Asymptotic analysis of operator families and applications to resonant media

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Abstract

We give an overview of operator-theoretic tools that have recently proved useful in the analysis of boundary-value and transmission problems for second-order partial differential equations, with a view to addressing, in particular, the asymptotic behaviour of resolvents of physically motivated parameter-dependent operator families. We demonstrate the links of this rich area, on the one hand, to functional frameworks developed by S. N. Naboko and his students, and on the other hand, to concrete applications of current interest in the physics and engineering communities.

In memoriam Sergey Naboko

1 Introduction

It has transpired recently that a number of operator-theoretical techniques which have been under active development for the past 60 years or so are extremely useful in the asymptotic analysis of highly inhomogeneous media. Apart from yielding sharp asymptotics of the corresponding Hamiltonians in the norm-resolvent topology, this research has resulted in a number of new important, yet mostly unexplored, connections between certain areas of the modern operator and spectral theory. These include the theory of dilations and functional models of dissipative and non-selfadjoint operators in Hilbert spaces, the boundary triples theory in the analysis of symmetric operators, zero-range models with an internal structure and, finally, the theory of generalised resolvents and their out-of-space "dilations".

The present survey, based on our results published in [41–45,45–48,76,117,118,120], attempts to shed some light on these connections and to thus present the subject area of strongly inhomogeneous media under the spotlight of modern spectral theory. We aim to show that in many ways this novel outlook allows one to gain a better understanding of the mentioned area by providing a universal abstraction layer for all the main objects to be found in the asymptotic analysis. Moreover, in most cases one can then proceed in the analysis on a purely abstract level surprisingly far, essentially postponing the use of the specific features of the problem at hand till the very last stages.

For readers' convenience, we have included a rather detailed exposition of the relevant areas of operator and spectral theory, keeping in mind that some papers laying the foundations of these areas have been poorly accessible to date.

We start with Section 2, devoted to the now-classical theory of dilations of dissipative operators. The role of dissipative operators as opposed to self-adjoint ones is that whereas the latter represent physical systems with the energy conservation law ("closed", or conservative, systems), the former allow for the consideration of a more realistic setup, where the loss of the total energy is factored in. The importance of dissipative systems has been a common place since at least the works of I. Prigogine; it is well-known that such systems may possess certain rather unexpected properties. The main difference between the self-adjoint and dissipative theories can be clarified, following M. G. Kreĭn, as follows: the major instruments of self-adjoint spectral analysis arise from the Hilbert space geometry, whereas this geometry doesn't work very well in the non-selfadjoint situation, with modern complex analysis taking the role of the main tool in the investigation.

Since the seminal contribution of B. Sz.-Nagy and C. Foiaş, the main object of dissipative spectral analysis has been the so-called dilation, representing an out-of-space self-adjoint extension, in the sense of (1) below, of the original dissipative operator L. Our argument actually goes as far as to suggest that this concept underpins the whole set of ideas and notions presented in the paper. B. S. Pavlov's explicit construction of dilation relies upon the second major ingredient, which is the characteristic function $S(z)$, see (5), which is an analytic operator-valued contraction in $\mathbb{C}_+$. The analysis of the dissipative operator L is reduced to the study of the function $S(z)$, and hence from this point onward it belongs to the domain of complex analysis. It turns out that the sole knowledge of $S(z)$ yields an explicit spectral representation of the dilation. Moreover, Naboko has shown that, in the same representation, a whole family of operators "close" to L, self-adjoint and non-selfadjoint alike, are modelled in an effective way. This idea in particular led to the description of absolutely continuous subspaces of all the operators considered as the closure of the so-called smooth vectors set. This latter is characterised as the collection of vectors such that the resolvent of the operator in question in the spectral representation maps them as the multiplication operator. An explicit construction of wave operators and scattering matrices then follows almost immediately.

In Section 2.3, we give a systematic exposition of this approach applied to the family of extensions of a symmetric densely defined operator on a Hilbert space H possessing equal deficiency indices. In so doing, we follow closely the strategy suggested by Sergey Naboko which he had applied in the analysis of additive relatively bounded perturbations of self-adjoint operators. We thus hope to provide a coherent presentation of the major contribution by Naboko to the spectral analysis of non-selfadjoint operators.

Our analysis is facilitated by the boundary triples theory, being an abstract framework, from which the extensions theory of symmetric operators, especially differential operators, greatly benefits. That's why we start our exposition by introducing the main concepts of this theory. The formula obtained for the scattering operator in the functional model representation allows us to derive an explicit formula for the scattering matrix, formulated in terms of Weyl-Titchmarsh M-matrices, i.e., in the natural terms associated with the problem. In Section 3, we consider an application of this technique to an inverse scattering problem on a quantum graph, where we are able to give an explicit solution to the problem of reconstructing matching conditions at graph vertices.

In Section 2.4, we consider the possible generalisation of the approach described above to the case of partial differential operators (PDO), associated with boundary value problems (BVP). Although the theory of boundary triples has been successfully applied to the spectral analysis of BVP for ordinary differential operators and related setups, in its original form this theory is not suited for dealing with BVP for partial differential equations (PDE), see [34, Section 7] for a relevant discussion. Recently, when the works [17,34,65,69,70,120] started to appear, it has transpired that, suitably modified, the boundary triples approach nevertheless admits a natural generalisation to the BVP setup, see also the seminal contributions by J. W. Calkin [37], M. S. Birman [25], L. Boutet de Monvel [31], M. S. Birman and M. Z. Solomyak [26], G. Grubb [68], and M. Agranovich [6], which provide the analytic backbone for the related operator-theoretic constructions.

In all cases mentioned above, one can see the fundamental rôle of a certain Herglotz operator-valued analytic function, which in problems where a boundary is present (and sometimes even without an explicit boundary [12]) turns out to be a natural generalisation of the classical notion of a Dirichlet-to-Neumann map. Moreover, it is precisely this object that permits to define the characteristic function which in turn facilitates the functional model construction.

In Section 4, we pass over to the discussion of zero-range models with an internal structure. The idea of replacing a model of short-range interactions by an explicitly solvable one with a zero-radius potential (possibly with an internal structure) [22, 24, 36, 79, 80, 111, 135] has paved the way for an influx of methods of the theory of extensions (both self-adjoint and non-selfadjoint) of symmetric operators to problems of mathematical physics. In particular, we view zero-range potentials with an internal structure as a particular case of out-of-space self-adjoint extensions of symmetric operators, the theory of which is intrinsically related to the analysis of generalised resolvents. The latter area is introduced in Section 2.5. We argue that out-of-space self-adjoint extensions corresponding to generalised resolvents naturally supersedes the dilation theory as presented in Section 2.2.

On yet another level, we claim that zero-range perturbations (and more precisely, zero-range perturbations with an internal structure) appear naturally as the norm-resolvent limits of Hamiltonians in the asymptotic analysis of inhomogeneous media. This relationship is established using the apparatus of generalised resolvents, as explained in Section 4.4.

Finally, we mention here that the theory of functional models as presented in Section 2 is directly applicable to the treatment of models of zero-range potentials with an internal structure. Its development yields a complete spectral analysis and an explicit construction of the scattering theory for the latter.

Two different models are considered in Section 4, one of these being a one-dimensional periodic model with critical contrast, unitary equivalent to the double porosity one. The PDE counterpart of the latter is discussed in Section 5. The second mentioned model pertains to the problem with a low-index inclusion in a homogeneous material. Our argument shows that the leading order term in the asymptotic expansion of its resolvent admits the same form as expected of a zero-range model; the difference is that here the effective model of the media is no longer "zero-range" per se; rather it pertains to a singular perturbation supported by a manifold. Therefore, this allows us to extend the notion of internal structure to the case of distributional perturbations supported by manifolds.

The discussion started in Section 4 is then continued in Section 5. We note that in every model considered so far, the internal structure of the limiting zero-range model is necessarily the simplest possible, i.e., pertains to the out-of-space extensions defined on $H \oplus \mathbb{C}^1$, where H is the original Hilbert space. It turns out that this is due to the fact that we only consider norm-resolvent convergence when the spectral parameter z is restricted to a compact set in $\mathbb{C}$.

Passing over to a generic setup with z not necessarily in a compact, we are able to claim that in some sense the internal structure can be arbitrarily complex, provided that the spectral parameter z is allowed to grow with the large parameter a, which describes the inhomogeneity, increasing to $+\infty$. This allows us to present an explicit example of a non-trivial internal structure in the leading order term of the norm-resolvent asymptotics in Section 4.4, which is supplemented with the discussion of the so-called scaling regimes which we introduce in Section 5.1.

The remainder of Section 5 is devoted to the analysis of a double porosity model of high-contrast homogenisation, where the leading order term of the asymptotic expansion is obtained by an application of the operator-theoretical technique based on the generalised resolvents, as in Section 4.

2 Functional models for dissipative and nonselfadjoint operators

Functional model construction for a contractive linear operator T acting on a Hilbert space H is a well developed domain of the operator theory. Since the pioneering works by B. Sz.-Nagy, C. Foiaş [130], P. D. Lax, R. S. Phillips [87], L. de Branges, J. Rovnyak [29,30], and M. S. Livšic [90], this field of research has attracted many specialists in operator theory, complex analysis, system control, Gaussian processes and other disciplines. Multiple studies culminated in the development of a comprehensive theory complemented by various applications, see [52, 63, 103, 104, 107] and references therein.

The underlying idea of a functional model is the fundamental theorem of B. Sz.-Nagy and C. Foias establishing the existence of a unitary dilation for any contractive (linear) Hilbert space operator T, $\|T\| \leq 1$. The unitary dilation U of T is a unitary operator on a Hilbert space $\mathcal{H} \supset H$ such that $P_H U^n|_H = T^n$ for all $n = 1, 2, \dots$. Here $P_H : \mathcal{H} \to H$ is an orthoprojection from $\mathcal{H}$ to its subspace H. The dilation U is called minimal if the linear set $\vee_{n>0} U^n H$ is dense in $\mathcal{H}$. The minimal dilation U of a contraction is unique up to unitary equivalence. The spectrum of U is absolutely continuous and covers the unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$. If one denotes by μ the spectral measure of U, the spectral theorem yields that operator T is unitarily equivalent to its model $T = P_H z|_H$, where $f \mapsto zf$ is the operator of multiplication on the spectral representation space $L^2(\mathbb{T}, \mu)$ of U.

Due to its abstract nature, a significant part of the functional model research for contractions took place among specialists in complex analysis and operator theory. The parallel theory for unbounded operators is based on the Cayley transform $T \mapsto -\mathrm{i}(T + I)(T - I)^{-1}$ applied to a contraction $\|T\| \leq 1$. Assuming that $\operatorname{clos}\operatorname{ran}(T - I) = H$, the Cayley transform of T, $\|T\| < 1$ is a dissipative densely defined operator $L = -\mathrm{i}(T + I)(T - I)^{-1}$, not necessarily bounded in H. It is easily seen that the spectrum of L is situated in the closed upper half plane $\overline{\mathbb{C}}_+$ of the complex plane. The imaginary part of L (defined in the sense of forms if needed) is a non-negative operator.

Alongside the developments in operator theory, the second half of the 20th century witnessed a huge progress in the spectral analysis of linear operators pertaining to physical disciplines. The principal tool of this was the method of Riesz projections, i.e., the contour integration of the operator's resolvent in the complex plane of spectral parameter. The spectral analysis of self-adjoint operators of quantum mechanics can be viewed as the prime example of highly successful application of contour integration in the study of conservative systems, i.e., closed systems with the energy preserved in the course of evolution.

Topical questions concerning the behavior of non-conservative systems, where the total energy is not preserved, and of resonant systems motivated in-depth studies of (unbounded) non-selfadjoint operators. The analysis of non-conservative dynamical systems and of non-selfadjoint operators especially relevant to the functional model theory was pioneered in the works of M. S. Brodskiĭ, M. S. Livšic and their colleagues, see [32,33,91]. Starting with a (bounded) self-adjoint operator $A = A^*$ as the main operator of a closed conservative system, these authors considered the coupling of this system to the outside world by means of externally attached channels. This construction represents a model of the so-called "open system", that is, of a physical system connected to its external environment. The energy of such modified system can dissipate through the external channels, while at the same time the energy can be fed into the system from the outside in the course of its evolution. In works of M. S. Brodskiĭ and M. S. Livšic, the external channels are modelled as an additive perturbation of the main self-adjoint operator A by a (bounded) non-selfadjoint perturbation: $A \to L = A + \mathrm{i}V$, $V = V^*$. The "channel vectors" form the Hilbert space $E = \operatorname{clos}\operatorname{ran}|V|$. If $V \geq 0$, the operator L is dissipative (i.e., $\operatorname{Im}(Lu, u) > 0$, $u \in H$); it describes a non-conservative system losing the total energy. In turn, and quite analogously to the case of contractions, under the assumption $\mathbb{C}_- \subset \rho(L)$ (recall that dissipative operators satisfying this condition are called *maximal*), the self-adjoint dilation of L is a self-adjoint operator $\mathscr{L}$ on a wider space $\mathcal{H} \supset H$ such that

$$(L - zI)^{-1} = P_H(\mathscr{L} - zI)^{-1}|_H, \quad z \in \mathbb{C}_-, \tag{1}$$

where P_H is an orthogonal projection from $\mathcal{H}$ onto H. The operator $\mathscr{L}$ describes a (larger) system with the state space $\mathcal{H}$, in which the energy is conserved, whereas L describes its subsystem losing its total energy. In the general case, a non-dissipative L corresponds to an open system where both the energy loss and the energy supply coexist.

The analysis of a non-selfadjoint operator L relies on the notion of its characteristic function [89, 127] discovered by M. S. Livšic in 1943–1944. It is a bounded analytic operator-function $\Theta(z)$, $z \in \rho(L^*)$ defined on the resolvent set of L^* and acting on the "channel vectors" from the space E. For dissipative L the function Θ coincides with the characteristic function of a contraction $T = (L - \mathrm{i}I)(L + \mathrm{i}I)^{-1}$ (the inverse Cayley transform of L), featured prominently in the works by B. Sz.-Nagy and C. Foias. The characteristic function of a non-selfadjoint operator L (or, alternatively, of its Cayley transform) determines the original operator L uniquely up to a unitary equivalence (see [90, 130]), provided L has no non-trivial self-adjoint "parts". Therefore, the study of non-selfadjoint operators is reduced to the study of operator-valued analytic functions. In and of itself, this does not mean much as these functions might be as complicated as the operators themselves. A simplification is achieved when the values of these functions are either matrices or belong to Schatten-von Neumann classes of compact operators, which is often the case in physical applications.

Closely related to the Sz.-Nagy-Foias model for contractions and to the open systems framework are the Lax-Phillips scattering theory [87] and the "canonical model" due to L. de Branges and J. Rovnyak [30]. The latter is developed for completely non-isometric contractions and their adjoints with quantum-mechanical applications in mind. The Lax-Phillips theory was originally developed to facilitate the analysis of scattering problems for hyperbolic wave equations in exterior domains to compact scatterers. It provides useful intuition into the underpinnings of the functional model construction and this connection will be exploited in the next section.

It was realized very early [2] that the three theories, i.e., the open systems theory, the Sz.-Nagy-Foiaş model, and the Lax-Phillips scattering, all deal with essentially the same objects. In particular, the characteristic function of a contraction (or of a dissipative operator) emerges, albeit under disguise, in all three theories. Being a purely theoretical abstract object in the Sz.-Nagy-Foiaş theory, the characteristic function emerges as a transfer function of a linear system according to M. S. Brodskiĭ and M. S. Livšic, and as the scattering matrix in the Lax-Phillips theory. The characteristic function of a contraction is also the central component in the L. de Branges and J. Rovnyak model theory [30]. Deep connections between the Sz-Nagy-Foias and the de Branges-Rovnyak models are clarified in a series of papers by N. Nikolskii and V. Vasyunin [105–107].

2.1 Lax-Phillips theory

The Lax-Phillips scattering theory [87] for the acoustic waves by a smooth compact obstacle in $\mathbb{R}^n$ with $n \geq 3$ odd provides an excellent illustration of the intrinsic links between the operator theory and mathematical physics. A number of concepts found in the theory of functional models of dissipative operators find their direct counterparts here, expressed in the language of realistic physical processes. For instance, the characteristic function of the operator governing the scattering process is realized as the scattering matrix, the self-adjoint dilation corresponds to the operator of "free" dynamics, i.e., the wave propagation process observed in absence of the obstacle, and the scattering channels are a direct analogue of the channels found in the Brodskiĭ-Livšic constructions. In this section we briefly recall the main concepts of Lax-Phillips scattering theory.

