda(H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)))$ by [45, Proposition 3.5].

Let $t \mapsto \mathcal{F}_t := \{(f, -\Theta_t f) : f \in H^{1/2}(\partial\Omega)\}$, then for $t_0 \in [0,1]$, there is an interval $\mathcal{I} \subset [0,1]$ centered at t_0 and a family of operators $t \mapsto \mathcal{M}_t, t \in \mathcal{I}$, which is in $C^1\big(\mathcal{I}, \mathcal{B}(\mathcal{F}_{t_0}, \mathcal{F}_{t_0}^\perp)\big)$ with $\mathcal{M}_{t_0} = 0$ and

$$\mathcal{F}_t = \big\{\mathbf{q} + \mathcal{M}_t\mathbf{q}\,\big|\,\mathbf{q} \in \mathcal{F}_{t_0}\big\}, t \in \mathcal{I},$$

see, for example, [44, Lemma 3.8]. In other words, $\mathcal{F}_t$ can be written locally as the graph of the operator $\mathcal{M}_t$, which is a replacement of $\mathcal{M}_{\lambda,t}$ from Section 4.5. We say that (λ, t_0) is a conjugate point if $\mathcal{K}_\lambda \cap \mathcal{F}_{t_0} \neq \{0\}$ or, equivalently, if $\ker(\mathcal{L}_{t_0} - \lambda) \neq \{0\}$.

We recall $\lambda(t_0) \in \mathrm{Spec}_{\mathrm{disc}}(\mathcal{L}_{t_0})$ from Theorem 5.2 and let $\lambda := \lambda(t_0)$. Then, (λ, t_0) is a conjugate point at which the Maslov crossing form $\mathfrak{m}_{t_0}$ for the path $t \mapsto \mathcal{K}_\lambda \oplus \mathcal{F}_t$ relative to the diagonal subspace $\mathfrak{D} = \{\mathbf{p} = (p,p) : p \in H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega))\}$ is defined by the formula

$$\mathfrak{m}_{t_0}(\mathbf{q}, \mathbf{p}) := \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=t_0} \widehat{\omega}(\mathbf{q}, \mathcal{M}_t\mathbf{p}) = \widehat{\omega}(\mathbf{q}, \dot{\mathcal{M}}_{t_0}\mathbf{p}),\ \mathbf{p}, \mathbf{q} \in (\mathcal{K}_\lambda \oplus \mathcal{F}_{t_0}) \cap \mathfrak{D}, \tag{5.31}$$

where $\widehat{\omega} = \omega \oplus (-\omega)$ and $\dot{\mathcal{M}}_{t_0} = \frac{\mathrm{d}}{\mathrm{d}t}\mathcal{M}_t\big|_{t=t_0}$. We stress that the pair of Lagrangian subspaces $\big(\mathcal{K}_\lambda, \mathcal{F}_{t_0}\big)$ is Fredholm since $\lambda = \lambda(t_0) \notin \mathrm{Spec}_{\mathrm{ess}}(\mathcal{L}_{t_0})$, see [93, Theorem 3.2]. Hence, $\dim\big((\mathcal{K}_\lambda \oplus \mathcal{F}_{t_0}) \cap \mathfrak{D}\big) < \infty$ and $\mathfrak{m}_{t_0}$ is a finite-dimensional bilinear form. In fact, the pair of Lagrangian subspaces $\big(\mathcal{K}_\lambda, \mathcal{F}_t\big)$ is Fredholm for t near t_0 due to continuity of the path of the resolvent operators $t \mapsto (\mathcal{L}_t - \mathbf{i})^{-1}$.

Proposition 5.8. *Let $\lambda(t_0)$, $\{\lambda_j(t)\}_{j=1}^m$ and $\{u_j\}_{j=1}^m$ be as in Theorem 5.2, and denote $\mathbf{q}_j := (\mathrm{T}u_j, \mathrm{T}u_j)$. Then, $\mathbf{q}_j \in (\mathcal{K}_{\lambda(t_0)} \oplus \mathcal{F}_{t_0}) \cap \mathfrak{D}$ and*

$$\dot{\lambda}_j(t_0) = \mathfrak{m}_{t_0}(\mathbf{q}_j, \mathbf{q}_j),\ 1 \leqslant j \leqslant m, \tag{5.32}$$

where $\mathfrak{m}_{t_0}$ is the Maslov crossing form introduced in (5.31).

Proof. The inclusion $\mathbf{q}_j \in (\mathcal{K}_{\lambda(t_0)} \oplus \mathcal{F}_{t_0}) \cap \mathfrak{D}$ holds since u_j is an eigenfunction of $\mathcal{L}_{t_0}$ corresponding to the eigenvalue $\lambda(t_0)$. For a fixed j, we abbreviate $\mathbf{q} := \mathbf{q}_j = \mathrm{T}u_j$ and introduce $g_t \in H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)$ as in (4.44) but with $\mathcal{M}_{\lambda,t}$ replaced by $\mathcal{M}_t$. In particular, $g_{t_0} = \mathrm{T}u_j$ because $\mathcal{M}_{t_0} = 0$. Since $g_t = Q_t g_t$ where Q_t is the orthogonal projection onto $\mathcal{F}_t$, we have

$$\dot{g}_{t_0} = \dot{Q}_{t_0} g_{t_0} + Q_{t_0} \dot{g}_{t_0} = \dot{Q}_{t_0} \mathrm{T}u_j + Q_{t_0} \dot{g}_{t_0}.$$