Let $\mathcal{H}$ be a Hilbert space with two mutually orthogonal subspaces $\mathcal{D}_\pm \subset \mathcal{H}$, $\mathcal{D}_- \oplus \mathcal{D}_+ \neq \mathcal{H}$. Denote by $\mathcal{K}$ the orthogonal complement of $\mathcal{D}_- \oplus \mathcal{D}_+$ in $\mathcal{H}$. Assume the existence of a single parameter evolution group of unitary operators $\{U(t)\}_{t\in\mathbb{R}}$ with the following properties

$$\begin{aligned} U(t)\mathcal{D}_- &\subseteq \mathcal{D}_-, \quad t \leq 0, \\ U(t)\mathcal{D}_+ &\subseteq \mathcal{D}_+, \quad t \geq 0, \\ \cap_{t\in\mathbb{R}} U(t)\mathcal{D}_\pm &= \{0\}, \\ \operatorname{clos} \cup_{t\in\mathbb{R}} U(t)\mathcal{D}_\pm &= \mathcal{H}. \end{aligned} \tag{2}$$

In the acoustic scattering, the space $\mathcal{H}$ consists of solutions to the wave equation (i.e., acoustic waves) and is endowed with the energy norm. The group $U(t)$ describes the evolution of "free" waves in $\mathcal{H}$, that is, the group $U(t)$ maps the Cauchy data of solutions at the time $t = 0$ to their Cauchy data at the time t. Since $U(t)$ is unitary for all $t \in \mathbb{R}$, the energy of solutions is preserved under the time evolution $f = U(0)f \mapsto U(t)f$, for any Cauchy data $f \in \mathcal{H}$. Correspondingly, the infinitesimal generator $\mathscr{B}$ of $U(t)$ is a self-adjoint operator in $\mathcal{H}$ with purely absolutely continuous spectrum covering the whole real line. The subspaces $\mathcal{D}_\pm$ are called incoming and outgoing subspaces of $U(t)$. These names are well justified. Indeed, the subspace $\mathcal{D}_-$ consists of solutions that do not interact with the obstacle prior to the moment $t = 0$, whereas $\mathcal{D}_+$ consists of scattered waves which do not interact with the obstacle after $t = 0$. There exist two representations for the generator $\mathscr{B}$ associated with $\mathcal{D}_\pm$ (the so called incoming and outgoing translation representations), in which the group $U(t)$ acts as the right shift operator $U(t) : u(x) \mapsto u(x - t)$ on $L^2(\mathbb{R}, E)$ with some auxiliary Hilbert space E. In these representations the subspaces $\mathcal{D}_\pm$ are mapped to $L^2(\mathbb{R}_\pm, E)$. It is not difficult to see that this construction satisfies the assumptions (2). Denote by $P_\pm : \mathcal{H} \to [\mathcal{D}_\pm]^\perp$ the orthogonal projections to the complements of $\mathcal{D}_\pm$ in $\mathcal{H}$. The elements of $\mathcal{K}$ are the scattering waves that are neither incoming in the past, nor outgoing in the future, i.e., the waves localized in the vicinity of the obstacle. The interaction of incoming waves with the obstacle, i.e., the scattering process, is then described by the compression of the group $U(t)$ to the neighborhood of the obstacle:

$$Z(t) = P_+ U(t) P_- = P_{\mathcal{K}} U(t) P_{\mathcal{K}}, \quad t \geq 0.$$

Here $P_{\mathcal{K}} = P_- P_+$ is an orthoprojection on $\mathcal{H}$. The operator family $\{Z(t)\}_{t\geq 0}$ forms a strongly continuous semigroup acting on $\mathcal{K}$. Since $Z(t)$ is a compression of the unitary group, it is clear that $\|Z(t)\| \leq 1$ for all $t \geq 0$. The infinitesimal generator B of the semigroup $\{Z(t)\}_{t\geq 0}$ turns out to be a linear operator with purely discrete spectrum $\{\lambda_k\}$ with $\mathrm{Re}(\lambda_k) < 0$, $k = 1, 2, \ldots$. The poles $\{\lambda_k\}$ of the resolvent of B and the corresponding eigenvectors are interpreted as the scattering resonances. These resonances correspond to the poles of the scattering matrix defined as an operator-valued function acting in the space $L^2(\mathbb{R}_-, E)$, i.e., the space of vector functions taking values in E.

The scattering matrix is mapped by the Fourier transform to the analytic in the lower half-plane operator function $S(z)$, $z \in \mathbb{C}_-$ with zeroes at $z_k = -\mathrm{i}\lambda_k$. The boundary values $S(k - \mathrm{i}0)$ on the real axis exist almost everywhere in the strong operator topology and are unitary for almost all $k \in \mathbb{R}$. The function $S(z)$ permits an analytic continuation $S(z) = [S^*(\bar{z})]^{-1}$ to the upper half-plane, where it is meromorphic.

The results of [2] show that $\theta(z) := S^*(\bar{z})$ coincides with the Livšic's characteristic function of a dissipative operator being unitary equivalent to the infinitesimal generator of $Z(t)$. Consequently, $\theta\big((z + \mathrm{i})/(z - \mathrm{i})\big)$ is the characteristic function of its Cayley transform as defined by B. Sz.-Nagy and C. Foiaş [130]. Finally, the resolvents of operators $\mathscr{L} = -\mathrm{i}\mathscr{B}$ and $L = -\mathrm{i}B$ satisfy the dilation equation (1). In other words, the operator corresponding to the free dynamics is the self-adjoint dilation of the dissipative operator that governs the scattering process.

2.1.1 Minimality, non-selfadjointness, resolvent

The beautiful geometric interpretation of scattering processes provided by the Lax-Phillips theory is not entirely transferable to the modelling of a general dissipative (or contractive) operator. For instance, given an arbitrary dissipative operator L on a Hilbert space K, its selfadjoint dilation $\mathscr{L}$ does not exists *a priori* and must be explicitly constructed first. In addition, such a dilation $\mathscr{L}$ should be *minimal*, that is, it must contain no reducing self-adjoint parts unrelated to the operator L. Mathematically, the minimality condition is expressed by the equality

$$\operatorname{clos} \bigvee_{z \notin R} (\mathscr{L} - zI)^{-1} |_K = \mathcal{H}$$

where $\mathcal{H}$ is the dilation space $\mathcal{H} \supset K$. The construction of a dilation satisfying this condition is a highly non-trivial task which was successfully addressed for contractions by B. Sz.-Nagy and C. Foiaş [130], aided by a theorem of M. A. Naĭmark [102], and then by B. Pavlov [109, 110] in two important cases of dissipative operators arising in mathematical physics. Later, this construction was generalized to a generic setting. We dwell on this further in the following sections.

For obvious reasons, the functional model theory of non-selfadjoint operators deals with operators possessing no non-trivial reducing self-adjoint parts. Such operators are called *completely non-selfadjoint* or, using a somewhat less accurate term, *simple*. The rationale behind this condition is easy to illustrate within the Lax-Phillips framework. Let the dissipative operator $L = -\mathrm{i}B$ governing the wave dynamics in a vicinity of an obstacle possess a non-trivial self-adjoint part. This part is then a self-adjoint operator acting on the subspace spanned by the eigenvectors of L

corresponding to its real eigenvalues. The restriction of $Z(t)$ to this subspace is an isometry for all $t \in \mathbb{R}$, and the energy of these states remains constant (recall that the space K is equipped with the energy norm). Therefore these waves stay in a bounded region adjacent to the obstacle at all times. These bound states do not participate in scattering, as they are invisible to the scattering process describing the asymptotic behaviour as $t \to \pm\infty$, so that the matrix S (or the characteristic function of L) contains no information pertaining to them. In operator theory, this is known as the claim that the characteristic function of a dissipative operator is oblivious to its self-adjoint part. It is also well-known, that the characteristic function uniquely determines the completely non-selfadjoint part of a dissipative operator.

The interaction dynamics of the Lax-Phillips scattering supposes neither minimality nor complete non-selfadjointness. One can envision incoming waves that do not interact with the obstacle during their evolution and eventually become outgoing as $t \to +\infty$. It is also easy to conceive of trapping obstacles preventing waves from leaving the neighbourhood of the obstacle at $t \to +\infty$. The geometry of such obstacles cannot be fully recovered from the scattering data because, as explained above, these standing waves do not participate in the scattering process.

In the applications discussed below, unless explicitly stated otherwise, all non-selfadjoint operators are assumed closed, densely defined with regular points in both lower and upper half planes. The latter condition can be relaxed but is adopted in what follows for the sake of convenience.

2.2 Pavlov's functional model and its spectral form

Functional models for prototypical dissipative operators of mathematical physics (as opposed to the model for contractions), alongside explicit constructions of self-adjoint dilations, were investigated by B. Pavlov in his works [108–110]. Two classes of dissipative operators were considered: the Schrödinger operator in $L^2(\mathbb{R}^3)$ with a complex-valued potential, and the operator generated by the differential expression $-y'' + q(x)y$ on the interval $[0, \infty)$ with a dissipative boundary condition at $x = 0$. In both cases the self-adjoint dilations are constructed explicitly in terms of the problem at hand, and supplemented by the model representations known today as "symmetric" and commonly referred to as the Pavlov's model. The results of [108–110] were extensively employed in various applications and provided a foundation for the subsequent constructions of self-adjoint dilations and functional models for general non-selfadjoint operators.

2.2.1 Additive perturbations [108, 109]

Let $A = A^*$ be a selfadjoint unbounded operator on a Hilbert space K and V a bounded non-negative operator $V = V^* = \alpha^2/2 \geq 0$, where $\alpha := (2V)^{1/2}$.

The paper [109] studies the dissipative Schrödinger operator $L = A + (\mathrm{i}/2)\alpha^2$ in $\mathbb{R}^3$ defined by the differential expression $-\Delta + q(x) + (\mathrm{i}/2)\alpha^2(x)$ with real continuous functions q and α such that $0 \leq \alpha \leq C < \infty$. The operators $A = -\Delta + q$ and $V = \alpha^2/2$ are the real and imaginary parts of L defined on $\mathrm{dom}(L) = \mathrm{dom}(A)$. Assuming the operator L has no non-trivial self-adjoint components and the resolvent set of L contains points in both upper and lower half planes, the operator L is a maximal completely non-selfadjoint, densely defined dissipative operator on K.

According to the general theory, there exists a minimal dilation of L, which is a self-adjoint operator $\mathscr{L}$ on a Hilbert space $\mathcal{H} \supset K$ such that

$$(L - zI)^{-1} = P_K(\mathscr{L} - zI)^{-1}|_K, \quad z \in \mathbb{C}_-, \tag{3}$$

where P_K is the orthogonal projection from $\mathcal{H}$ onto its subspace K.

The dilation constructed in [109] closely resembles the generator $\mathscr{B}$ of the unitary group $U(t)$ in the Lax-Phillips theory: Pavlov realised that a natural way to construct a self-adjoint dilation would be to add the missing "incoming" and "outgoing" energy channels to the original non-conservative dynamics, thus mimicking the starting point of Lax and Phillips. The challenge here is to determine the operator that describes the "free" evolution of the dynamical system given only its "internal" part, thus in some sense "reversing" the Lax-Phillips approach.

Denote $E := \operatorname{clos}\operatorname{ran}\alpha$ and define the dilation space as the direct sum of K and the equivalents of incoming and outgoing channels $\mathcal{D}_\pm = L^2(\mathbb{R}_\pm, E)$,

$$\mathcal{H} = \mathcal{D}_- \oplus K \oplus \mathcal{D}_+$$

Elements of $\mathcal{H}$ are represented as three-component vectors (v_-, u, v_+) with $v_\pm \in \mathcal{D}_\pm$ and $u \in K$. The Lax-Phillips theory suggests that the dilation $\mathscr{L}$ restricted to $\mathcal{D}_- \oplus \{0\} \oplus \mathcal{D}_+$ should be the self-adoint generator A of the continuous unitary group of right shifts $\exp(\mathrm{i}At) = U(t) : v(x) \mapsto v(x-t)$ in $L^2(\mathbb{R}, E)$. By Stone's theorem, one has

$$\mathrm{i}Av = \lim_{t\downarrow 0} t^{-1}[U(t)v - v] = \lim_{t\downarrow 0} t^{-1}\big(v(x-t) - v(x)\big) = -v'(x),$$

so that the generator of $U(t)$ is the operator $A : v \mapsto \mathrm{i}dv/dx$. Hence, the action of $\mathscr{L}$ on the channels $\mathcal{D}_\pm$ is defined by $\mathscr{L} : (v_-, 0, v_+) \mapsto (\mathrm{i}v'_-, 0, \mathrm{i}v'_+)$. The self-adjointness of $\mathscr{L} = \mathscr{L}^*$ and the requirement (3) yield the form of dilation $\mathscr{L}$ as found in [109],

$$\mathscr{L}\begin{pmatrix} v_- \\ u \\ v_+ \end{pmatrix} = \begin{pmatrix} \mathrm{i}\dfrac{dv_-}{dx} \\ Au + \dfrac{\alpha}{2}\left[v_+(0) + v_-(0)\right] \\ \mathrm{i}\dfrac{dv_+}{dx} \end{pmatrix}, \tag{4}$$

defined on the domain

$$\operatorname{dom}(\mathscr{L}) = \big\{(v_-, u, v_+) \in \mathcal{H} \mid v_\pm \in W_2^1(\mathbb{R}_\pm, E), u \in \operatorname{dom}(A), v_+(0) - v_-(0) = i\alpha u\big\}$$

Embedding theorems for the Sobolev space W_2^1 guarantee the existence of boundary values $v_\pm(0)$. The "boundary condition" $v_+(0) - v_-(0) = \mathrm{i}\alpha u$ can be interpreted as a concrete form of coupling between the incoming and outgoing channels $\mathcal{D}_\pm$ realized by the imaginary part of L acting on E.

When $\alpha = 0$, the right hand side of (4) is the orthogonal sum of two self-adjoint operators, that is, the operator A on K and the operator $\mathrm{i}d/dx$ acting in the orthogonal sum of channels $L^2(\mathbb{R}, E) = \mathcal{D}_- \oplus \mathcal{D}_+$. The characteristic function of L is the contractive operator-valued function defined by the formula

$$S(z) = I_E + \mathrm{i}\alpha(L^* - zI)^{-1}\alpha : E \to E, \quad z \in \mathbb{C}_+ \tag{5}$$

According to the fundamental result of Adamyan and Arov [2], the function S coincides with the scattering operator of the pair $(\mathscr{L}, \mathscr{L}_0)$ where $\mathscr{L}_0$ is defined by (4) with $u = 0$ and $\alpha = 0$.

2.2.2 Extensions of symmetric operators [110]

Consider the differential expression

$$\ell y = -y'' + q(x)y$$

in $K = L^2(\mathbb{R}_+)$ with a real function q such that the Weyl limit point case takes place. Denote by φ and ψ the standard solutions to the equation $\ell y = zy$ with $z \in \mathbb{C}_+$, satisfying the boundary conditions

$$\varphi(0,z) = 0, \quad \varphi'(0,z) = -1, \quad \psi(0,z) = 1, \quad \psi'(0,z) = 0$$

Then the Weyl solution $\chi = \varphi + m_\infty(z)\psi \in L^2(\mathbb{R}_+)$, where $m_\infty(z)$ is the Weyl function pertaining to ℓ and corresponding to the boundary condition $y(0) = 0$, is defined uniquely. The function $m_\infty(z)$ is analytic with positive imaginary part for $z \in \mathbb{C}_+$.

Define the operator L in $K = L^2(\mathbb{R}_+)$ by the expression ℓ supplied with the non-selfadjoint boundary condition at $x = 0$

$$(y' - hy)|_{x=0} = 0, \quad \text{where} \quad \operatorname{Im} h = \frac{\alpha^2}{2}, \quad \alpha > 0$$

A short calculation ascertains that L is dissipative indeed.

The Pavlov's dilation of L is the operator $\mathscr{L}$ in the space $\mathcal{H} = \mathcal{D}_- \oplus K \oplus \mathcal{D}_+$, where $\mathcal{D}_\pm = L^2(\mathbb{R}_\pm)$, defined on elements $(v_-, u, v_+) \in \mathcal{H}$ which satisfy

$$\begin{aligned} &v_\pm \in W_2^1(\mathbb{R}_\pm), \quad u, \ell u \in L^2(\mathbb{R}_+), \\ &u' - hu\big|_0 = \alpha v_-(0), \quad u' - \bar{h}u\big|_0 = \alpha v_+(0) \end{aligned} \tag{6}$$

The action of the operator $\mathscr{L}$ on this domain is set by the formula

$$\mathscr{L}\begin{pmatrix} v_- \\ u \\ v_+ \end{pmatrix} = \begin{pmatrix} \mathrm{i}\dfrac{dv_-}{dx} \\ \ell u \\ \mathrm{i}\dfrac{dv_+}{dx} \end{pmatrix}. \tag{7}$$

The characteristic function of L is the scalar analytic in the upper half-plane function $S(z)$ given by

$$S(z) = \frac{m_\infty(z) - h}{m_\infty(z) - \bar{h}}, \quad \operatorname{Im}(z) > 0.$$

Note that since $\operatorname{Im} h = \alpha^2/2$, the function $S(z)$ can be rewritten in a form similar to that of the characteristic function (5), i. e.,

$$S(z) = 1 + \mathrm{i}\alpha\big(\bar{h} - m_\infty(z)\big)^{-1}\alpha. \tag{8}$$

2.2.3 Pavlov's symmetric form of the dilation

According to the general theory [130], once the characteristic function S is known, the analysis of the completely non-selfadjoint part of the operator L is reduced to the analysis of S. Hence, the typical questions of the operator theory (the spectral analysis, description of invariant subspaces) are reformulated as problems pertaining to analytic (operator-valued) functions.

Assume that L is completely non-selfadjoint and $\rho(L) \cap \mathbb{C}_\pm \neq \varnothing$. Let $\mathscr{L}$ be its minimal self-adjoint dilation, S being the characteristic function of L. Owing to the general theory [130], the operator L is unitary equivalent to its model acting in the spectral representation of $\mathscr{L}$ in accordance with (3). Recall that the characteristic function $S(z)$, $z \in \mathbb{C}_+$ is analytic in the upper half-plane taking values in the set of contractions of E,

$$S(z) : E \to E, \quad \|S(z)\| \leq 1, \quad z \in \mathbb{C}_+$$

Due to the operator version of Fatou's theorem [130], the nontangential boundary values of the function S exist in the strong operator topology almost everywhere on the real line. Put $S = S(k) := \text{s-lim}_{\varepsilon \downarrow 0} S(k + \mathrm{i}\varepsilon)$ and $S^* = S^*(k) := \text{s-lim}_{\varepsilon \downarrow 0}[S(k + \mathrm{i}\varepsilon)]^*$, both limits existing for almost all $k \in \mathbb{R}$. The Fatou theorem guarantees that the operators $S(k)$ and $S^*(k)$ are contractions on E for almost all $k \in \mathbb{R}$. The symmetric form of the dilation is obtained by completion of the dense linear set in $L^2(E) \oplus L^2(E)$ with respect to the norm

$$\left\| \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\|^2_{\mathscr{H}} := \int_{\mathbb{R}} \left\langle \begin{pmatrix} I & S^* \\ S & I \end{pmatrix} \begin{pmatrix} \tilde{g} \\ g \end{pmatrix}, \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\rangle_{E \oplus E} dk, \tag{9}$$

followed by factorisation by the elements of zero norm. In the symmetric representation, the incoming and outgoing subspaces $\mathcal{D}_\pm$ admit their simplest possible form. On the other hand, calculations related to the space K can meet certain difficulties, since the "weight" in (9) can be singular. Also note that the elements of $\mathscr{H}$ are not individual functions from $L^2(E) \oplus L^2(E)$ but rather equivalence classes [104,106]. Despite these complications, the Pavlov's symmetric model has been widely accepted in the analysis of non-selfadjoint operators, and in particular of the operators of mathematical physics. Two alternative and equivalent forms of the norm $\| \cdot \|_{\mathscr{H}}$ that are easy to derive,

$$\left\| \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\|^2_{\mathscr{H}} = \|S\tilde{g} + g\|^2_{L^2(E)} + \|\Delta_* g\|^2_{L^2(E)} = \|\tilde{g} + S^* g\|^2_{L^2(E)} + \|\Delta \tilde{g}\|^2_{L^2(E)},$$

where $\Delta := \sqrt{I - S^*S}$ and $\Delta_* := \sqrt{I - SS^*}$, show that for each $\binom{\tilde{g}}{g} \in \mathscr{H}$ expressions $S\tilde{g} + g$, $\tilde{g} + S^* g$, $\Delta \tilde{g}$, and $\Delta_* g$ are in fact usual square summable vector-functions from $L^2(E)$. Moreover, due to these equalities the form (9) is positive-definite indeed and thus represents a norm.

The space

$$\mathscr{H} = L^2 \begin{pmatrix} I & S^* \\ S & I \end{pmatrix}$$

with the norm defined by (9) is the space of spectral representation for the self-adjoint dilation $\mathscr{L}$ of the operator L. Henceforth we will denote the corresponding unitary mapping of $\mathcal{H}$ onto $\mathscr{H}$ by Φ. It means that the operator of multiplication by the independent variable acting on $\mathscr{H}$, i.e., the operator $f(k) \mapsto kf(k)$, is unitary equivalent to the dilation $\mathscr{L}$. Hence, for $z \in \mathbb{C} \setminus \mathbb{R}$, the mapping $\binom{\tilde{g}}{g} \mapsto (k - z)^{-1} \binom{\tilde{g}}{g}$ is unitary equivalent to the resolvent $(\mathscr{L} - z)^{-1}$ and therefore

$$(L - zI)^{-1} \simeq P_{\mathscr{K}} (k - z)^{-1} \big|_{\mathscr{K}}, \quad z \in \mathbb{C}_-,$$

where the $\simeq$ sign is utilised to denote unitary equivalence.

The incoming and outgoing subspaces of the dilation space $\mathscr{H}$ admit the form

$$\mathscr{D}_+ := \begin{pmatrix} H^2_+(E) \\ 0 \end{pmatrix}, \quad \mathscr{D}_- := \begin{pmatrix} 0 \\ H^2_-(E) \end{pmatrix}, \quad \mathscr{K} := \mathscr{H} \ominus [\mathscr{D}_+ \oplus \mathscr{D}_-]$$

where $H_2^{\pm}(E)$ are the Hardy classes of E-valued vector functions analytic in $\mathbb{C}_{\pm}$. As usual [115], the functions from vector-valued Hardy classes $H_2^{\pm}(E)$ are identified with their boundary values existing almost everywhere on the real line. They form two complementary mutually orthogonal subspaces so that $L^2(E) = H_+^2(E) \oplus H_-^2(E)$.

The image $\mathscr{K}$ of K under the spectral mapping Φ of the dilation space $\mathcal{H}$ to $\mathscr{H}$ is the subspace

$$\mathscr{K} = \left\{ \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \in \mathscr{H} \; : \; \tilde{g} + S^* g \in H_-^2(E), \, S\tilde{g} + g \in H_+^2(E) \right\}$$

The orthogonal projection $P_{\mathscr{K}}$ from $\mathscr{H}$ onto $\mathscr{K}$ is defined by formula (10) on a dense set of functions from $L^2(E) \oplus L^2(E)$ in $\mathscr{H}$

$$P_{\mathscr{K}} \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = \begin{pmatrix} \tilde{g} - P_+(\tilde{g} + S^* g) \\ g - P_-(S\tilde{g} + g) \end{pmatrix}, \quad \tilde{g} \in L^2(E), \; g \in L^2(E). \tag{10}$$

Here $P_{\pm}$ are the orthogonal projections of L^2 onto the Hardy classes $H_2^{\pm}$.

Further information on model representations can be found in the series of papers [104–107] and the treatise [103].

2.2.4 Naboko's functional model of non-selfadjoint operators

The development of the functional model approach for contractions inspired the search for such models of non-dissipative operators. The attempts to follow the blueprints of Sz.-Nagy-Foias and Lax-Philitps meet serious challenges rooted in the absence of a proper self-adjoint dilation for non-dissipative operators: the dilatation in this case is a self-adjoint operator acting on a space with an indefinite metric [49]. Consequently, the characteristic function of a non-dissipative operator is an analytic operator-function, contractive with respect to an indefinite metric [50], which considerably hinders any further progress in this direction. We mention the works [16, 93], the monograph [83] and references therein for more details and examples.

An alternative approach was suggested in the late seventies with the publication of papers [95,96] and especially [97] by S. Naboko who found a way to represent a non-dissipative operator in a model space of a suitably chosen dissipative one. We refer the reader to the relevant section of the paper on Sergey Naboko's mathematical heritage in the present volume for the details of the mentioned approach and the relevant references. In the next section of the present paper we outline the main ingredients of an adaptation of the latter to the setting of extensions of symmetric operators, which was developed by Sergey's students.

We mention that this set of techniques allows one to significantly advance the spectral analysis of non-selfadjoint operators, including the definition of the absolutely continuous and singular subspaces and the study of spectral resolutions of identity. In particular, of major importance is the possibility to construct the wave and scattering operators in a natural representation. It should be noted that the self-adjoint scattering theory (and all the major versions of the latter) turns out to be included as a particular case of a much more general non-selfadjoint one.

2.3 Functional model for a family of extensions of a symmetric operator

The generic model constructed in [92, 118] lends itself as a powerful and universal tool for the analysis of (completely) non-selfadjoint and (completely) non-unitary operators. Since characteristic functions of such operators are essentially unique and define the operators up to unitary equivalence, all model considerations are immediately available once this function is known. In many applications, however, the results sought need to be formulated in terms of the problem itself (i.e., in the natural terms), rather than in the abstract language of characteristic functions (and their transforms). One prominent example when the general theory is not sufficient is the setting of extensions of symmetric operators and the associated setting of operators pertaining to boundary-value problems. Within this setup, the results are expected to be formulated as statements concerning the symmetric operator itself and the relevant properties of the extension parameters. Some results in this direction were obtained by B. Solomyak in [124], but the related calculations tend to be rather tedious due to the reduction to the case of contractions which is required.

The extension theory of symmetric operators, especially differential operators, greatly benefits from the abstract framework known as the boundary triples theory. The basic concepts of this operator-theoretic approach can be found in the textbook [122] by K. Schmüdgen. The recent monograph [20] contains a detailed treatment of this area.

It is therefore quite natural to utilise this approach in conjunction with the functional models techniques outlined above in the analysis of non-selfadjoint extensions of symmetric operators. This section briefly outlines the results pertaining to the functional model construction for dissipative and non-dissipative extensions of symmetric operators and the related developments, including an explicit construction of the wave and scattering operators and of the scattering matrices. Since all the considerations in this area are essentially parallel to the ones of Naboko in his development of spectral theory for additive perturbations of self-adjoint operators, one can consider this narrative as a rather detailed exposition of Naboko's ideas and results in a particular case, important for applications.

2.3.1 Boundary triples

The fundamentals of the boundary triples theory have been introduced in [20, 122], see also references therein.

Denote by A a closed and densely defined symmetric operator on the separable Hilbert space H with the domain $\operatorname{dom} A$, having equal deficiency indices $0 < n_+(A) = n_-(A) \leq \infty$.

Definition 2.1 ([77]). *A triple $\{\mathcal{K}, \Gamma_0, \Gamma_1\}$ consisting of an auxiliary Hilbert space $\mathcal{K}$ and linear mappings Γ_0, Γ_1 defined everywhere on $\operatorname{dom} A^*$ is called a* boundary triple *for A^* if the following conditions are satisfied:*

1. *The abstract Green's formula is valid*

$$(A^*f, g)_H - (f, A^*g)_H = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{K}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{K}}, \quad f, g \in \operatorname{dom} A^* \tag{11}$$

2. *For any $Y_0, Y_1 \in \mathcal{K}$ there exist $f \in \operatorname{dom} A^*$, such that $\Gamma_0 f = Y_0$, $\Gamma_1 f = Y_1$. In other words, the mapping $f \mapsto \Gamma_0 f \oplus \Gamma_1 f$, $f \in \operatorname{dom} A^*$ to $\mathcal{K} \oplus \mathcal{K}$ is surjective.*

It can be shown (see [77]) that a boundary triple for A^* exists assuming only $n_+(A) = n_-(A)$. Note also that a boundary triple is not unique. Given any bounded self-adjoint operator $\Lambda = \Lambda^*$ on $\mathcal{K}$, the collection $\{\mathcal{K}, \Gamma_0, \Gamma_1 + \Lambda\Gamma_0\}$ is a boundary triple for A^* as well, provided that $\Gamma_1 + \Lambda\Gamma_0$ is surjective.

Definition 2.2. *Let $\mathscr{T} = \{\mathcal{K}, \Gamma_0, \Gamma_1\}$ be a boundary triple of A^*. The Weyl function of A^* corresponding to $\mathscr{T}$ and denoted $M(z)$, $z \in \mathbb{C} \setminus \mathbb{R}$ is an analytic operator-function with a positive imaginary part for $z \in \mathbb{C}_+$ (i.e., an operator R-function) with values in the algebra of bounded operators on $\mathcal{K}$ such that*

$$M(z)\Gamma_0 f_z = \Gamma_1 f_z, \quad f_z \in \ker(A^* - zI), \quad z \notin \mathbb{R}$$

For $z \in \mathbb{C} \setminus \mathbb{R}$ we have $(M(z))^* = (M(\bar{z}))$ and $\operatorname{Im}(z) \cdot \operatorname{Im}(M(z)) > 0$.

Definition 2.3. *An extension $\mathcal{A}$ of a closed densely defined symmetric operator A is called* almost solvable (a.s.) *and denoted $\mathcal{A} = A_B$ if there exist a boundary triple $\{\mathcal{K}, \Gamma_0, \Gamma_1\}$ for A^* and a bounded operator $B : \mathcal{K} \to \mathcal{K}$ defined everywhere in $\mathcal{K}$ such that*

$$f \in \operatorname{dom} A_B \iff \Gamma_1 f = B\Gamma_0 f$$

This definition implies the inclusion $\operatorname{dom} A_B \subset \operatorname{dom} A^*$ and that A_B is a restriction of A^* to the linear set $\operatorname{dom} A_B := \{f \in \operatorname{dom} A^* : \Gamma_1 f = B\Gamma_0 f\}$. In this context, the operator B plays the role of a parameter for the family of extensions $\{A_B \mid B : \mathcal{K} \to \mathcal{K}\}$.

It can be shown (see [47] for references) that if the deficiency indices $n_\pm(A)$ are equal and A_B is an almost solvable extension of A, then the resolvent set of A_B is not empty (i.e. A_B is maximal), both A_B and $(A_B)^* = A_{B^*}$ are restrictions of A^* to their domains, and A_B and B are selfadjont (dissipative) simultaneously. The spectrum of A_B coincides with the set of points $z_0 \in \mathbb{C}$ such that $(M(z_0) - B)^{-1}$ does not admit analytic continuation into it.

2.3.2 Characteristic functions

Assume that the parameter B of an almost solvable extension A_B is completely non-selfadjoint. It can be represented as the sum of its real and imaginary part

$$B = B_R + \mathrm{i}B_I, \quad B_R = B_R^*, \quad B_I = B_I^*$$

These parts are well defined since B is bounded. The Green's formula implies that for $B_I \neq 0$ the imaginary part of A_B (in the sense of its form) is non-trivial, i. e., $\operatorname{Im}(A_B u, u) \neq 0$ at least for some $u \in \operatorname{dom}(A_B)$. Hence A_B in this case is not a self-adjoint operator. It appears highly plausible that complete non-selfadjointness of A_B can be derived solely from complete non-selfadjointness of B, assuming that A has no reducing self-adjoint parts. However, no direct proof of this assertion seems to be available in the existing literature.

According to (5), the characteristic function of B has the form

$$\Theta_B(z) = I_E + \mathrm{i}J\alpha(B^* - zI)^{-1}\alpha : E \to E, \quad z \in \rho(B^*),$$

where $\alpha := \sqrt{2|B_I|}$, $J := \operatorname{sign} B_I$, and $E := \operatorname{clos}\operatorname{ran}(\alpha)$. On the other hand, direct calculations according to [127] lead to the following representation for the characteristic function $\Theta_{A_B} : E \to E$ of the non-selfadjoint part of the extension A_B

$$\Theta_{A_B} = I_E + \mathrm{i}J\alpha(B^* - M(z))^{-1}\alpha, \quad z \in \rho(A_B^*).$$

These two formulae confirm an earlier observation that goes back to B. S. Pavlov's work [110], see (8) above. The function Θ_{A_B} is obtained from Θ_B by the substitution of $M(z)$ for zI_E, $z \in \mathbb{C}_+$

$$\Theta_{A_B}(z) = \Theta_B(M(z)), \quad z \in \rho(A_B^*).$$

Alongside A_B introduce the dissipative almost solvable extension A_+ parameterized by $B_+ := B_R + \mathrm{i}|B_I|$. Note that the characteristic function S of A_+ is given by (*cf.* (5))

$$S(z) = I_E + \mathrm{i}\alpha(B_+^* - zI)^{-1}\alpha : E \to E, \quad z \in \mathbb{C}_+. \tag{12}$$

Calculations of [117] (cf. [95]) show that the characteristic functions of A_B and A_+ are related via an operator linear-fractional transform known as Potapov-Ginzburg transformation, or PG-transform [14]. This fact is essentially geometric. It connects contractions on Kreĭn spaces (i.e., the spaces with an indefinite metric defined by the involution $J = J^* = J^{-1}$) with contractions on Hilbert spaces endowed with the regular metric. The PG-transform is invertible and the following assertion pointed out in [95] holds.