This and that $\mathrm{ran}(Q_{t_0})$ is Lagrangian yields, as in (4.50),

$$\omega(\mathrm{T}u_j,\, \dot{g}_{t_0}) = \omega(\mathrm{T}u_j, \dot{Q}_{t_0} \mathrm{T}_{t_0} u_j).$$

As in (4.51), by definition of $\mathfrak{m}_{t_0}$, this implies

$$\mathfrak{m}_{t_0}(\mathbf{q}_j, \mathbf{q}_j) = -\omega(\mathrm{T}u_j,\, \dot{g}_{t_0}) = -\omega(\mathrm{T}u_j, \dot{Q}_{t_0} \mathrm{T}u_j) = \omega(\dot{Q}_{t_0} \mathrm{T}u_j, \mathrm{T}u_j).$$

By formula (5.9) in Theorem 5.2, we have $\dot{\lambda}_j(t_0) = -\langle \dot{\Theta}_{t_0} \gamma_{_D} u_j, \gamma_{_D} u_j \rangle_{L^2(\partial\Omega)}$. Thus, it remains to show that

$$\omega(\dot{Q}_{t_0} \mathrm{T}u_j, \mathrm{T}u_j) = -\langle \dot{\Theta}_{t_0} \gamma_{_D} u_j, \gamma_{_D} u_j \rangle_{L^2(\partial\Omega)}.$$

The latter assertion follows from (3.46) with $\phi_j = -\gamma_{_D} u_j$ and $X_t = \Theta_t$, $Y_t = I$ as

$$\mathcal{F}_t = \mathrm{graph}(-\Theta_t) = \ker([X_t, Y_t])$$

with this choice of X_t and Y_t. $\square$

Remark 5.9. As discussed in Remark 4.23, formula (5.32) relating the derivative of the eigenvalues of the elliptic operators $\mathcal{L}_t$ with respect to the parameter t and the value of the (Maslov) crossing form for the flow $t \mapsto \mathcal{K}_{\lambda(t)} \oplus \mathcal{F}_t$ of Lagrangian planes could be viewed as an infinitesimal version of the fundamental relation between the spectral flow and the Maslov index. Indeed, as in Remark 4.23, formula (5.32) implies relation (4.54) with H_t replaced by $\mathcal{L}_t$ and $\Upsilon_{\lambda,t}$ replaced by $\mathcal{K}_{\lambda(t)} \oplus \mathcal{F}_t$.

Example 5.10. We will now briefly return to the Robin eigenvalue problem (5.16) related to the Friedlander inequalities but at once for the general elliptic operator $\mathcal{L}$ described in Subsection 5.1. We recall that for $\lambda \notin \mathrm{Spec}(\mathcal{L}_D)$, the Dirichlet-to-Neumann operator $M_{D,N}(\lambda)$ is defined by $f \mapsto -\gamma_{_N} u$ (in the relevant papers [46, 62], $M_{D,N}$ is defined by $f \mapsto \gamma_{_N} u$) where u is the solution to $\mathcal{L}u = \lambda u, \gamma_{_D} u = f$. It is easy to see that (5.16) has a nontrivial solution if and only if $\mu = \cot(\frac{\pi}{2} t)$ is an eigenvalue of $M_{DN}(\lambda)$. Combining Remarks 4.23 and 5.9 and Example 5.5 with Proposition 5.8 can be used to show the following formula relating the spectral counting functions of the Dirichlet and Neumann realizations $\mathcal{L}_D$ and $\mathcal{L}_N$ and the Dirichlet-to-Neuman map $M_{D,N}(0)$,

$$\begin{aligned} \#\{\lambda \in \mathrm{Spec}(\mathcal{L}_N) : \lambda < 0\} - \#\{\lambda \in \mathrm{Spec}(\mathcal{L}_D) : \lambda < 0\} \\ = \#\{\mu \in \mathrm{Spec}(M_{D,N}(0)) : \mu \geqslant 0\}, \end{aligned} \tag{5.33}$$

see [62] and, specifically, [46, Theorem 3] and the literature therein (in [46, 62] the RHS of (5.33) is given by the number of *negative* eigenvalues of $M_{D,N}(\lambda)$, this is due to sign discrepancy in the definition of $M_{D,N}(\lambda)$). We omit details and just mention that the monotonicity of the eigenvalue curves $\lambda_k(t)$, $k = 1, 2, \dots$, established in Example 5.5 and formula (5.32) show that the Maslov crossing form is sign definite at each conjugate point on the vertical line through λ when t changes from 0 to 1 (Figure 1 serves as a schematic illustration of this assertion). By a standard calculation, see, for example, Step 1 in the proof of [93, Theorem 3.3], the Maslov crossing form is also sign definite at each conjugate point on the horizontal lines through $t = 0$ and $t = 1$ when λ is changing. These two properties are sometimes referred to as the monotonicity of the Maslov index. Thus, cf. Remark 4.23, the spectral flow through zero given by the LHS of (5.33) is equal to the Maslov index along the vertical line through λ that, in turn, is equal to the RHS.

6 | SYMPLECTIC RESOLVENT DIFFERENCE FORMULAS FOR DUAL PAIRS

In this section, we give a generalization of the resolvent difference formula (2.12) to the case of boundary triplets for an adjoint pair $A, \widetilde{A}$, see, for example, [1, 30, 32] and the literature cited therein. The theory of adjoint pairs goes back to [99, 124], see also [7, 16, 31, 102]. It allows one to describe nonself-adjoint extensions for an adjoint pair of densely defined closed (but not necessarily symmetric) operators. A typical example of the adjoint pair, see, for example, [30, 32], is furnished by a nonsymmetric elliptic second-order partial differential operator and its formal adjoint; this example is discussed in detail in the end of this section.

We follow [32] to recall the definition of the adjoint pair and its boundary triplet. Let $A, \widetilde{A}$ be closed densely defined operators on a Hilbert space $\mathcal{H}$ forming an adjoint pair, that is, we assume that $\widetilde{A} \subseteq A^*$ and $A \subseteq (\widetilde{A})^*$. We denote by $\mathcal{H}_+$, respectively, $\widetilde{\mathcal{H}}_+$ the domain $\mathrm{dom}(A^*)$, respectively, $\mathrm{dom}((\widetilde{A})^*)$ equipped with the graph-scalar product and graph norm for A^*, respectively, $(\widetilde{A})^*$, cf. Section 2. Let $\mathfrak{H}$ and $\mathfrak{K}$ be some "boundary" Hilbert spaces and

$$\Gamma_0 : \widetilde{\mathcal{H}}_+ \to \mathfrak{H}, \quad \Gamma_1 : \widetilde{\mathcal{H}}_+ \to \mathfrak{K}, \quad \widetilde{\Gamma}_0 : \mathcal{H}_+ \to \mathfrak{K}, \quad \widetilde{\Gamma}_1 : \mathcal{H}_+ \to \mathfrak{H}$$

be some "boundary trace operators." The collection $\{\mathfrak{H}, \mathfrak{K}, \Gamma_0, \Gamma_1, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is called a *boundary triplet for the adjoint pair* $A, \widetilde{A}$ when the following hypothesis is satisfied.

Hypothesis 6.1. Suppose that $A, \widetilde{A}$ is an adjoint pair of densely defined closed operators such that $\widetilde{A} \subseteq A^*$ and $A \subseteq (\widetilde{A})^*$. Consider linear operators, called the *trace operators*,

$$\mathrm{T} := [\Gamma_0, \Gamma_1]^\top : \widetilde{\mathcal{H}}_+ \to \mathfrak{H} \times \mathfrak{K}, \ \widetilde{\mathrm{T}} := [\widetilde{\Gamma}_0, \widetilde{\Gamma}_1]^\top : \mathcal{H}_+ \to \mathfrak{K} \times \mathfrak{H}.$$

Assume that the operators T and $\widetilde{\mathrm{T}}$ are surjective and satisfy

$$\langle (\widetilde{A})^* u, v\rangle_{\mathcal{H}} - \langle u, A^* v\rangle_{\mathcal{H}} = \langle \Gamma_1 u, \widetilde{\Gamma}_0 v\rangle_{\mathfrak{K}} - \langle \Gamma_0 u, \widetilde{\Gamma}_1 v\rangle_{\mathfrak{H}}, \tag{6.1}$$

for all $u \in \widetilde{\mathcal{H}}_+$ and $v \in \mathcal{H}_+$.

The existence of a boundary triplet for every adjoint pair $A, \widetilde{A}$ was proved in [99], where, in addition, it was shown that

$$\mathrm{dom}(A) = \mathrm{dom}((\widetilde{A})^*) \cap \ker \Gamma_0 \cap \ker \Gamma_1, \ \mathrm{dom}(\widetilde{A}) = \mathrm{dom}(A^*) \cap \ker \widetilde{\Gamma}_0 \cap \ker \widetilde{\Gamma}_1.$$

It is well known that the operators $T, \widetilde{T}$ are bounded, cf. [102, 120, Lemma 14.13].

The following resolvent difference formula is a direct generalization of Theorem 2.6. It gives the difference of the resolvent operators of any two (not necessarily sel-adjoint) extensions of the operator A that are parts of $(\widetilde{A})^*$.

Theorem 6.2. *Let $\{\mathfrak{H}, \mathfrak{K}, \Gamma_0, \Gamma_1, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ be a boundary triplet for an adjoint pair $A, \widetilde{A}$, and let $\mathcal{A}_j$ for $j = 1, 2$ be any two closed extensions of A acting in $\mathcal{H}$ and satisfying $A \subseteq \mathcal{A}_j \subseteq (\widetilde{A})^*$. Suppose that $\zeta \in \mathbb{C} \setminus (\mathrm{Spec}(\mathcal{A}_1) \cup \mathrm{Spec}(\mathcal{A}_2))$ and denote $R_j(\zeta) := (\mathcal{A}_j - \zeta)^{-1}$ for $j = 1, 2$. Then one has*

$$R_2(\zeta) - R_1(\zeta) = \big(\widetilde{\Gamma}_0 R_2^*(\zeta)\big)^* \Gamma_1 R_1(\zeta) - \big(\widetilde{\Gamma}_1 R_2^*(\zeta)\big)^* \Gamma_0 R_1(\zeta), \tag{6.2}$$

$$R_2(\zeta) - R_1(\zeta) = \big(\widetilde{\mathrm{T}} R_2^*(\zeta)\big)^* Q_2 J Q_1 (\mathrm{T} R_1(\zeta)), \tag{6.3}$$