Proposition 2.1. *The characteristic function Θ_{A_B} is J-contractive on its domain and the PG-transform maps it to the contractive characteristic function S of A_+ as follows:*

$$\Theta_{A_B} \mapsto S = -(\chi^+ - \Theta_{A_B}\chi^-)^{-1}(\chi^- - \Theta_{A_B}\chi^+), \qquad S \mapsto \Theta_{A_B} = (\chi^- + \chi^+ S)(\chi^+ + \chi^- S)^{-1} \tag{13}$$

where $\chi^\pm = (I_E \pm J)/2$ are orthogonal projections onto subspaces of χ^+E and χ^-E, respectively.

It appears somewhat unexpected that two operator-valued functions connected by formulae (13) can be explicitly written down in terms of their "main operators" A_B and A_+. This relationship between the characteristic functions of A_B and A_+ goes in fact much deeper, see [13, 14]. In particular, the self-adjoint dilation of A_+ and the J-self-adjoint dilation of A_B are also related via a suitably adjusted version of the PG-transform. Similar statements hold for the corresponding linear systems or "generating operators" of the functions Θ_{A_B} and S, cf. [13,14]. This fact is crucial for the construction of a model of a general closed and densely defined non-selfadjoint operator, see [118].

2.3.3 Functional model for a family of extensions

Formulae of the previous secion are essentially the same as the formulae of [95] connecting characteristic functions of non-dissipative and dissipative operators. Reasoning by analogy, this suggests an existence of certain identities that would connect the resolvents of A_B and A_+ corresponding to parameters $B = B_R + iB_I$ and $B_+ = B_R + i|B_I|$. Such identities indeed exist; they are the celebrated Kreĭn formulae for resolvents of two extensions of a symmetric operator. Their variant is readily derived within the framework of boundary triplets, see [117] for calculations, where all details of the following results can also be found.

The functional model of the dissipative extension A_+ begins with the derivation of its minimal selfadjoint dilation $\mathscr{A}$. It is constructed following the recipe of B. Pavlov [108–110] and takes a form quite similar to (6), (7)

$$\mathscr{A}\begin{pmatrix} v_- \\ u \\ v_+ \end{pmatrix} = \begin{pmatrix} \mathrm{i}v_-' \\ A_+^* u \\ \mathrm{i}v_+' \end{pmatrix}, \quad \begin{pmatrix} v_- \\ u \\ v_+ \end{pmatrix} \in \operatorname{dom}(\mathscr{A})$$

where $\operatorname{dom}(\mathscr{A})$ consists of vectors $(v_-, u, v_+) \in \mathcal{H} = \mathcal{D}_- \oplus H \oplus \mathcal{D}_+$, with $v_\pm \in W_2^1(\mathbb{R}_\pm, E)$, $u \in \operatorname{dom}(A_+^*)$ under two "boundary conditions" imposed on $v_\pm$ and u:

$$\Gamma_1 u - B_+\Gamma_0 u = \alpha v_-(0), \quad \Gamma_1 u - B_+^*\Gamma_0 u = \alpha v_+(0)$$

The functional model construction for A_+ follows the recipe by S. Naboko [97]. The following theorem holds.

Theorem 2.2. *There exists a mapping Φ from the dilation space $\mathcal{H}$ onto Pavlov's model space $\mathscr{H}$ defined by (9) with the following properties*

1. *Φ is isometric.*
2. *$\tilde{g} + S^*g = \mathscr{F}_+ h$, $S\tilde{g} + g = \mathscr{F}_- h$, where $\binom{\tilde{g}}{g} = \Phi h$, $h \in \mathcal{H}$*
3. *$\Phi \circ (\mathscr{L} - zI)^{-1} = (k - z)^{-1} \circ \Phi, \quad z \in \mathbb{C} \setminus \mathbb{R}$*
4. *$\Phi\mathcal{H} = \mathscr{H}, \quad \Phi\mathcal{D}_\pm = \mathscr{D}_\pm, \quad \Phi\mathcal{K} = \mathscr{K}$*
5. *$\mathscr{F}_\pm \circ (\mathscr{L} - zI)^{-1} = (k - z)^{-1} \circ \mathscr{F}_\pm, \quad z \in \mathbb{C} \setminus \mathbb{R}.$*

where bounded maps $\mathscr{F}_\pm : \mathcal{H} \to L^2(\mathbb{R}, E)$ are defined by the formulae

$$\mathscr{F}_+ : h \mapsto -\frac{1}{\sqrt{2\pi}} \alpha\Gamma_0(A_+ - k + \mathrm{i}0)^{-1}u + S_+^*(k)\hat{v}_-(k) + \hat{v}_+(k),$$
$$\mathscr{F}_- : h \mapsto -\frac{1}{\sqrt{2\pi}} \alpha\Gamma_0(A_+^* - k - \mathrm{i}0)^{-1}u + \hat{v}_-(k) + S_+(k)\hat{v}_+(k),$$

where $h = (v_-, u, v_+) \in \mathcal{H}$ and $\hat{v}_\pm$ are the Fourier transforms of $v_\pm \in L^2(\mathbb{R}_\pm, E)$.

Using the Kreĭn formulae, which play the same role as Hilbert resolvent identities in the case of additive perturbations, one can obtain results similar to those of [97] and obtain an explicit description of $(A_+ - z)^{-1}$ in the functional model representation. An analogue of this result for more general extensions of A corresponding to a choice of parameter B in the form $B_R + \alpha\varkappa\alpha/2$ with bounded $\varkappa : E \to E$ and $B_R = B_R^*$ is proven along the same lines. This program was realized in [118] for a particular case $\varkappa = \mathrm{i}J$ and in [47] for the family of extensions $A_\varkappa$ parameterized by $B_\varkappa = \alpha\varkappa\alpha/2$. The latter form of extension parameter utilizes the possibility of "absorbing" the part $B_R = B_R^*$ into the map Γ_1, i. e., passing from the boundary triple $\{\mathcal{K}, \Gamma_0, \Gamma_1\}$ to the triple $\{\mathcal{K}, \Gamma_0, \Gamma_1 + B_R\Gamma_0\}$.

2.3.4 Smooth vectors and the absolutely continuous subspace

Here we characterise the absolutely continuous spectral subspace for an almost solvable extension of a densely defined symmetric operator with equal (possibly infinite) deficiency indices. The procedure we follow is heavily influenced by the ideas of Sergey Naboko, see [97, 99] and is carried out essentially in parallel to the exposition of [97]. In contrast to the mentioned works, dealing with additive perturbations of self-adjoint operators, we are dealing with the case of extensions, self-adjoint and non-self-adjoint alike. The narrative below follows the argument presented in our papers [46, 47].

Since we are not limiting the consideration to the case of self-adjoint operators, we first require the notion of the absolutely continuous spectral subspace applicable in the non-self-adjoint setup. In the functional model space $\mathscr{H}$ introduced in Section 2.2.3 constructed based on the characteristic function $S(z)$ introduced in Section 2.3.2 consider two subspaces $\mathscr{N}_\pm^\varkappa$ defined as follows:

$$\mathscr{N}_\pm^\varkappa := \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathscr{H} : P_\pm \left(\chi_\varkappa^+(\widetilde{g} + S^*g) + \chi_\varkappa^-(S\widetilde{g} + g) \right) = 0 \right\},$$

where

$$\chi_\varkappa^\pm := \frac{I \pm \mathrm{i}\varkappa}{2}.$$

and $P_\pm$ are orthogonal projections onto their respective Hardy classes, as above.

These subspaces have a characterisation in terms of the resolvent of the operator $A_\varkappa$. This, again, can be seen as a consequence of a much more general argument (see *e.g.* [116, 118]).

Theorem 2.3. *Suppose that* $\ker \alpha = 0$. *The following characterisation holds:*

$$\mathscr{N}_\pm^\varkappa = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathscr{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{k-z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \ \textit{for all } z \in \mathbb{C}_\pm \right\}.$$

Here Φ *denotes the unitary mapping of the dilation space* $\mathcal{H}$ *onto* $\mathscr{H}$, *as above.*

Consider the counterparts of $\mathscr{N}_\pm^\varkappa$ in the original Hilbert space H :

$$\widetilde{N}_\pm^\varkappa := \Phi^* P_K \mathscr{N}_\pm^\varkappa ,$$

which are linear sets albeit not necessarily subspaces. In a way similar to [97], one introduces the set

$$\widetilde{N}_{\mathrm{e}}^\varkappa := \widetilde{N}_+^\varkappa \cap \widetilde{N}_-^\varkappa$$

of so-called *smooth vectors* and its closure $N_{\mathrm{e}}^\varkappa := \operatorname{clos}(\widetilde{N}_{\mathrm{e}}^\varkappa)$.

The next assertion (*cf. e.g.* [116, 118], for the case of general non-selfadjoint operators), is an alternative non-model characterisation of the linear sets $\widetilde{N}_\pm^\varkappa$.

Theorem 2.4. *The sets* $\widetilde{N}_\pm^\varkappa$ *are described as follows:*

$$\widetilde{N}_\pm^\varkappa = \{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\}.$$

Moreover, one shows that for the functional model image of $\tilde{N}_{\mathrm{e}}^\varkappa$ the following representation holds:

$$\Phi\widetilde{N}_{\mathrm{e}}^\varkappa = \left\{ P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathscr{H} : \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathscr{H} \text{ satisfies } \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{k-z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \quad \forall z \in \mathbb{C}_- \cup \mathbb{C}_+ \right\}, \tag{14}$$

which motivates the term "the set of smooth vectors" used for $\widetilde{N}_{\mathrm{e}}^\varkappa$. (Note that the inclusion of the right-hand side of (14) into $\Phi\widetilde{N}_{\mathrm{e}}^\varkappa$ follows immediately from Theorem 2.3.)

The above Theorem together with Theorem 2.5 below motivates generalising the notion of the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ to the case of non-selfadjoint extensions $A_\varkappa$ of a symmetric operator A, by identifying it with the set $N_{\mathrm{e}}^\varkappa$. This generalisation follows in the footsteps of the corresponding definition by Naboko [97] in the case of additive perturbations (see also [116, 118] for the general case).

Definition 2.4. *For a symmetric operator* A, *in the case of a non-selfadjoint extension* $A_\varkappa$ *the absolutely continuous subspace* $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ *is defined by the formula* $\mathcal{H}_{\mathrm{ac}}(A_\varkappa) := N_{\mathrm{e}}^\varkappa$.

In the case of a self-adjoint extension $A_\varkappa$, *we understand* $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ *in the sense of the classical definition of the absolutely continuous subspace of a self-adjoint operator.*

It turns out that in the case of self-adjoint extensions a rather mild additional condition guarantees that the non-self-adjoint definition above is equivalent to the classical self-adjoint one. Namely, we have the following

Theorem 2.5. *Assume that* $\varkappa = \varkappa^*$, $\ker(\alpha) = \{0\}$ *and let* $\alpha\Gamma_0(A_\varkappa - zI)^{-1}$ *be a Hilbert-Schmidt operator for at least one point* $z \in \rho(A_\varkappa)$. *If* A *is completely non-selfadjoint, then the definition* $\mathcal{H}_{\rm ac}(A_\varkappa) = N_{\rm e}^\varkappa$ *is equivalent to the classical definition of the absolutely continuous subspace of a self-adjoint operator, i.e.*

$$N_{\rm e}^\varkappa = \mathcal{H}_{\rm ac}(A_\varkappa)\,.$$

Remark 1. *Alternative conditions, which are even less restrictive in general, that guarantee the validity of the assertion of Theorem 2.5 can be obtained along the lines of [99].*

2.3.5 Wave and scattering operators

The results of the preceding section allow us, see [46, 47], to calculate the wave operators for any pair $A_{\varkappa_1}, A_{\varkappa_2}$, where $A_{\varkappa_1}$ and $A_{\varkappa_2}$ are two different extensions of a symmetric operator A, under the additional assumption that the operator α has a trivial kernel. For simplicity, in what follows we set $\varkappa_2 = 0$ and write $\varkappa$ instead of $\varkappa_1$. Note that A_0 is a self-adjoint operator, which is convenient for presentation purposes.

In order to compute the wave operators of this pair, one first establishes the model representation for the function $\exp(iA_\varkappa t)$, $t \in \mathbb{R}$, of the operator $A_\varkappa$, evaluated on the set of smooth vectors $\widetilde{N}_{\rm e}^\varkappa$. Due to (14), it is easily shown that on this set $\exp(iA_\varkappa t)$ acts as an operator of multiplication by $\exp(ikt)$. We then utilise the following result.

Proposition 2.6. *([97, Section 4]) If* $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^\varkappa$ *and* $\Phi^* P_K\binom{\widehat{g}}{g} \in \widetilde{N}_{\rm e}^0$ *(with the same element*[1] g*), then*

$$\left\|\exp(-{\rm i}A_\varkappa t)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - \exp(-{\rm i}A_0 t)\Phi^* P_K\begin{pmatrix}\widehat{g}\\ g\end{pmatrix}\right\|_{\mathscr{H}} \xrightarrow[t\to-\infty]{} 0.$$

It follows from Proposition 2.6 that whenever $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^\varkappa$ and $\Phi^* P_K\binom{\widehat{g}}{g} \in \widetilde{N}_{\rm e}^0$ (with the same second component g), formally one has

$$\begin{aligned}\lim_{t\to-\infty} {\rm e}^{{\rm i}A_0 t}{\rm e}^{-{\rm i}A_\varkappa t}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} &= \Phi^* P_K\begin{pmatrix}\widehat{g}\\ g\end{pmatrix}\\ &= \Phi^* P_K\begin{pmatrix}-(I+S)^{-1}(I+S^*)g\\ g\end{pmatrix}.\end{aligned}$$

In view of the classical definition of the wave operator of a pair of self-adjoint operators, see *e.g.* [75],

$$W_\pm(A_0, A_\varkappa) := \operatorname*{s-lim}_{t\to\pm\infty} {\rm e}^{{\rm i}A_0 t}{\rm e}^{-{\rm i}A_\varkappa t}P_{\rm ac}^\varkappa,$$

where $P_{\rm ac}^\varkappa$ is the projection onto the absolutely continuous subspace of $A^\varkappa$, we obtain that, at least formally, for $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^\varkappa$ one has

$$W_-(A_0, A_\varkappa)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\begin{pmatrix}-(I+S)^{-1}(I+S^*)g\\ g\end{pmatrix}. \tag{15}$$

[1] Despite the fact that $\binom{\widetilde{g}}{g} \in \mathscr{H}$ is nothing but a symbol, still $\widetilde{g}$ and g can be identified with vectors in certain $L^2(E)$ spaces with operators "weights", see details below in Section 2.3.6. Further, we recall that even then for $\binom{\widetilde{g}}{g} \in \mathscr{H}$, the components $\widetilde{g}$ and g are not, in general, *independent* of each other.

By considering the case $t \to +\infty$, one also obtains

$$W_+(A_0, A_\varkappa)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \lim_{t \to +\infty} \mathrm{e}^{\mathrm{i}A_0 t} \mathrm{e}^{-\mathrm{i}A_\varkappa t} \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -(I+S^*)^{-1}(I+S)\widetilde{g} \end{pmatrix}$$

again for $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$.

Further, the definition of the wave operators $W_\pm(A_\varkappa, A_0)$

$$\left\| \mathrm{e}^{-\mathrm{i}A_\varkappa t} W_\pm(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - \mathrm{e}^{-\mathrm{i}A_0 t}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathscr{H}} \xrightarrow[t \to \pm\infty]{} 0$$

yields, for all $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$,

$$W_-(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} -(I+\chi_\varkappa^-(S-I))^{-1}(I+\chi_\varkappa^+(S^*-I))g \\ g \end{pmatrix}$$

and

$$W_+(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -(I+\chi_\varkappa^+(S^*-I))^{-1}(I+\chi_\varkappa^-(S-I))\widetilde{g} \end{pmatrix}. \tag{16}$$

In order to rigorously justify the above formal argument, *i.e.* in order to prove the existence and completeness of the wave operators, one needs to first show that the right-hand sides of the formulae (15)–(16) make sense on dense subsets of the corresponding absolutely continuous subspaces, which is done in a similar way to [99]. Below, we show how this argument works in relation to the wave operator (15) only, skipping the technical details in view of making the exposition more transparent.