where $R_2^*(\zeta) = ((\mathcal{A}_2)^* - \overline{\zeta})^{-1}$, the operator $\widetilde{\mathrm{T}} R_2^*(\zeta) = \big(\widetilde{\Gamma}_0 R_2^*(\zeta), \widetilde{\Gamma}_1 R_2^*(\zeta)\big)$ is considered as an operator in $\mathcal{B}(\mathcal{H}, \mathfrak{K} \times \mathfrak{H})$ and the adjoint operators in (6.2), (6.3) are defined correspondingly, Q_1, respectively, Q_2 denotes the orthogonal projection onto $\overline{\mathrm{T}(\mathrm{dom}(\mathcal{A}_1))}$ in the space $\mathfrak{H} \times \mathfrak{K}$, respectively, onto $\overline{\widetilde{\mathrm{T}}(\mathrm{dom}((\mathcal{A}_2)^*))}$ in the space $\mathfrak{K} \times \mathfrak{H}$, and the operator J maps a pair (f, g) from $\mathfrak{H} \times \mathfrak{K}$ into the pair $(g, -f)$ from $\mathfrak{K} \times \mathfrak{H}$.

Proof. The inclusion $A \subseteq \mathcal{A}_j \subseteq (\widetilde{A})^*$ yields $\widetilde{A} \subseteq (\mathcal{A}_j)^* \subseteq A^*$ for $j = 1, 2$ [83, Section III.5.5]. The operator $R_2^*(\zeta) \in \mathcal{B}(\mathcal{H})$ is also bounded from $\mathcal{H}$ onto $\mathrm{dom}((\mathcal{A}_2)^*) \subseteq \mathcal{H}_+ = \mathrm{dom}(A^*)$. Thus, the operator $\widetilde{\mathrm{T}} R_2^*(\zeta)$ is well defined, and, analogously, the operator $\mathrm{T} R_1(\zeta)$ is well defined. Moreover, for all $u, v \in \mathcal{H}$, one has

$$(A^* - \overline{\zeta}) R_2^*(\zeta) v = (\mathcal{A}_2 - \zeta)^* R_2^*(\zeta) v = v, \ \big((\widetilde{A})^* - \zeta\big) R_1(\zeta) u = (\mathcal{A}_1 - \zeta) R_1(\zeta) u = u. \tag{6.4}$$

We also have $Q_2 \widetilde{\mathrm{T}} R_2^*(\zeta) = \widetilde{\mathrm{T}} R_2^*(\zeta)$ and $Q_1 \mathrm{T} R_1(\zeta) = \mathrm{T} R_1(\zeta)$ by the definition of the orthogonal projections Q_2 and Q_1. Thus, (6.3) is just a reformulation of (6.2). For the proof of (6.2), we use (6.1) and (6.4) to write

$$\begin{aligned}
\langle (R_2(\zeta) - R_1(\zeta)) u, v \rangle_{\mathcal{H}} &= \langle R_2(\zeta) u - R_1(\zeta) u, (\mathcal{A}_2 - \overline{\zeta})^* R_2^*(\zeta) v \rangle_{\mathcal{H}} \\
&= \langle (\mathcal{A}_2 - \zeta) R_2(\zeta) u, R_2^*(\zeta) v \rangle_{\mathcal{H}} - \langle R_1(\zeta) u, (A^* - \overline{\zeta}) R_2^*(\zeta) v \rangle_{\mathcal{H}} \\
&= \langle u, R_2^*(\zeta) v \rangle_{\mathcal{H}} - \langle \big((\widetilde{A})^* - \zeta\big) R_1(\zeta) u, R_2^*(\zeta) v \rangle_{\mathcal{H}} \\
&\quad + \langle \Gamma_1 R_1(\zeta) u, \widetilde{\Gamma}_0 R_2^*(\zeta) v \rangle_{\mathfrak{K}} - \langle \Gamma_0 R_1(\zeta) u, \widetilde{\Gamma}_1 R_2^*(\zeta) v \rangle_{\mathfrak{H}} \\
&= \langle \big(\widetilde{\Gamma}_0 R_2^*(\zeta)\big)^* \Gamma_1 R_1(\zeta) u, v \rangle_{\mathcal{H}} - \langle \big(\widetilde{\Gamma}_1 R_2^*(\zeta)\big)^* \Gamma_0 R_1(\zeta) u, v \rangle_{\mathcal{H}},
\end{aligned}$$

for all $u, v \in \mathcal{H}$, yielding (6.2). □

In particular, for $j = 1, 2$, given an operator $\Psi_j \in \mathcal{B}(\mathfrak{H}, \mathfrak{K})$ (not necessarily self-adjoint), we consider in $\mathcal{H}$ the extension $\mathcal{A}_j$ of A satisfying $A \subseteq \mathcal{A}_j \subseteq (\widetilde{A})^*$ and defined by the formulas

$$\mathcal{A}_j u = (\widetilde{A})^* u \ \text{ for } \ u \in \mathrm{dom}(\mathcal{A}_j) := \{u \in \widetilde{\mathcal{H}}_+ : \Gamma_1 u = \Psi_j \Gamma_0 u\}, \quad j = 1, 2.$$

Corollary 6.3. *Under assumptions in Theorem 6.2, one has*

$$R_2(\zeta) - R_1(\zeta) = \big(\widetilde{\Gamma}_0 R_2^*(\zeta)\big)^* (\Psi_1 - \Psi_2) \Gamma_0 R_1(\zeta).$$

The proof of this corollary is similar to the poof of Theorem 6.2 and is omitted here, but it is presented in the electronic version of this manuscript [92].