Let $S(z) - I$ be of the class $\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, *i.e.* a compact analytic operator function in the upper half-plane up to the real line. Then so is $(S(z)-I)/2$, which is also uniformly bounded in the upper half-plane along with $S(z)$. We next use the result of [99, Theorem 3] about the non-tangential boundedness of operators of the form $(I+T(z))^{-1}$ for $T(z)$ compact up to the real line. We infer that, provided $(I+(S(z_0)-I)/2)^{-1}$ exists for some $z_0 \in \mathbb{C}_+$ (and hence, see [32], everywhere in $\mathbb{C}_+$ except for a countable set of points accumulating only to the real line), one has non-tangential boundedness of $(I+(S(z)-I)/2)^{-1}$, and therefore also of $(I+S(z))^{-1}$, for almost all points of the real line.

On the other hand, the latter inverse can be computed in $\mathbb{C}_+$:

$$\big(I+S(z)\big)^{-1} = \frac{1}{2}\big(I + \mathrm{i}\alpha M(z)^{-1}\alpha/2\big). \tag{17}$$

It follows from (17) and the analytic properties of $M(z)$ that the inverse $(I+S(z))^{-1}$ exists everywhere in the upper half-plane. Thus, Theorem 3 of [99] is indeed applicable, which yields that $(I+S(z))^{-1}$ is $\mathbb{R}$-a.e. nontangentially bounded and, by the operator generalisation of the Calderon theorem (see [125]), which was extended to the operator context in [99, Theorem 1], it admits measurable non-tangential limits in the strong operator topology almost everywhere on $\mathbb{R}$. As it is easily seen, these limits must then coincide with $(I+S(k))^{-1}$ for almost all $k \in \mathbb{R}$.

Then the correctness of the formula (15) for the wave operators follows: indeed, consider $\mathbb{1}_n(k)$, the indicator of the set $\{k \in \mathbb{R} : \|(I+S(k))^{-1}\| \le n\}$. Clearly, $\mathbb{1}_n(k) \to 1$ as $n \to \infty$ for almost all $k \in \mathbb{R}$. Next, suppose that $P_K(\tilde{g}, g) \in \tilde{N}_{\mathrm{e}}^{\varkappa}$. Then $P_K \mathbb{1}_n(\tilde{g}, g)$ is shown to be a smooth vector as well as

$$\begin{pmatrix} -(I+S)^{-1}\mathbb{1}_n(I+S^*)g \\ \mathbb{1}_n g \end{pmatrix} \in \mathscr{H}.$$

It follows, by the Lebesgue dominated convergence theorem, that the set of vectors $P_K \mathbb{1}_n(\tilde{g}, g)$ is dense in $N_{\rm e}^{\varkappa}$.

Thus the following theorem holds.

Theorem 2.7. *Let A be a closed, symmetric, completely nonselfadjoint operator with equal deficiency indices and consider its extension $A_\varkappa$ under the assumptions that $\ker(\alpha) = \{0\}$ and that $A_\varkappa$ has at least one regular point in $\mathbb{C}_+$ and in $\mathbb{C}_-$. If $S - I \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, then the wave operators $W_\pm(A_0, A_\varkappa)$ and $W_\pm(A_\varkappa, A_0)$ exist on dense sets in $N_{\rm e}^{\varkappa}$ and $\mathcal{H}_{\rm ac}(A_0)$, respectively, and are given by the formulae (15)–(16). The ranges of $W_\pm(A_0, A_\varkappa)$ and $W_\pm(A_\varkappa, A_0)$ are dense in $\mathcal{H}_{\rm ac}(A_0)$ and $N_{\rm e}^{\varkappa}$, respectively.*[2]

Remark 2. *1. The condition $S(z) - I \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ can be replaced by the following equivalent condition: $\alpha M(z)^{-1}\alpha$ is nontangentially bounded almost everywhere on the real line, and $\alpha M(z)^{-1}\alpha \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ for $\Im z \geq 0$.*

2. The latter condition is satisfied [66], as long as the scalar function $\|\alpha M(z)^{-1}\alpha\|_{\mathfrak{S}_p}$ is nontangentially bounded almost everywhere on the real line for some $p < \infty$, where $\mathfrak{S}_p$, $p \in (0, \infty]$, are the standard Schatten – von Neumann classes of compact operators.

3. An alternative sufficient condition is the condition $\alpha \in \mathfrak{S}_2$ (and therefore $B_\varkappa \in \mathfrak{S}_1$), or, more generally, $\alpha M(z)^{-1}\alpha \in \mathfrak{S}_1$, see [98] for details.

Finally, the scattering operator Σ for the pair $A_\varkappa$, A_0 is defined by

$$\Sigma = W_+^{-1}(A_\varkappa, A_0) W_-(A_\varkappa, A_0).$$

The above formulae for the wave operators lead (*cf.* [97]) to the following formula for the action of Σ in the model representation:

$$\Phi \Sigma \Phi^* P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = P_K \begin{pmatrix} -(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \\ (I + S^*)^{-1}(I + S)(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \end{pmatrix}, \tag{18}$$

whenever $\Phi^* P_K \binom{\tilde{g}}{g} \in \widetilde{N}_{\rm e}^0$. In fact, as explained above, this representation holds on a dense linear set in $\widetilde{N}_{\rm e}^0$ within the conditions of Theorem 2.7, which guarantees that all the objects on the right-hand side of the formula (18) are correctly defined.

2.3.6 Spectral representation for the absolutely continuous part of the operator A_0 and the scattering matrix

The identity

$$\left\| P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\|_{\mathscr{H}}^2 = \langle (I - S^*S)\tilde{g}, \tilde{g} \rangle$$

which is derived in [97, Section 7] for all $P_K \binom{\tilde{g}}{g} \in \widetilde{N}_{\rm e}^0$ allows us to consider the isometry $F : \Phi \widetilde{N}_{\rm e}^0 \mapsto L^2(E; I - S^*S)$ defined by the formula

$$F P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = \tilde{g}.$$

[2] In the case when $A_\varkappa$ is self-adjoint, or, in general, the named wave operators are bounded, the claims of the theorem are equivalent (by the classical Banach-Steinhaus theorem) to the statement of the existence and completeness of the wave operators for the pair $A_0, A_\varkappa$. Sufficient conditions of boundedness of these wave operators are contained in *e.g.* [97, Section 4], [99] and references therein.

Here $L^2(E; I - S^*S)$ is the Hilbert space of E-valued functions on $\mathbb{R}$ square summable with the matrix "weight" $I - S^*S$.

Under the assumptions of Theorem 2.7 one can show that the range of the operator F is dense in the space $L^2(E; I - S^*S)$. Thus, the operator F admits an extension to the unitary mapping between $\Phi N_{\rm e}^0$ and $L^2(E; I - S^*S)$.

It follows that the self-adjoint operator $(A_0 - z)^{-1}$ considered on $\widetilde{N}_{\rm e}^0$ acts as the multiplication by $(k - z)^{-1}$, $k \in \mathbb{R}$, in $L^2(E; I - S^*S)$. In particular, if one considers the absolutely continuous "part" of the operator A_0, namely the operator $A_0^{(\rm e)} := A_0|_{N_{\rm e}^0}$, then $F\Phi A_0^{(\rm e)}\Phi^* F^*$ is the operator of multiplication by the independent variable in the space $L^2(E; I - S^*S)$.

In order to obtain a spectral representation from the above result, it is necessary to diagonalise the "weight" in the definition of the above L^2-space. The corresponding transformation is straightforward when, e.g., $\alpha = \sqrt{2}I$. (This choice of α satisfies the conditions of Theorem 2.7 *e.g.* when the boundary space $\mathcal{K}$ is finite-dimensional). In this particular case one has

$$S = (M - {\rm i}I)(M + {\rm i}I)^{-1},$$

and consequently

$$I - S^*S = -2i(M^* - {\rm i}I)^{-1}(M - M^*)(M + {\rm i}I)^{-1}.$$

Introducing the unitary transformation

$$G : L^2(E; I - S^*S) \mapsto L^2(E; -2{\rm i}(M - M^*)),$$

by the formula $g \mapsto (M + {\rm i}I)^{-1}g$, one arrives at the fact that $GF\Phi A_0^{(\rm e)}\Phi^* F^* G^*$ is the operator of multiplication by the independent variable in the space $L^2(E; -2{\rm i}(M - M^*))$.

Remark 3. *The weight $M^* - M$ can be assumed to be naturally diagonal in many physically relevant settings, including the setting of quantum graphs considered in Section 3.*

The above result only pertains to the absolutely continuous part of the self-adjoint operator A_0, unlike *e.g.* the passage to the classical von Neumann direct integral, under which the whole of the self-adjoint operator gets mapped to the multiplication operator in a weighted L^2-space (see *e.g.* [27, Chapter 7]). Nevertheless, it proves useful in scattering theory, since it yields an explicit expression for the scattering matrix $\widehat{\Sigma}$ for the pair $A_\varkappa$, A_0, which is the image of the scattering operator Σ in the spectral representation of the operator A_0. Namely, one arrives at:

Theorem 2.8. *The following formula holds:*

$$\widehat{\Sigma} = GF\Sigma(GF)^* = (M - \varkappa)^{-1}(M^* - \varkappa)(M^*)^{-1}M, \tag{19}$$

where the right-hand side represents the operator of multiplication by the corresponding function in the space $L^2(E; -2{\rm i}(M - M^*))$.

2.4 Functional models for operators of boundary value problems

The surjectivity condition in Definition 2.1 is a strong limitation that excludes many important problems for extensions of symmetric operators with infinite deficiency indices. The standard textbook version of a boundary value problem for the Laplace operator in a bounded domain $\Omega \subset \mathbb{R}^3$ with smooth boundary $\partial\Omega$ is a typical example. The "natural" boundary maps Γ_0 and Γ_1 are two trace operators $\Gamma_0 : u \mapsto u|_{\partial\Omega}$, $\Gamma_1 : u \mapsto -\partial u/\partial n|_{\partial\Omega}$, where $\partial/\partial n$ denotes the derivative along the exterior normal to the boundary $\partial\Omega$. The ranges of these operators do not coincide with $\mathcal{H} = L^2(\Omega)$ (the simplest possible Hilbert space of functions defined on the boundary) so the assumption of surjectivity does not hold. A simple argument reveals the source of this problem: it appears due to the limited compatibility of the Green's formula required to hold on all of $\mathrm{dom}(A^*)$ and the required surjectivity of both boundary maps Γ_0, Γ_1 also defined on the same domain $\mathrm{dom}(A^*)$. This limitation of the boundary triples formalism can be relaxed and the framework extended to cover more general cases, albeit at the cost of increased complexity, see [17, 18], the book [20] and the references therein for a detailed account.

Formally a more restrictive approach applicable to semibounded symmetric operators A and not based on the description of $\mathrm{dom}\, A^*$ was developed by M. Birman, M. Kreĭn and M. Vishik. Despite its limited scope, this theory proves to be indispensable in applications to various problems of ordinary and partial differential operators. The publication [5] contains a concise exposition of these results. It was realized later that the Birman-Kreĭn-Vishik method is closely related to the theory of linear systems with boundary control and to the original ideas of M. Livšic from the open systems theory, see e. g. [119, 120] in this connection. Let us give a brief account of relevant results derived from the works cited above and tailored to the purposes of current presentation.

2.4.1 Boundary value problem

Let H, E be two separable Hilbert spaces, A_0 an unbounded closed linear operator on H with the dense domain $\mathrm{dom}\, A_0$ and $\Pi : E \to H$ a bounded linear operator defined everywhere in E.

Theorem 2.9. *Assume the following:*

- *A_0 is self-adjoint and boundedly invertible;*
- *There exists the left inverse $\tilde{\Gamma}_0$ of Π so that $\tilde{\Gamma}_0\Pi\varphi = \varphi$ for all $\varphi \in E$;*
- *The intersection of $\mathrm{dom}\, A_0$ and $\mathrm{ran}\, \Pi$ is trivial: $\mathrm{dom}\, A_0 \cap \mathrm{ran}\, \Pi = \{0\}$.*

Since $\mathrm{dom}\, A_0$ and $\mathrm{ran}\, \Pi$ have trivial intersection, the direct sum $\mathrm{dom}\, A_0 \dot{+} \mathrm{ran}\, \Pi$ form a dense linear set in H that can be described as $\{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in E\}$. Define two linear operators A and Γ_0 with the common domain $\mathrm{dom}\, A_0 \dot{+} \mathrm{ran}\, \Pi$ as "null extensions" of A_0 and $\tilde{\Gamma}_0$ to the complementary component of $\mathrm{dom}\, A_0 \dot{+} \mathrm{ran}\, \Pi$

$$A : A_0^{-1}f + \Pi\varphi \mapsto f, \quad \Gamma_0 : A_0^{-1}f + \Pi\varphi \mapsto \varphi, \qquad f \in H, \varphi \in E$$

The spectral "boundary value problem" associated with the pair $\{A_0, \Pi\}$ satisfying these conditions is the system of two linear equations for the unknown vector $u \in \mathrm{dom}\, A := \mathrm{dom}\, A_0 \dot{+} \mathrm{ran}\, \Pi$:

$$\begin{cases} (A - zI)u = f \\ \Gamma_0 u = \varphi \end{cases} \qquad f \in H, \quad \varphi \in E, \tag{20}$$

where $z \in \mathbb{C}$ is the spectral parameter.

Let $z \in \rho(A_0)$, $f \in H$, $\varphi \in E$. Then the system (20) admits the unique solution $u_z^{f,\varphi}$ given by the formula

$$u_z^{f,\varphi} = (A_0 - zI)^{-1}f + (I - zA_0^{-1})^{-1}\Pi\varphi$$

If the expression on the right hand side is null for some $f \in H$, $\varphi \in E$, then $f = 0$ and $\varphi = 0$.

Let Λ be a linear operator on E with the domain $\operatorname{dom}\Lambda \subset E$ not necessarily dense in E. Define the linear operator Γ_1 on $\operatorname{dom}\Gamma_1 := \{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \operatorname{dom}\Lambda\}$ as the mapping

$$\Gamma_1 : A_0^{-1}f + \Pi\varphi \mapsto \Pi^* f + \Lambda\varphi, \qquad f \in H, \quad \varphi \in \operatorname{dom}\Lambda$$

This definition implies $\Lambda = \Gamma_1 \Pi|_{\operatorname{dom}\Lambda}$.

Denote $\mathscr{D} := \operatorname{dom}\Gamma_1 = \{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \operatorname{dom}\Lambda\}$. Obviously $\mathscr{D} \subset \operatorname{dom} A$. The next theorem is a form of the Green's formula for the operator A.

Theorem 2.10. *Assume that Λ is selfadjoint (and therefore densely defined) in E. Then*

$$(Au, v) - (u, Av) = (\Gamma_1 u, \Gamma_0 v)_E - (\Gamma_0 u, \Gamma_1 v)_E, \qquad u, v \in \mathscr{D}$$

Notice the difference with the boundary triples version (11), where the operator on the left hand side is the adjoint of a symmetric operator. In contrast, Theorem 2.10 has no relation to symmetric operators. The Green's formula is valid on a set defined by the selfadjoint A_0 and an arbitrarily chosen selfadjoint operator Λ.

Under the assumptions of Theorems 2.9 and 2.10 the operator-valued analytic function

$$M(z) = \Lambda + z\Pi^*(I - zA_0^{-1})^{-1}\Pi, \quad z \in \rho(A_0)$$

defined on $\operatorname{dom} M(z) = \operatorname{dom}\Lambda$ is the Weyl function (cf. [20]) of the boundary value problem (20) in the sense of equality (cf. Definition 2.2)

$$M(z)\Gamma_0 u_z = \Gamma_1 u_z, \quad z \in \rho(A_0)$$

where $u_z = u_z^{f,\varphi}$ is the solution to (20) with $f = 0$ and $\varphi \in \operatorname{dom}\Lambda$.

For the boundary value problem pertaining to the Laplace operator in a bounded domain $\Omega \subset \mathbb{R}^3$ with a smooth boundary $\partial\Omega$ the boundary maps Γ_0, Γ_1 are defined as $\Gamma_0 : u \mapsto u|_{\partial\Omega}$, $\Gamma_1 : u \mapsto -\partial u/\partial n|_{\partial\Omega}$. Then A_0 is the Dirichlet Laplacian in $L^2(\Omega)$ and Π is the operator of harmonic continuation from the boundary space $E = L^2(\partial\Omega)$ to Ω. The conditions $\operatorname{dom}(A_0) \cap \operatorname{ran}(\Pi) = \{0\}$ and $\Gamma_0\Pi = I_E$ are satisfied by virtue of the embedding theorems for Sobolev classes. In this setting $M(\cdot)$ is known as the Dirichlet-to-Neumann map, which is a pseudodifferential operator defined on $H^1(\partial\Omega)$. A special role of the operator $\Lambda = M(0)$ for the study of boundary value problems was pointed out by M. Vishik in his work [135] and sometimes Λ in the settings of elliptic partial differential operators is referred to as the *Vishik operator*.