Remark 6.4. We note that both the Weyl function and the γ-field for an adjoint pair were originally introduced and studied in [101, 102], where the Krein-type formula written in terms of these objects was derived for the first time.

Remark 6.5. The formulas for resolvent difference presented in Theorem 6.2 are applicable to a pair of formally adjoint uniformly elliptic operators on domains with C^∞ boundaries. The celebrated work of M.I. Višik [124, 125] and G. Grubb [73] provides boundary triplets for dual pairs in this setting. We elaborate on this point in the electronic version of this paper available on ArXiv [92].

APPENDIX A: LAGRANGIAN PLANES AND SELF-ADJOINT EXTENSIONS

In this appendix, we elaborate on the assumption of the second part of Theorem 2.6—that the image of the domain of a self-adjoint extension is a Lagrangian plane. It is well known that self-adjoint extensions of A can be parameterized by Lagrangian planes, see, for example, [71, Theorem 3.1.6], [77, 106], and [120, Proposition 14.7]. Such parameterization depends on the choice of the trace operator T and the "boundary" space $\mathfrak{H}$, see, for example, [14, Proposition 2.4] and [71, Chapter 3]. Theorems A.1 and A.2 and Corollary A.5 below give yet another variant of the parameterization. The proofs amount to checking basic definitions and therefore omitted for the sake of brevity. They are, however, presented in the electronic version of this paper available on ArXiv [92].

Theorem A.1. *Assume Hypothesis 2.1 and that $\mathcal{F} \in \Lambda(\mathfrak{H} \times \mathfrak{H})$ is a Lagrangian subspace in $\mathfrak{H} \times \mathfrak{H}$ such that*

$$\mathcal{F} \cap \mathrm{T}(\mathcal{D}) = \mathrm{T}\big(\mathrm{T}^{-1}(\mathcal{F})\big) \textit{ is } (\mathfrak{H} \times \mathfrak{H})\textit{-dense in } \mathcal{F}. \tag{A.1}$$

Then, the operator $\mathcal{A} = A^*|_{\mathrm{T}^{-1}(\mathcal{F})}$ is essentially self-adjoint, that is, $\overline{\mathcal{A}} = \mathcal{A}^*$, if and only if

$$\mathrm{dom}(\mathcal{A}^*) \cap \mathcal{D} \textit{ is } (\mathcal{H}_+)\textit{-dense in } \mathrm{dom}(\mathcal{A}^*). \tag{A.2}$$

Next, we present a result saying that the traces of the domains of self-adjoint extensions of A form Lagrangian planes in $\mathfrak{H} \times \mathfrak{H}$.

Theorem A.2. *Assume Hypothesis 2.1 and that there exists a self-adjoint restriction $\mathcal{A}$ of A^* on a subspace* $\mathrm{dom}(\mathcal{A}) \subset \mathcal{H}_+$ *such that*

$$\mathrm{dom}(\mathcal{A}) \cap \mathcal{D} \textit{ is } (\mathcal{H}_+)\textit{-dense in } \mathrm{dom}(\mathcal{A}). \tag{A.3}$$

Then the $(\mathfrak{H} \times \mathfrak{H})$-closure of the subspace $\mathcal{F}$ defined by $\mathcal{F} := \mathrm{T}(\mathrm{dom}(\mathcal{A}) \cap \mathcal{D})$ is Lagrangian, that is, $\overline{\mathcal{F}} = \mathcal{F}^\circ$, if and only if

$$\mathcal{F}^\circ \cap \mathrm{T}(\mathcal{D}) \textit{ is } (\mathfrak{H} \times \mathfrak{H})\textit{-dense in } \mathcal{F}^\circ. \tag{A.4}$$

We note that conditions (A.1)–(A.4) automatically hold for all classes of PDE, ODE, and quantum graphs operators and all examples that we know; these conditions trivially hold provided

$\mathcal{D} = \mathcal{H}_+$ and $\mathrm{T}(\mathcal{D}) = \mathfrak{H} \times \mathfrak{H}$, that is, when $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ is an abstract boundary triplet, see Section 4. We recall Remark 2.5 regarding the existence of self-adjoint extensions of A under Hypothesis 2.1.

Remark A.3. The density assumptions $\overline{\mathrm{dom}(A)} = \mathcal{H}, \overline{\mathrm{ran}(\mathrm{T})} = \mathfrak{H} \times \mathfrak{H}$ introduced in Hypothesis 2.1 are absolutely critical for Theorems A.1 and A.2 to hold. Indeed, [53, Example 6.6] gives a scenario in which dropping the above-mentioned density assumptions facilitates a Lagrangian plane in $\mathfrak{H} \times \mathfrak{H}$ whose preimage is equal to $\mathrm{dom}(A)$, which is evidently not a domain of self-adjoint extension of A.

Assuming Hypothesis 2.1, for the sake of brevity, in the sequel, we will use the following terminology.

Definition A.4.