2.4.2 Family of boundary value problems

General boundary value problems for the operator A have the form (cf. [135])

$$\begin{cases} (A - zI)u = f \\ (\alpha\Gamma_0 + \beta\Gamma_1)u = \varphi \end{cases} \qquad f \in H, \quad \varphi \in E. \tag{21}$$

Here α, β are linear operators on E such that β is bounded (and defined everywhere in E) and α can be unbounded in which case $\operatorname{dom}\alpha \supset \operatorname{dom}\Lambda = \mathscr{D}$. Under certain verifiable conditions the solutions to (21) exist and are described by the following theorem.

Theorem 2.11 (see [120]). *Assume that the conditions of Theorems 2.9 and 2.10 are satisfied and that the operator sum* $\alpha + \beta\Lambda$ *is correctly defined on* $\operatorname{dom}\Lambda$ *and closable in* E*. Then* $\alpha + \beta M(z)$*,* $z \in \rho(A_0)$ *is also closable as an additive perturbation of* $\alpha + \beta\Lambda$ *by the bounded operator* $M(z) - \Lambda$*. Denote by* $\mathscr{B}(z)$ *the closure of* $\alpha + \beta M(z)$*,* $z \in \rho(A_0)$ *and let* $\mathscr{B} = \mathscr{B}(0)$*.*

- *Consider the Hilbert space* $\mathscr{H}_{\mathscr{B}}$ *formed by the vectors* $\left\{u = A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \operatorname{dom}\mathscr{B}\right\}$ *and endowed with the norm*

$$\|u\|_{\mathscr{B}} = \left(\|f\|^2 + \|\varphi\|^2 + \|\mathscr{B}\varphi\|^2\right)^{1/2}$$

  The formal sum $\alpha\Gamma_0 + \beta\Gamma_1$ *is a bounded map from the Hilbert space* $\mathscr{H}_{\mathscr{B}}$ *to* E*. Note that the summands in* $(\alpha\Gamma_0 + \beta\Gamma_1)u$*,* $u \in \mathscr{H}_{\mathscr{B}}$ *need not be defined individually.*

- *Assume that for some* $z \in \rho(A_0)$ *the operator* $\mathscr{B}(z)$ *has a bounded inverse* $[\mathscr{B}(z)]^{-1}$*. Then the problem (21) is uniquely solvable. Under this condition there exists a closed operator* $A_{\alpha,\beta}$ *with dense domain*

$$\operatorname{dom} A_{\alpha,\beta} = \{u \in \mathscr{H}_{\mathscr{B}} \mid (\alpha\Gamma_0 + \beta\Gamma_1)u = 0\} = \operatorname{Ker}(\alpha\Gamma_0 + \beta\Gamma_1)$$

  and the resolvent (Kreĭn formula) holds:

$$(A_{\alpha,\beta} - zI)^{-1} = (A_0 - zI)^{-1} - (I - zA_0^{-1})^{-1}\Pi[\mathscr{B}(z)]^{-1}\beta\Pi^*(I - zA_0^{-1})^{-1}$$

- *Denote by* A_{00} *the restriction of* A_0 *to the set* $\operatorname{Ker}\Gamma_1$*, that is,* $A_{00} = A|_{\operatorname{Ker}\Gamma_0 \cap \operatorname{Ker}\Gamma_1}$*. Then* A_{00} *is a symmetric operator with its domain not necessarily dense in* H *and*

$$A_{00} \subset A_{\alpha,\beta} \subset A$$

Notice that A_0 is a self-adjoint extension of A_{00} contained in A. It is not difficult to recognize the parallel with the von Neumann theory of self-adjoint extensions of symmetric operators. The operator A_{00} is the "minimal" operator with the "maximal" equal to A_{00}^* (whenever the latter exists) and all self-adjoint extensions $A_{s.a.}$ of A_{00} satisfy $A_{00} \subset A_{s.a.} \subset A_{00}^*$. Within the framework of Theorem 2.11 the equivalent of A_{00}^* is the operator A of the boundary value problem (20) defined on the domain $\operatorname{dom}(A)$. The semiboundness condition for A_{00} is relaxed and replaced by the bounded invertibility of A_0, i. e., the existence of a regular point of A_0 on the real line.

2.4.3 Functional model

The results of previous sections hint at the possibility of a functional model construction for the family of operators $A_{\alpha,\beta}$ with a suitably chosen pair (α, β). Having in mind the model space (9), the selection of a "close" dissipative operator is typically guided by the properties of the problem at hand. In the most general case when parameters (α, β) are unspecified, a reasonable approach seems to be to construct a model suitable for the widest possible range of (α, β). In accordance with the work by S. Naboko [97], the action of the operator $A_{\alpha,\beta}$ will then be explicitly described in the functional model representation.

This program is realized in the recent paper [48]. The "model" dissipative operator $L = A_{-iI,I}$ corresponds to the boundary condition $(\Gamma_1 - i\Gamma_0)u = 0$ for $u \in \operatorname{dom}(L)$ in the notation (21). The characteristic function of L then coincides with the Cayley transform of the Weyl function,

$$S(z) = (M(z) - \mathrm{i}I)(M(z) + \mathrm{i}I)^{-1} : E \to E, \quad z \in \mathbb{C}_+.$$

Under the mapping of the upper half plane to the unit disk, the function $S((z-\mathrm{i})/(z+\mathrm{i}))$ is the Sz.Nagy-Foiaş characteristic function of a contraction, namely, the Cayley transform V_0 of A_{00} extended to $H \ominus \mathrm{dom}(V_0)$ by the null operator, hence resulting in a partial isometry. If A_{00} has no non-trivial self-adjoint parts, the dissipative operator $L = A_{-\mathrm{i}I,I}$ is also completely non-selfadjoint. The standard assumptions of complete non-selfadjointness and maximality of L are thus met. The minimal self-adjoint dilation $\mathscr{A}$ of L formally coincides with the dilation obtained in Section 2.3.3 for the case of boundary triples with $A_+^* = A$, $B_+ = \mathrm{i}I_E$, $B_+^* = -\mathrm{i}I_E$ and $\alpha = \sqrt{2}I_E$.

The description of operators $A_{\alpha,\beta}$ in the spectral representation of dilation $\mathscr{A}$, i.e. in the model space (9), cannot be easily obtained for arbitrary (α, β). However, under certain conditions imposed on the parameters (α, β) the model construction becomes tractable. Namely, one assumes that the operator β is boundedly invertible, the operator $B = \beta^{-1}\alpha$ is bounded in E and that the operator-valued function $M(z)$ is invertible and $BM(z)^{-1}$ is compact at least for some z in the upper and lower half-plane of $\mathbb{C}$ (and therefore for all $z \in \mathbb{C} \setminus \mathbb{R}$).

It follows, that the operator $A_{\alpha,\beta}$ has at most discrete spectrum in $\mathbb{C} \setminus \mathbb{R}$ with possible accumulation to the real line only. Moreover, the resolvent set of $A_{\alpha,\beta}$ coincides with the open set of complex numbers $z \in \mathbb{C}$ such that the closed operator $\overline{B + M(z)}$ has a bounded inverse, i. e. $\rho(A_{\alpha,\beta}) = \{z \in \mathbb{C} \mid 0 \in \rho(\overline{B + M(z)})\}$.

Finally, the model representation of the resolvent $(A_{\alpha,\beta} - zI)^{-1}$, $z \in \rho(A_{\alpha,\beta})$ is explicitly computed in the model space (9).

Once the latter are established, it is natural to expect that the absolutely continuous subspaces can be characterised for the operators of boundary value problems in the case of exterior domains and the scattering theory can then be constructed following the recipe of Naboko, as presented in Section 2.2. If this programme is pursued, this would yield a natural representation of the corresponding scattering matrix purely in terms of the $M-$operator defined above. A paper devoted to this subject is presently being prepared for publication.

2.5 Generalised resolvents

In the present Section, we briefly recall the notion of generalised resolvents (see [7] for details) of symmetric operators, which play a major role in the asymptotic analysis of highly inhomogeneous media as presented in the present paper. It turns out that generalised resolvents and their underlying self-adjoint operators in larger (dilated) spaces feature prominently in our approach; moreover, their setup turns out to be natural in the theory of time-dispersive and frequency-dispersive media. On the mathematical level, this area is closely interrelated with the theory of dilations and functional models of dissipative operators, the latter (at least, in the case of dissipative extensions of symmetric operators) being an important particular case of the former.

We start with an operator-function $R(z)$ in the Hilbert space H, analytic in $z \in \mathbb{C}_+$. Assuming that $\mathrm{Im}\, R(z) \geq 0$ for $z \in \mathbb{C}_+$, and under the well-known asymptotic condition

$$\limsup_{\tau \to +\infty} \tau \|R(\mathrm{i}\tau)\| < +\infty,$$

one has due to the operator generalisation of Herglotz theorem by Neumark [102]:

$$R(z) = \int_{-\infty}^{\infty} \frac{1}{t-z} dB(t),$$

where $B(t)$ is a uniquely defined left-continuous operator-function such that $B(-\infty) = 0$, $B(t_2) - B(t_1) \geq 0$ for $t_2 > t_1$ and $B(+\infty)$ bounded. By the argument of [59], it follows from the Neumark theorem [101,102] (cf., e.g., [98]) that there exists a bounded operator $X : \mathcal{H} \mapsto H$ with an auxiliary Hilbert space $\mathcal{H}$ and a self-adjoint operator $\mathcal{A}$ in $\mathcal{H}$ such that

$$R(z) = X(\mathcal{A} - z)^{-1}X^*$$

with

$$XX^* = \text{s-}\lim_{t\to+\infty} B(t) = \text{s-}\limsup_{\tau\to+\infty} \tau \operatorname{Im} R(i\tau).$$

A particular case of this result, see [126], holds when (a) for some $z_0 \in \mathbb{C}_+$ there exists a subspace $\mathfrak{L} \subset H$ such that (i) for all non-real z and all $f \in \mathfrak{L}$ one has

$$R(z)f - R(z_0)f = (z - z_0)R(z)R(z_0)f,$$

(ii) for any $z \in \mathbb{C}_+$ and any $g \in \mathfrak{L}^\perp$ one has

$$\|R(z)g\|^2 \leq \frac{1}{\operatorname{Im} z} \operatorname{Im}\langle R(z)g, g\rangle,$$

(iii) for all $g \in \mathfrak{L}^\perp$ the function $R(z)g$ is regular in $\mathbb{C}_+$; (b) $\overline{R(z_0)\mathfrak{L}} = H$.

Under these assumptions, the function $R(z)$ is ascertained to be a generalised resolvent of a densely defined symmetric operator A in H. Moreover, the deficiency index of A in $\mathbb{C}_+$ is equal to $\dim \mathfrak{L}^\perp$. Precisely, this means that $\mathcal{H} \supset H$ and $X = P$, where P is the orthogonal projection of $\mathcal{H}$ to H, i.e.,

$$R(z) = P(\mathcal{A} - z)^{-1}|_H, \quad \operatorname{Im} z \neq 0, \tag{22}$$

where $\mathcal{A}$ is a self-adjoint out-of-space extension of the symmetric operator A (or, alternatively, a zero-range model with an internal structure, see Section 4 below). Moreover, under the minimality condition $\bigvee_{\operatorname{Im} z\neq 0}(\mathcal{A} - z)^{-1}H = \mathcal{H}$, it is defined uniquely up to a unitary transform which acts as unity on H, see [101].

The latter representation takes precisely the same form as the dilation condition (3) in the case of maximal dissipative extensions of symmetric operators, with the generalised resolvent $R(z)$ replacing the resolvent of a dissipative operator. It is in fact shown that the property (22) generalises (3).

Namely, it turns out [126, 128] that

$$R(z) = (A_{B(z)} - z)^{-1} \text{ for } z \in \mathbb{C}_+ \cup \mathbb{C}_-.$$

Here in the particular case of equal deficiency indices, which is of interest to us from the point of view of zero-range models with an internal structure, $A_{B(z)}$ is a $z-$dependant extension of A such that there exists a boundary triple $(\mathscr{K}, \Gamma_0, \Gamma_1)$ defining this extension as follows:

$$\operatorname{dom} A_{B(z)} = \{u \in \operatorname{dom} A^* | \Gamma_1 u = B(z)\Gamma_0 u\}$$

with $B(z)$ being a $-R$ function (i.e., an analytic operator-function with a non-positive imaginary part in $\mathbb{C}_+$).

Because of $B^*(\bar{z}) = B(z)$, which is the standard extension of an $R-$function into $\mathbb{C}_-$ implied here, the extension $A_{B(z)}$ turns out to be dissipative for $z \in \mathbb{C}_-$ and anti-dissipative for $z \in \mathbb{C}_+$. We henceforth refer to $\mathcal{A}$ as the Neumark-Strauss dilation of the generalised resolvent $R(z) = (A_{B(z)} - z)^{-1}$. In a particular case of constant $B(z) = B$ such that $\operatorname{Im} B \leq 0$, we have

$$(A_B - z)^{-1} = P(\mathcal{A} - z)^{-1}|_H \text{ for } z \in \mathbb{C}_- \text{ and } (A_{B^*} - z)^{-1} = P(\mathcal{A} - z)^{-1}|_H \text{ for } z \in \mathbb{C}_+,$$

which are precisely (3) for both A_B and A_{B^*} at the same time.

From what has been said above it follows that generalised resolvents appear when one conceals certain degrees of freedom in a conservative physical system, either for the sake of convenience or because these are not known. In particular, we refer the reader to the papers [59, 60], where systems with time dispersion are analysed, with prescribed "memory" term. It turns out that passing over to the frequency domain one ends up with a generalised resolvent. It then proves possible to explicitly restore a conservative Hamiltonian (the operator $\mathcal{A}$ in our notation) which yields precisely the postulated time dispersion. In a nutshell, the idea here is to work with an explicit and simple enough model of the part of the space pertaining to the "hidden degrees of freedom" instead of the unnecessarily complicated physical equations which govern them. Similar ideas have been utilised in [131, 132]. The same technique has found its applications in numerics, and in particular in the so-called theory of absorbing boundary conditions, see, e.g., [53, 71].

The problem of constructing a spectral representation for a Neumark-Strauss dilation of a given generalised resolvent thus naturally arises. In a number of special cases, where $\mathcal{H}$ and $\mathcal{A}$ admit an explicit construction (and in particular one has $\mathcal{H} = H \oplus \mathbb{C}^k$ for $k \geq 1$), this can be done following essentially the same path as outlined in Section 2.3 above. This is due to the fact that in this case the operator $\mathcal{A}$ can be realised as a von Neumann extension of a symmetric operator in $\mathcal{H}$ with equal and finite deficiency indices. The corresponding construction in the case when $k = 1$ is presented in [45]. Surprisingly, this rather simple model already has a number of topical applications, see Sections 4 and 5 of the present paper, and also the papers [57, 81, 82], where a generalised resolvent of precisely the same class appears in the setting of thin networks converging to quantum graphs.

The generic case has been studied by Strauss in [129], where three spectral representations of the dilation are constructed, analogous to the ones of L. de Branges and J. Rovnyak, B. S. Pavlov, and B. Sz.-Nagy and C. Foiaş. These results however present but theoretical interest, as they are formulated in terms which apparently cannot be related to the original problem setup and are therefore not usable in applications.

A different approach was suggested by M. D. Faddeev and B. S. Pavlov in [112], where a problem originally studied by P. D. Lax and R. S. Phillips in [88] was considered. In [112], a five-component representation of the dilation was constructed, which further allowed to obtain the scattering matrix in an explicit form. It therefore comes as no surprise that, precisely as in the Lax-Phillips approach, the resonances are revealed to play a fundamental role in this analysis (cf. the analysis of the so-called Regge poles in the physics literature).

Later on, and again motivated in particular by applications to scattering, Neumark-Strauss dilations were constructed in some special cases by J. Behrndt et al., see [11, 19].

We remark that all the above results, except [45] and [129], have stopped short of attempting to construct a spectral form of the Neumark-Strauss dilation. Any generic construction leading to the latter and formulated in "natural" terms is presently unknown, to the best of our knowledge.

2.6 Universality of the model construction

The general form of the functional model of an unbounded closed operator [118] is a generalization of the special cases, as developed in the papers by B. Pavlov and S. Naboko cited above. This section aims to clarify the relationship between the models pertaining to different representations of the characteristic function of a non-selfadjoint operator. As an illustration, we consider two special cases of operators of mathematical physics described above and link them to the general model construction of [118].

2.6.1 Characteristic function of a linear operator [127]

Let L be a closed linear operator on a (separable) Hilbert space H with the domain $\mathrm{dom}(L)$. Consider the form $\Psi_L(\cdot,\cdot)$ defined on $\mathrm{dom}(L)\times\mathrm{dom}(L)$:

$$\Psi_L(f,g)=\frac{1}{\mathrm{i}}\left[(Lf,g)_H-(f,Lg)_H\right],\quad f,g\in\mathrm{dom}(L) \tag{23}$$

Definition 2.5. *The boundary space of L is a linear space E with a possibly indefinite scalar product $(\cdot,\cdot)_E$ such that there exists a closed linear operator Γ defined on $\mathrm{dom}(\Gamma)=\mathrm{dom}(L)$ and the following identity holds*

$$\Psi_L(f,g)=(\Gamma f,\Gamma g)_E,\quad f,g\in\mathrm{dom}(L) \tag{24}$$

The operator Γ is called the boundary operator of L.

This definition is meaningful for any linear operator on H. For the purposes of model construction, it is sufficient to focus only on the case when L is densely defined and dissipative. The model representation of a non-dissipative operator is given in the model space of an auxiliary dissipative one, as explained above. When L is dissipative, one has $\Psi_L(f,f)\geq 0$, $f\in\mathrm{dom}(L)$ and therefore the space E can be chosen as the Hilbert space obtained by factorization and completion of $\{\Gamma f\mid f\in\mathrm{dom}(L)\}$ with respect to the norm $\|\Gamma f\|_E$, $f\in\mathrm{dom}(L)$. Note that the boundary operator Γ defined in (24) is not uniquely defined. Due to the Hilbert structure of E, for any isometry π on E the operator $\pi\Gamma$ also satisfies the condition (24). Moreover, if (24) holds for some operator Γ' and space E', then there exists an isometry $\pi:E'\to E$ such that $\Gamma=\pi\Gamma'$.

Denote by E_* and Γ_* the boundary space and the boundary operator for the dissipative operator $-L^*$ endowed with the Hilbert metric. Assume that L is maximal, i. e., $\mathbb{C}_-\subset\rho(L)$. Then L^* is also maximal and $\mathbb{C}_+\subset\rho(L^*)$. The following definition is valid for general non-selfadjiont operators.

Definition 2.6. *Let E and Γ be the boundary space and the boundary operator for a closed densely defined operator L. Let E_* and Γ_* be the boundary space and the boundary operator for the operator $-L^*$. The characteristic function of the operator L is the analytic operator-valued function $S(z):E\to E_*$ defined by*

$$S(z)\Gamma f=\Gamma_*(L^*-zI)^{-1}(L-zI)f,\quad f\in\mathrm{dom}(L),\quad z\in\rho(L^*)$$

If L is dissipative, then the spaces E and E_* are Hilbert spaces, and the operator $S(z)$ is a contraction on E for each $z\in\mathbb{C}_+$.

Note that the actual form of $S(z)$ depends on the choice of boundary spaces and boundary operators. If $\Gamma':\mathrm{dom}(L)\to E'$ and $\Gamma'_*:\mathrm{dom}(L^*)\to E'_*$ satisfy the condition (24) and $S'(z)$ is the corresponding characteristic function, then there exist two isometries $\pi_*:E_*\to E'_*$ and $\pi:E\to E'$ such that $\pi_*S(z)=S'(z)\pi$, $z\in\rho(L^*)$. Such characteristic functions of the operator L are often called *equivalent.*

All steps involved in the model construction outlined above do not depend on the concrete form of the characteristic function [35]. In particular cases when the characteristic function can be expressed in terms of the original problem, the model admits a "natural" form in relation to the problem setup. Examples of such calculations are provided towards the end of this section.

In order to compute a characteristic function of L one has to come up with a suitable definition of boundary spaces and operators. Consider first the general case where no specific assumptions on the operator L are made, and introduce the Cayley transform of L, i.e., $T = (L - \mathrm{i}I)(L + \mathrm{i}I)^{-1}$. The operator T is clearly contractive. The operators

$$Q := \frac{1}{\sqrt{2}}(I - T^*T)^{1/2}, \qquad Q_* := \frac{1}{\sqrt{2}}(I - TT^*)^{1/2}$$

are thus non-negative. A straightforward calculation [118] shows that the boundary spaces E, E_* and the boundary operators Γ, Γ_* can be defined as follows:

$$E = \operatorname{clos}\operatorname{ran}(Q), \quad E_* = \operatorname{clos}\operatorname{ran}(Q_*), \quad \Gamma = \operatorname{clos} Q(L + \mathrm{i}I), \quad \Gamma_* = \operatorname{clos} Q_*(L^* - \mathrm{i}I).$$

Here the operators Γ and Γ_* are the closures of the respective mappings initially defined on $\operatorname{dom}(L)$ and $\operatorname{dom}(L^*)$. This choice leads to the following expression for the characteristic function of the operator L :

$$S(z) = \left(T - (z - \mathrm{i})\Gamma_*(L^* - zI)^{-1}Q\right)\big|_E, \quad z \in \mathbb{C}_+. \tag{25}$$

An explicit calculation reveals that $S(z)$ is closely related to the characteristic function of T,

$$S(z) = -\vartheta_T\left(\frac{z - \mathrm{i}}{z + \mathrm{i}}\right), \quad z \in \mathbb{C}_+,$$

where

$$\vartheta_T(\lambda) = \left(-T + 2\lambda Q_*(I - \lambda T^*)^{-1}Q\right)\big|_E, \qquad |\lambda| < 1$$

is the Sz.-Nagy-Foiaş characteristic function of the contractive operator T. Therefore, the formula (25) is the abstract form of the characteristic function of L regardless the "concrete" realization of the operator L.

2.6.2 Examples

The actual choice of boundary spaces and operators is guided by the specifics of the problem at hand. Let us demonstrate the "natural" selection for these objects for some of the models introduced in Section 2.

Additive perturbations This is the simplest (and canonical) case of the characteristic function calculations included here solely for the completeness of exposition. Let L be a dissipative operator of Section 2.2.1, defined as an additive perturbation of a self-adjoint operator. Then for $f, g \in \operatorname{dom}(A) = \operatorname{dom}(L)$ one has

$$\Psi_L(f, g) = \frac{1}{\mathrm{i}}\left[(Lf, g) - (f, Lg)\right] = \frac{1}{\mathrm{i}}\left[\left(\mathrm{i}\frac{\alpha^2}{2}f, g\right) - \left(f, \mathrm{i}\frac{\alpha^2}{2}g\right)\right] = (\alpha f, \alpha g)$$

and therefore, the boundary space can be chosen as $E = \operatorname{clos}\operatorname{ran}(\alpha)$ with the boundary operator Γ defined as a mapping $\Gamma f \mapsto \alpha f$. In a similar way, $E_* = E$ and $\Gamma_* = \Gamma$.

The characteristic function of L corresponding to this selection of boundary spaces and operators is then computed as (5). As explained above, this characteristic function is equivalent to the function (25).

Almost solvable extensions In the notation of Section 2.3, let $L = A_B$ be a dissipative almost solvable extension of a symmetric operator A corresponding to the bounded operator $B = B_R + iB_I$ with $B_R = B_R^*$ and $B_I = B_I^* \geq 0$ defined on the space $\mathcal{K}$. Denote $\alpha := \sqrt{2}(B_I)^{1/2}$. From the Green's formula (11) and the condition $\Gamma_1 f = B\Gamma_0 f,\ f \in \mathrm{dom}(L)$ we obtain for $f, g \in \mathrm{dom}(L)$:

$$\Psi_L(f,g) = \frac{1}{\mathrm{i}}\left[(Lf,g) - (f,Lg)\right] = \frac{1}{\mathrm{i}}\big((B - B^*)\Gamma_0 f, \Gamma_0 g\big)_{\mathcal{K}} = (\alpha\Gamma_0 f, \alpha\Gamma_0 g)_{\mathcal{K}}.$$

Next we demonstrate two alternative approaches to the derivation of the characteristic function of L.

Approach 1. Define the boundary space $\mathcal{E}$ of the operator $L = A_B$ as the factorization and completion of the linear set $\mathcal{L} = \{\Gamma_0 f, |\ f \in \mathrm{dom}(L)\}$ endowed with the norm $\|u\|_{\mathcal{E}} = \|\alpha^2 u\|_{\mathcal{K}}$, $u \in \mathcal{L}$. The norm $\|\cdot\|_{\mathcal{E}}$ is degenerate if $\ker(\alpha)$ is non-trivial, thus the factorization becomes necessary. The corresponding boundary operator Γ is the map $\Gamma : f \mapsto \Gamma_0 f$ on the domain $\mathrm{dom}(\Gamma) = \mathrm{dom}(L)$. In a similar way, $\mathscr{E}_*$ is defined as the factorization and completion of the linear set $\mathcal{L}_* = \{\Gamma_0 g, |\ g \in \mathrm{dom}(L^*)\}$ with respect to the norm $\|u\|_{\mathcal{E}_*} = \|\alpha^2 u\|_{\mathcal{K}}$, $u \in \mathcal{L}_*$. The boundary operator Γ_* is the mapping $\Gamma_* : g \mapsto \Gamma_0 g$ defined on $\mathrm{dom}(\Gamma_*) = \mathrm{dom}(L^*)$. Thus, both boundary spaces $\mathcal{E}$ and $\mathcal{E}_*$ are Hilbert spaces with the norm associated with the "weight" equal to α^2.

An explicit computation then yields the following expression for the characteristic function $\mathscr{S}$:

$$\mathscr{S}(z) = \big(B^* - M(z)\big)^{-1}\big(B - M(z)\big), \quad z \in \rho(L^*),$$

where $M(z)$ is the Weyl-Titchmarsh $M-$function of Section 2.3.

Approach 2. An alternative form of the characteristic function is obtained based on the boundary operators Γ and Γ_* introduced as the closures of the mappings $f \mapsto \alpha\Gamma_0 f$ and $g \mapsto \alpha\Gamma_0 g$ defined on the linear sets $\mathrm{dom}(L)$ and $\mathrm{dom}(L^*)$, respectively. The boundary spaces E and E_* in this case are chosen as

$$E = \mathrm{clos}\,\mathrm{ran}\big(\alpha\Gamma_0|_{\mathrm{dom}(L)}\big), \qquad E_* = \mathrm{clos}\,\mathrm{ran}\big(\alpha\Gamma_0|_{\mathrm{dom}(L^*)}\big).$$

In all applications considered in this paper, these spaces coincide: $E = E_*$. Similarly to the situation of additive perturbations, it is often convenient (and common) to extend these spaces to $\mathrm{clos}\,\mathrm{ran}(\alpha)$.

The corresponding characteristic function is then represented by the formula (12) repeated here for the sake of readers' convenience:

$$S(z) = I_E + \mathrm{i}\alpha\big(B^* - M(z)\big)^{-1}\alpha : E \to E, \quad z \in \rho(L^*).$$

In contrast to Approach 1, this form captures the specifics of the extension parameter B. In particular, the dimension of the space E equals the dimension of the range of α. If the operator B is a compact perturbation of a self-adjoint, i. e., $B_I = \alpha^2/2 \in \mathfrak{S}_\infty$, then the characteristic function $S(z)$ is an operator-valued function of the form $I + \mathfrak{S}_\infty$ defined on the (unweighted) Hilbert space $\mathrm{clos}\,\mathrm{ran}(\alpha)$.

Equivalence of $\mathscr{S}$ and S. The mapping $\widehat{\alpha} : f \mapsto \alpha f$, $f \in \mathcal{E}$ is an isometry from the "weighted" space $\mathcal{E}$ to the space $\mathcal{K}$. The equality $\widehat{\alpha}\mathscr{S}(z) = S(z)\widehat{\alpha}$, $z \in \rho(L^*)$ expresses equivalence of the characteristic functions $\mathscr{S}$ and S corresponding to different choices of boundary spaces and operators. Both $\mathscr{S}$ and S functions are equivalent to the characteristic function of L written in its abstract form (25). It is easy to see that the boundary operators of Approach 1 and Approach 2 are also related by means of the isometric mapping $\widehat{\alpha}$.

In conclusion, we point out the recent paper [35] where the construction of the selfadjoint dilation and the functional model of a dissipative operator is based entirely on the concept of Strauss boundary spaces and operators (23), (24) with no reference to their "concrete" realizations.

3 An application: inverse scattering problem for quantum graphs

In the present section, we present an application of the theory introduced in Section 2.3, and in particular of the explicit construction of wave operators and scattering matrices facilitated by the approach based on the functional model due to Sergey Naboko. We first obtain an explicit expression for the scattering matrix of a quantum graph which we take to be the Laplacian on a finite non-compact metric graph, subject to $\delta-$type coupling at graph vertices. Then we present an explicit constructive solution to the inverse scattering problem for this graph, i.e., explicit formulae for the coupling constants at graph vertices. The narrative of this Section is based upon the papers [46, 47].

For simplicity of presentation we will only consider the case of a finite non-compact quantum graph, when the deficiency indices are finite. However, the same approach allows us to consider the general setting of infinite deficiency indices, which in the quantum graph setting leads to an infinite graph. In particular, one could consider the case of an infinite compact part of the graph.

In what follows, we denote by $\mathbb{G}=\mathbb{G}(\mathcal{E},\sigma)$ a finite metric graph, *i.e.* a collection of a finite non-empty set $\mathcal{E}$ of compact or semi-infinite intervals $e_j=[x_{2j-1},x_{2j}]$ (for semi-infinite intervals we set $x_{2j}=+\infty$), $j=1,2,\dots,n$, which we refer to as *edges*, and of a partition σ of the set of endpoints $\mathcal{V}:=\{x_k : 1\le k\le 2n,\ x_k<+\infty\}$ into N equivalence classes V_m, $m=1,2,\dots,N$, which we call *vertices*: $\mathcal{V}=\bigcup_{m=1}^N V_m$. The degree, or valence, $\deg(V_m)$ of the vertex V_m is defined as the number of elements in V_m, *i.e.* $\operatorname{card}(V_m)$. Further, we partition the set $\mathcal{V}$ into the two non-overlapping sets of *internal* $\mathcal{V}^{(\mathrm{i})}$ and *external* $\mathcal{V}^{(\mathrm{e})}$ vertices, where a vertex V is classed as internal if it is incident to no non-compact edge and external otherwise. Similarly, we partition the set of edges $\mathcal{E}=\mathcal{E}^{(\mathrm{i})}\cup\mathcal{E}^{(\mathrm{e})}$, into the collection of compact ($\mathcal{E}^{(\mathrm{i})}$) and non-compact ($\mathcal{E}^{(\mathrm{e})}$) edges. We assume for simplicity that the number of non-compact edges incident to any graph vertex is not greater than one.

For a finite metric graph $\mathbb{G}$, we consider the Hilbert spaces

$$L^2(\mathbb{G}):=\bigoplus_{j=1}^n L^2(e_j),\qquad W^{2,2}(\mathbb{G}):=\bigoplus_{j=1}^n W^{2,2}(e_j).$$

Further, for a function $f\in W^{2,2}(\mathbb{G})$, we define the normal derivative at each vertex along each of the adjacent edges, as follows:

$$\partial_n f(x_j):=\begin{cases} f'(x_j), & \text{if } x_j \text{ is the left endpoint of the edge,}\\ -f'(x_j), & \text{if } x_j \text{ is the right endpoint of the edge.}\end{cases}$$

In the case of semi-infinite edges we only apply this definition at the left endpoint of the edge.

Definition 3.1. *For $f\in W^{2,2}(\mathbb{G})$ and $a_m\in\mathbb{C}$ (below referred to as the "coupling constant"), the condition of continuity of the function f through the vertex V_m (i.e. $f(x_j)=f(x_k)$ if $x_j,x_k\in V_m$)*

together with the condition

$$\sum_{x_j \in V_m} \partial_n f(x_j) = a_m f(V_m)$$

is called the δ-type matching at the vertex V_m.

Remark 4. *Note that the δ-type matching condition in a particular case when $a_m = 0$ reduces to the standard Kirchhoff matching condition at the vertex V_m, see e.g. [23].*

Definition 3.2. *The quantum graph Laplacian A_a, $a := (a_1, ..., a_N)$, on a graph $\mathbb{G}$ with δ-type matching conditions is the operator of minus second derivative $-d^2/dx^2$ in the Hilbert space $L^2(\mathbb{G})$ on the domain of functions that belong to the Sobolev space $W^{2,2}(\mathbb{G})$ and satisfy the δ-type matching conditions at every vertex V_m, $m = 1, 2, \dots, N$. The Schrödinger operator on the same graph is defined likewise on the same domain in the case of summable edge potentials (cf. [54]).*

If all coupling constants a_m, $m = 1, \dots, N$, are real, it is shown that the operator A_a is a proper self-adjoint extension of a closed symmetric operator A in $L^2(\mathbb{G})$ [56]. Note that, without loss of generality, each edge e_j of the graph $\mathbb{G}$ can be considered to be an interval $[0, l_j]$, where $l_j := x_{2j} - x_{2j-1}$, $j = 1, \dots, n$ is the length of the corresponding edge. Throughout the present Section we will therefore only consider this situation.