(i) Given a subspace $\mathcal{F}$ in $\mathfrak{H} \times \mathfrak{H}$, we call $\mathcal{A} = A^*|_{\mathrm{T}^{-1}(\mathcal{F})}$ the *operator associated with* $\mathcal{F}$.
(ii) Given an operator $\mathcal{A}$, we call $\mathcal{F} = \mathrm{T}\big(\mathrm{dom}(\mathcal{A}) \cap \mathcal{D}\big)$ the *subspace associated with* $\mathcal{A}$.
(iii) We say that a Lagrangian subspace $\mathcal{F} \in \Lambda(\mathfrak{H} \times \mathfrak{H})$ is $(\mathrm{T}, \mathcal{D})$-*aligned* or, when there is no confusion, simply *aligned* if (A.1) holds and the adjoint to the associated with $\mathcal{F}$ operator $\mathcal{A}$ satisfies (A.2).
(iv) We say that a self-adjoint restriction $\mathcal{A}$ of A^* is $(\mathrm{T}, \mathcal{D})$-*aligned* or, when there is no confusion, simply *aligned* if (A.3) holds and the annihilator of the associated with $\mathcal{A}$ subspace $\mathcal{F}$ satisfies (A.4).

Employing Definition A.4, let us state a result overarching Theorems A.1 and A.2.

Corollary A.5. *If $\mathcal{F}$ is an aligned Lagrangian subspace, then the operator $\mathcal{A}$ associated with $\mathcal{F}$ is essentially self-adjoint and its closure $\overline{\mathcal{A}}$ is aligned; in particular, the closure of the subspace associated with $\overline{\mathcal{A}}$ is equal to $\mathcal{F}$.*

Conversely, if $\mathcal{A}$ is an aligned self-adjoint restriction of A^*, then the closure $\overline{\mathcal{F}}$ of the subspace $\mathcal{F}$ associated with $\mathcal{A}$ is an aligned Lagrangian subspace; in particular, the closure of the operator associated with $\overline{\mathcal{F}}$ is equal to $\mathcal{A}$.

A particularly transparent and widely studied scenario of aligned Lagrangian subspaces and self-adjoint operators is discussed in Section 4, see, in particular, Remark 4.2.

APPENDIX B: THE KREIN–NAIMARK RESOLVENT FORMULA REVISITED

In this appendix, we revisit the classical Krein–Naimark (B.4) formula for the difference of resolvents of two self-adjoint extensions of an abstract symmetric operator, see, for example, [120, Section 14.6]. As we demonstrate in the proof of Proposition B.1, the Krein–Naimark formula (B.4) can be naturally derived from formula (2.12) in Theorem 2.6 by specializing it to the case of ordinary boundary triplets. Conversely, in Remark B.2, we show how to derive (2.12) from (B.4).

Let $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ be an ordinary boundary triplet as described in Definition 4.1. Following common convention, we define one of the two self-adjoint extensions of A in the Krein–Naimark formula by

$$\mathcal{A}_0 := A^* \upharpoonright_{\ker(\Gamma_0)}, \tag{B.1}$$

and subtract from its resolvent the resolvent of yet another, arbitrary, self-adjoint extension.

First, we recall some known facts, see, for example, [120, Section 14]. Since

$$\mathrm{dom}(A^*) = \mathrm{dom}(A_0) \dot{+} \ker(A^* - \zeta) \text{ for } \zeta \in \mathbb{C} \setminus \mathbb{R},$$

the map $\Gamma_0 \restriction_{\ker(A^*-\zeta)} : \ker(A^* - \zeta) \to \mathfrak{H}$ is bijective, and thus, we define $\gamma(\zeta) := (\Gamma_0 \restriction_{\ker(A^*-\zeta)})^{-1}$ and notice that $\gamma(\zeta) \in \mathcal{B}(\mathfrak{H}, \mathcal{H})$ and $\Gamma_0\gamma(\zeta)h = h$ for any $h \in \mathfrak{H}$. In particular, $\gamma(\zeta)$ is injective. We will use the well-known Derkach–Malamud lemma saying that $\gamma^*(\overline{\zeta}) = \Gamma_1(\mathcal{A}_0 - \zeta)^{-1}$, see [55, Lemma 1] or [120, Proposition 14.14(i)]. The operator-valued function $\gamma(\cdot)$ can be extended analytically to $\mathbb{C} \setminus \mathrm{Spec}(\mathcal{A}_0)$ giving rise to the abstract Weyl function $M(\zeta) := \Gamma_1\gamma(\zeta)$, $\zeta \in \mathbb{C} \setminus \mathrm{Spec}(\mathcal{A}_0)$.

Next, let $\mathcal{A}$ be an arbitrary self-adjoint extension of A, and let $\mathcal{F} \in \Lambda(\mathfrak{H} \times \mathfrak{H})$ be the Lagrangian subspace such that $\mathcal{F} = \mathrm{T}(\mathrm{dom}(\mathcal{A}))$, cf. Theorems A.1 and A.2 and Remark 4.2. We will treat $\mathcal{F}$ as a linear relation, see, for example, [120, Section 14.1]. Slightly abusing notation, we do not distinguish between the operator $M(\zeta)$ and its graph, in particular, we write $\mathcal{F} - M(\zeta) := \mathcal{F} - \mathrm{graph}(M(\zeta))$ and treat both terms in the right-hand side as linear relations. The linear relation $\mathcal{F} - M(\zeta)$ is called *invertible* whenever

$$\ker(\mathcal{F} - M(\zeta)) := \{f \in \mathfrak{H} : (f, 0) \in (\mathcal{F} - M(\zeta))\} = \{0\}, \text{ and} \tag{B.2}$$

$$\mathrm{ran}(\mathcal{F} - M(\zeta)) := \{g \in \mathfrak{H} : \exists f \in \mathfrak{H} \; s.t. \, (f, g) \in (\mathcal{F} - M(\zeta))\} = \mathfrak{H}. \tag{B.3}$$

In this case, there exists an operator in $\mathcal{B}(\mathfrak{H})$ whose graph is given by

$$\{(g, f) \in \mathfrak{H} \times \mathfrak{H} : (f, g) \in (\mathcal{F} - M(\zeta))\};$$

this operator is denoted by $(\mathcal{F} - M(\zeta))^{-1}$.

Proposition B.1. *Let $(\mathfrak{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet for the symmetric operator A, see Definition 4.1, let $\mathcal{A}_0$ be the self-adjoint extension of A from (B.1), let $\mathcal{A}$ be an arbitrary self-adjoint extension of A and $\mathcal{F} = \mathrm{T}(\mathrm{dom}(\mathcal{A}))$. Then $\mathcal{F} - M(\zeta)$ is invertible and*

$$(\mathcal{A} - \zeta)^{-1} = (\mathcal{A}_0 - \zeta)^{-1} + \gamma(\zeta)(\mathcal{F} - M(\zeta))^{-1}\gamma^*(\overline{\zeta}) \text{ for } \zeta \notin \mathrm{Spec}(\mathcal{A}_0) \cup \mathrm{Spec}(\mathcal{A}). \tag{B.4}$$

Proof. We denote $R_0(\zeta) := (\mathcal{A}_0 - \zeta)^{-1}$ and $R(\zeta) = (\mathcal{A} - \zeta)^{-1}$. Since $\Gamma_0 R_0(\overline{\zeta}) = 0$ by (B.1), the resolvent difference formula from Theorem 2.6 and the Derkach–Malamud lemma above yield

$$R_0(\zeta) - R(\zeta) = (\Gamma_0 R_0(\overline{\zeta}))^*\Gamma_1 R(\zeta) - (\Gamma_1 R_0(\overline{\zeta}))^*\Gamma_0 R(\zeta) = -\gamma(\zeta)\Gamma_0 R(\zeta).$$

It remains to prove (B.2) and (B.3), and that

$$\Gamma_0 R(\zeta) = (\mathcal{F} - M(\zeta))^{-1}\gamma^*(\overline{\zeta}). \tag{B.5}$$

The main identity needed for the proofs is that

$$\gamma^*(\overline{\zeta})u = \Gamma_1 R_0(\zeta)u = \Gamma_1 R(\zeta)u - M(\zeta)\Gamma_0 R(\zeta)u \text{ for all } u \in \mathcal{H}. \tag{B.6}$$

To justify the second equality in (B.6), we use $(A^* - \zeta)\gamma(\zeta) = 0$ and $\Gamma_0(I_{\mathcal{H}} - \gamma(\zeta)\Gamma_0) = 0$, yielding $\mathrm{ran}(I_{\mathcal{H}} - \gamma(\zeta)\Gamma_0) \subset \mathrm{dom}(\mathcal{A}_0)$, and write

$$\Gamma_1 R_0(\zeta) = \Gamma_1 R_0(\zeta)(\mathcal{A} - \zeta)R(\zeta) = \Gamma_1 R_0(\zeta)(A^* - \zeta)R(\zeta)$$

$$= \Gamma_1 R_0(\zeta)(A^* - \zeta)(I_{\mathcal{H}} - \gamma(\zeta)\Gamma_0)R(\zeta)$$
$$= \Gamma_1 R_0(\zeta)(\mathcal{A}_0 - \zeta)(I_{\mathcal{H}} - \gamma(\zeta)\Gamma_0)R(\zeta)$$
$$= \Gamma_1(I_{\mathcal{H}} - \gamma(\zeta)\Gamma_0)R(\zeta) = \Gamma_1 R(\zeta) - M(\zeta)\Gamma_0 R(\zeta),$$

thus proving (B.6). Since $R(\zeta)$ is a bijection of $\mathcal{H}$ onto $\mathrm{dom}(\mathcal{A})$, we have $\mathcal{F} = \{(\Gamma_0 R(\zeta)u, \Gamma_1 R(\zeta)u) : u \in \mathcal{H}\}$. This and (B.6) yield

$$\begin{aligned}\mathcal{F} - M(\zeta) &= \{(f, g - M(\zeta)f) : (f,g) \in \mathcal{F}\} \\ &= \left\{(\Gamma_0 R(\zeta)u, \Gamma_1 R(\zeta)u - M(\zeta)\Gamma_0 R(\zeta)u) : u \in \mathcal{H}\right\} \\ &= \left\{\left(\Gamma_0 R(\zeta)u, \gamma^*(\overline{\zeta})u\right) : u \in \mathcal{H}\right\}.\end{aligned} \tag{B.7}$$

Since T is surjective, (B.3) follows from (B.7). Indeed, for any $g \in \mathfrak{H}$, there is some $v \in \mathrm{dom}(A^*)$ such that $\Gamma_0 v = 0$ and $\Gamma_1 v = g$. Since $v \in \mathrm{dom}(\mathcal{A}_0)$, there is some $u \in \mathcal{H}$ such that $v = R_0(\zeta)u$ and so $g = \Gamma_1 R_0(\zeta)u \in \mathrm{ran}(\mathcal{F} - M(\zeta))$ by (B.7) and (B.6). To begin the proof of (B.2), we first notice that $\gamma(\zeta)\ker(\mathcal{F} - M(\zeta)) \subset \mathrm{dom}(\mathcal{A})$. Indeed, by (B.7) and (B.6), we have $\ker(\mathcal{F} - M(\zeta)) = \left\{\Gamma_0 R(\zeta)u : \Gamma_1 R(\zeta)u = M(\zeta)\Gamma_0 R(\zeta)u, u \in \mathcal{H}\right\}$, and thus,

$$\begin{aligned}&\mathrm{T}\gamma(\zeta)\ker(\mathcal{F} - M(\zeta)) \\ &= \{(\Gamma_0\gamma(\zeta)\Gamma_0 R(\zeta)u, \Gamma_1\gamma(\zeta)\Gamma_0 R(\zeta)u) : \Gamma_1 R(\zeta)u = M(\zeta)\Gamma_0 R(\zeta)u, u \in \mathcal{H}\} \\ &= \{(\Gamma_0 R(\zeta)u, M(\zeta)\Gamma_0 R(\zeta)u) : \Gamma_1 R(\zeta)u = M(\zeta)\Gamma_0 R(\zeta)u, u \in \mathcal{H}\} \\ &= \mathcal{F} \cap \mathrm{graph}(M(\zeta)).\end{aligned}$$

Therefore, $(\mathcal{A} - \zeta)\gamma(\zeta)\ker(\mathcal{F} - M(\zeta)) = (A^* - \zeta)\gamma(\zeta)\ker(\mathcal{F} - M(\zeta)) = \{0\}$ yields the inclusion $\gamma(\zeta)\ker(\mathcal{F} - M(\zeta)) \subset \ker(\mathcal{A} - \zeta) = \{0\}$ and thus $\ker(\mathcal{F} - M(\zeta)) = \{0\}$ because $\gamma(\zeta)$ is injective, thus finishing the proof of (B.2). Finally, using (B.7) again,

$$\begin{aligned}\mathrm{graph}(\mathcal{F} - M(\zeta))^{-1} &= \left\{(g,f) \in \mathfrak{H} \times \mathfrak{H} : (f,g) \in (\mathcal{F} - M(\zeta))\right\} \\ &= \left\{\left(\gamma^*(\overline{\zeta})u, \Gamma_0 R(\zeta)u\right) : u \in \mathcal{H}\right\}\end{aligned}$$

yielding $(\mathcal{F} - M(\zeta))^{-1}\gamma^*(\overline{\zeta}) = \Gamma_0 R(\zeta)$, as required to finish the proof of (B.5) and thus (B.4). □

Remark B.2. In the course of proof of the Krein–Naimark formula (B.4), we established relation (B.5). Using this relation, we now show how to derive formula (2.12) in Theorem 2.6 from formula (B.4), cf. the proofs of Theorem 2 and Corollary 4 in [55]. For any two self-adjoint extensions $\mathcal{A}_1$ and $\mathcal{A}_2$ and the extension $\mathcal{A}_0$ given by (B.1), we denote $R_j(\zeta) = (\mathcal{A}_j - \zeta)^{-1}$ for any ζ that is not in the spectrum of $\mathcal{A}_j$, $j = 0, 1, 2$. Applying (B.4) and using (B.5) for $\mathcal{A}_1$ and $\mathcal{A}_2$ yields

$$R_1(\zeta) = R_0(\zeta) + \gamma(\zeta)\Gamma_0 R_1(\zeta), \quad R_2(\zeta) = R_0(\zeta) + \gamma(\zeta)\Gamma_0 R_2(\zeta). \tag{B.8}$$

Multiplying (B.8) by Γ_1 and using formulas $\gamma^*(\overline{\zeta}) = \Gamma_1 R_0(\zeta)$ and $M(\zeta) = \Gamma_1\gamma(\zeta)$ gives

$$\Gamma_1 R_1(\zeta) = \gamma^*(\overline{\zeta}) + M(\zeta)\Gamma_0 R_1(\zeta), \quad \Gamma_1 R_2(\overline{\zeta}) = \gamma^*(\zeta) + M(\overline{\zeta})\Gamma_0 R_2(\overline{\zeta}).$$

Plugging this in the RHS of formula (2.12) and using the property $M^*(\zeta) = M(\overline{\zeta})$ of the Weyl function, see, for example, [120, Proposition 14.15(ii)], yields

$$\begin{aligned}
&\left(\Gamma_0 R_2(\overline{\zeta})\right)^* \Gamma_1 R_1(\zeta) - \left(\Gamma_1 R_2(\overline{\zeta})\right)^* \Gamma_0 R_1(\zeta) \\
&= \left(\Gamma_0 R_2(\overline{\zeta})\right)^* \left(\gamma^*(\overline{\zeta}) + M(\zeta)\Gamma_0 R_1(\zeta)\right) - \left(\gamma^*(\zeta) + M(\overline{\zeta})\Gamma_0 R_2(\overline{\zeta})\right)^* \Gamma_0 R_1(\zeta) \\
&= \left(\gamma(\overline{\zeta})\Gamma_0 R_2(\overline{\zeta})\right)^* - (\gamma(\zeta)\Gamma_0 R_1(\zeta)) + \left(\Gamma_0 R_2(\overline{\zeta})\right)^* \left(M(\zeta) - M^*(\overline{\zeta})\right)\Gamma_0 R_1(\zeta) \\
&= \left(R_2(\overline{\zeta}) - R_0(\overline{\zeta})\right)^* - (R_1(\zeta) - R_0(\zeta)) = R_2(\zeta) - R_1(\zeta),
\end{aligned}$$

where, to pass to the last line, we used (B.8) again. This proves (2.12) as required.

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