In [54], the following result is obtained for the case of finite *compact* metric graphs.

Proposition 3.1 ([54])**.** *Let $\mathbb{G}$ be a finite compact metric graph with δ-type coupling at all vertices. There exists a closed densely defined symmetric operator A and a boundary triple such that the operator A_a is an almost solvable extension of A, for which the parametrising matrix $\varkappa$ is given by $\varkappa = \operatorname{diag}\{a_1, \dots, a_N\}$, whereas the Weyl function is an $N \times N$ matrix with elements*

$$m_{jk}(z) = \begin{cases} -\sqrt{z}\Bigg(\sum\limits_{e_p \in E_k} \cot \sqrt{z} l_p - 2 \sum\limits_{e_p \in L_k} \tan \dfrac{\sqrt{z} l_p}{2} \Bigg), & j = k, \\ \sqrt{z} \sum\limits_{e_p \in C_{jk}} \dfrac{1}{\sin \sqrt{z} l_p}, & j \neq k;\ V_j, V_k \text{ adjacent}, \\ 0, & j \neq k;\ V_j, V_k \text{ non-adjacent}. \end{cases} \tag{26}$$

Here the branch of the square root is chosen so that $\Im \sqrt{z} \geq 0$, l_p is the length of the edge e_p, E_k is the set of non-loop graph edges incident to the vertex V_k, L_k is the set of loops at the vertex V_k, and C_{jk} is the set of graph edges connecting vertices V_j and V_k.

In [46] this is extended to non-compact metric graphs as follows. Denote by $\mathbb{G}^{(\mathrm{i})}$ the compact part of the graph $\mathbb{G}$, *i.e.* the graph $\mathbb{G}$ with all the non-compact edges removed. Proposition 3.1 yields an expression for the Weyl function $M^{(\mathrm{i})}$ pertaining to the graph $\mathbb{G}^{(\mathrm{i})}$.

Lemma 3.2. *The matrix functions M, $M^{(\mathrm{i})}$ described above are related by the formula*

$$M(z) = M^{(\mathrm{i})}(z) + \mathrm{i}\sqrt{z} P_{\mathrm{e}}, \qquad z \in \mathbb{C}_+, \tag{27}$$

where P_{e} is the orthogonal projection in the boundary space $\mathcal{K}$ onto the set of external vertices $V_{\mathbb{G}}^{(\mathrm{e})}$, i.e. the matrix P_{e} such that $(P_{\mathrm{e}})_{ij} = 1$ if $i = j$, $V_i \in V_{\mathbb{G}}^{(\mathrm{e})}$, and $(P_{\mathrm{e}})_{ij} = 0$ otherwise.

The formula (27) leads to $M(s) - M^*(s) = 2\mathrm{i}\sqrt{s}P_\mathrm{e}$ a.e. $s \in \mathbb{R}$, and the expression (19) for $\widehat{\Sigma}$ leads to the classical scattering matrix $\widehat{\Sigma}_\mathrm{e}(k)$ of the pair of operators A_0 (which is the Laplacian on the graph $\mathbb{G}$ with standard Kirchhoff matching at all the vertices) and $A_\varkappa$, where $\varkappa = \varkappa = \operatorname{diag}\{a_1, \dots, a_N\}$:

$$\widehat{\Sigma}_\mathrm{e}(s) = P_\mathrm{e}(M(s) - \varkappa)^{-1}(M(s)^* - \varkappa)(M(s)^*)^{-1}M(s)P_\mathrm{e}, \qquad s \in \mathbb{R}, \tag{28}$$

which acts as the operator of multiplication in the space $L^2(P_\mathrm{e}\mathcal{K}; 4\sqrt{s}ds)$.

We remark that in the more common approach to the construction of scattering matrices, based on comparing the asymptotic expansions of solutions to spectral equations, see *e.g.* [58], one obtains $\widehat{\Sigma}_\mathrm{e}$ as the scattering matrix. Our approach yields an explicit factorisation of $\widehat{\Sigma}_\mathrm{e}$ into expressions involving the matrices M and $\varkappa$ only, sandwiched between two projections. (Recall that M and $\varkappa$ contain the information about the geometry of the graph and the coupling constants, respectively.) From the same formula (28), it is obvious that without the factorisation the pieces of information pertaining to the geometry of the graph and the coupling constants at the vertices are present in the final answer in an entangled form.

We reiterate that the analysis above pertains not only to the cases when the coupling constants are real, leading to self-adjoint operators A_a, but also to the case of non-selfadjoint extensions, *cf.* Theorem 2.7.

In what follows we often drop the argument $s \in \mathbb{R}$ of the Weyl function M and the scattering matrices $\widehat{\Sigma}$, $\widehat{\Sigma}_\mathrm{e}$.

It is easily seen that a factorisation of $\widehat{\Sigma}_\mathrm{e}$ into a product of $\varkappa-$dependent and $\varkappa-$independent factors (*cf.* (19)) still holds in this case in $P_\mathrm{e}\mathcal{K}$, namely

$$\widehat{\Sigma}_\mathrm{e} = \big[P_\mathrm{e}(M - \varkappa)^{-1}(M^* - \varkappa)P_\mathrm{e}\big]\big[P_\mathrm{e}(M^*)^{-1}MP_\mathrm{e}\big]. \tag{29}$$

We will now exploit the above approach in the analysis of the inverse scattering problem for Laplace operators on finite metric graphs, whereby the scattering matrix $\widehat{\Sigma}_\mathrm{e}(s)$, defined by (29), is assumed to be known for almost all positive "energies" $s \in \mathbb{R}$, along with the graph $\mathbb{G}$ itself. The data to be determined is the set of coupling constants $\{a_j\}_{j=1}^N$. For simplicity, in what follows we treat the inverse problem for graphs with real coupling constants, which corresponds to self-adjoint operators.

First, for given M, $\widehat{\Sigma}_\mathrm{e}$ we reconstruct the expression $P_\mathrm{e}(M^{(\mathrm{i})} - \varkappa)^{-1}P_\mathrm{e}$ for almost all $s > 0$:

$$P_\mathrm{e}(M^{(\mathrm{i})} - \varkappa)^{-1}P_\mathrm{e} = \frac{1}{\mathrm{i}\sqrt{s}}\left(2\big(P_\mathrm{e} + \widehat{\Sigma}_\mathrm{e}[P_\mathrm{e}(M^*)^{-1}MP_\mathrm{e}]^{-1}\big)^{-1} - I\right)P_\mathrm{e}. \tag{30}$$

In particular, due to the property of analytic continuation, the expression $P_\mathrm{e}(M^{(\mathrm{i})} - \varkappa)^{-1}P_\mathrm{e}$ is determined uniquely in the whole of $\mathbb{C}$ with the exception of a countable set of poles, which coincides with the set of eigenvalues of the self-adjoint Laplacian $A_\varkappa^{(\mathrm{i})}$ on the compact part $\mathbb{G}^{(\mathrm{i})}$ of the graph $\mathbb{G}$ with matching conditions at the graph vertices given by the matrix $\varkappa$, *cf.* Proposition 3.1.

Definition 3.3. *Given a partition $\mathcal{V}_1 \cup \mathcal{V}_2$ of the set of graph vertices, for $z \in \mathbb{C}$ consider the linear set $U(z)$ of functions that satisfy the differential equation $-u_z'' = zu_z$ on each edge, subject to the conditions of continuity at all vertices of the graph and the δ-type matching conditions at the vertices in the set $\mathcal{V}_2$. For each function $f \in U(z)$, consider the vectors*

$$\Gamma_1^{\mathcal{V}_1}u_z := \Big\{\sum_{x_j \in V_m} \partial_n f(x_j)\Big\}_{V_m \in \mathcal{V}_1}, \qquad \Gamma_0^{\mathcal{V}_1}u_z := \big\{f(V_m)\big\}_{V_m \in \mathcal{V}_1}.$$

The Robin-to-Dirichlet map of the set $\mathcal{V}_1$ maps the vector $(\Gamma_1^{\mathcal{V}_1} - \varkappa^{\mathcal{V}_1}\Gamma_0^{\mathcal{V}_1})u_z$ to $\Gamma_0^{\mathcal{V}_1}u_z$, where $\varkappa^{\mathcal{V}_1} := \operatorname{diag}\{a_m : V_m \in \mathcal{V}_1\}$. (Note that the function $u_z \in U(z)$ is determined uniquely by $(\Gamma_1^{\mathcal{V}_1} - \varkappa^{\mathcal{V}_1}\Gamma_0^{\mathcal{V}_1})u_z$ for all $z \in \mathbb{C}$ except a countable set of real points accumulating to infinity).

The above definition is a natural generalisation of the corresponding definitions of Dirichlet-to-Neumann and Neumann-to-Dirichlet maps pertaining to the graph boundary, considered in *e.g.* [23], [84].

We argue that the matrix $P_{\rm e}(M^{(\rm i)} - \varkappa)^{-1}P_{\rm e}$ is the Robin-to-Dirichlet map for the set $\mathcal{V}^{(\rm e)}$. Indeed, assuming $\phi := \Gamma_1 u_z - \varkappa\Gamma_0 u_z$ and $\phi = P_{\rm e}\phi$, where the latter condition ensures the correct δ-type matching on the set $\mathcal{V}^{(\rm i)}$, one has $P_{\rm e}\phi = (M^{(\rm i)} - \varkappa)\Gamma_0 u_z$ and hence $\Gamma_0 u_z = (M^{(\rm i)} - \varkappa)^{-1}P_{\rm e}\phi$. Applying $P_{\rm e}$ to the last identity yields the claim, in accordance with Definition 3.3.

We thus have the following theorem.

Theorem 3.3. *The Robin-to-Dirichlet map for the vertices $\mathcal{V}^{(\rm e)}$ is determined uniquely by the scattering matrix $\widehat{\Sigma}_{\rm e}(s)$, $s \in \mathbb{R}$, via the formula (30).*

The following definition, required for the formulation of the next theorem, is a generalisation of the procedure of graph contraction, well studied in the algebraic graph theory, see *e.g.* [133].

Definition 3.4 (Contraction procedure for graphs and associated quantum graph Laplacians)**.** *For a given graph $\mathbb{G}$ vertices V and W connected by an edge e are "glued" together to form a new vertex (VW) of the contracted graph $\widetilde{\mathbb{G}}$ while simultaneously the edge e is removed, whereas the rest of the graph remains unchanged. We do allow the situation of multiple edges, when V and W are connected in $\mathbb{G}$ by more than one edge, in which case all such edges but the edge e become loops of their respective lengths attached to the vertex (VW). The corresponding quantum graph Laplacian A_a defined on $\mathbb{G}$ is contracted to the quantum graph Laplacian $\widetilde{A}_{\widetilde{a}}$ by the application of the following rule pertaining to the coupling constants: a coupling constant at any unaffected vertex remains the same, whereas the coupling constant at the new vertex (VW) is set to be the sum of the coupling constants at V and W. Here it is always assumed that all quantum graph Laplacians are described by Definition 3.2.*

Theorem 3.4. *Suppose that the edge lengths of the graph $\mathbb{G}^{(\rm i)}$ are rationally independent. The element*[3] *$(1,1)$ of the Robin-to-Dirichlet map described above yields the element $(1,1)$ of the "contracted" graph $\widetilde{\mathbb{G}}^{(\rm i)}$ obtained from the graph $\mathbb{G}^{(\rm i)}$ by removing a non-loop edge e emanating from V_1. The procedure of passing from the graph $\mathbb{G}^{(\rm i)}$ to the contracted graph $\widetilde{\mathbb{G}}^{(\rm i)}$ is given in Definition 3.4.*

Proof. Due to the assumption that the edge lengths of the graph $\mathbb{G}^{(\rm i)}$ are rationally independent, the element (1,1), which we denote by f_1, is expressed explicitly as a function of $\sqrt{z}$ *and* all the edge lengths l_j, $j = 1, 2, \dots, n$, in particular, of the length of the edge e, which we assume to be l_1 without loss of generality. This is an immediate consequence of the explicit form of the matrix $M^{(\rm i)}$, see (26). Again without loss of generality, we also assume that the edge e connects the vertices V_1 and V_2.

Further, consider the expression $\lim_{l_1 \to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a)$. On the one hand, this limit is known from the explicit expression for f_1 mentioned above. On the other hand, f_1 is the ratio of the determinant $\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)$ of the principal minor of the matrix $M^{(\rm i)}(z) - \varkappa$ obtained by

[3] By renumbering if necessary, this does not lead to loss of generality.

removing its first row and and first column and the determinant of $M^{(\mathrm{i})}(z) - \varkappa$ itself:

$$f_1(\sqrt{z}; l_1, \dots, l_n; a) = \frac{\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)}{\det\bigl(M^{(\mathrm{i})}(z) - \varkappa\bigr)}$$

Next, we multiply by $-l_1$ both the numerator and denominator of this ratio, and pass to the limit in each of them separately:

$$\lim_{l_1 \to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a) = \frac{\lim\limits_{l_1 \to 0} (-l_1)\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)}{\lim\limits_{l_1 \to 0} (-l_1)\det\bigl(M^{(\mathrm{i})}(z) - \varkappa\bigr)} \tag{31}$$

The numerator of (31) is easily computed as the determinant $\mathcal{D}^{(2)}(z; l_1, \dots, l_n; a)$ of the minor of $M^{(\mathrm{i})}(z) - \varkappa$ obtained by removing its first two rows and first two columns.

As for the denominator of (31), we add to the second row of the matrix $M^{(\mathrm{i})}(z) - \varkappa$ its first row multiplied by $\cos(\sqrt{z} l_1)$, which leaves the determinant unchanged. This operation, due to the identity

$$-\cot(\sqrt{z} l_1)\cos(\sqrt{z} l_1) + \frac{1}{\sin(\sqrt{z} l_1)} = \sin(\sqrt{z} l_1),$$

cancels out the singularity of all matrix elements of the second row at the point $l_1 = 0$. We introduce the factor $-l_1$ (*cf.* 31) into the first row and pass to the limit as $l_1 \to 0$. Clearly, all rows but the first are regular at $l_1 = 0$ and hence converge to their limits as $l_1 \to 0$. Finally, we add to the second column of the limit its first column, which again does not affect the determinant, and note that the first row of the resulting matrix has one non-zero element, namely the $(1, 1)$ entry. This procedure reduces the denominator in (31) to the determinant of a matrix of the size reduced by one. As in [55], it is checked that this determinant is nothing but $\det(\widetilde{M}^{(\mathrm{i})} - \widetilde{\varkappa})$, where $\widetilde{M}^{(\mathrm{i})}$ and $\widetilde{\varkappa}$ are the Weyl matrix and the (diagonal) matrix of coupling constants pertaining to the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$. This immediately implies that the ratio obtained as a result of the above procedure coincides with the entry (1,1) of the matrix $(\widetilde{M}^{(\mathrm{i})} - \widetilde{\varkappa})^{-1}$, *i.e.*

$$\lim_{l_1 \to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a) = f_1^{(1)}(\sqrt{z}; l_2, \dots, l_n; \widetilde{a}),$$

where $f_1^{(1)}$ is the element (1,1) of the Robin-to-Dirichlet map of the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$, and $\widetilde{a}$ is given by Definition 3.4. □

The main result of this section is the theorem below, which is obtained as a corollary of Theorems 3.3 and 3.4. We assume without loss of generality that $V_1 \in \mathcal{V}^{(\mathrm{e})}$ and denote by $f_1(\sqrt{z})$ the (1,1)-entry of the Robin-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$. We set the following notation. Fix a spanning tree $\mathbb{T}$ (see *e.g.* [133]) of the graph $\mathbb{G}^{(\mathrm{i})}$. We let the vertex V_1 to be the root of $\mathbb{T}$ and assume, again without loss of generality, that the number of edges in the path γ_m connecting V_m and the root is a non-decreasing function of m. Denote by $N^{(m)}$ the number of vertices in the path γ_m, and by $\{l_k^{(m)}\}$, $k = 1, \dots, N^{(m)} - 1$, the associated sequence of lengths of the edges in γ_m, ordered along the path from the root V_1 to V_m. Note that each of the lengths $l_k^{(m)}$ is clearly one of the edge lengths l_j of the compact part of the original graph $\mathbb{G}$.

Theorem 3.5. *Assume that the graph $\mathbb{G}$ is connected and the lengths of its compact edges are rationally independent. Given the scattering matrix $\widehat{\Sigma}_{\mathrm{e}}(s)$, $s \in \mathbb{R}$, the Robin-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$ and the matrix of coupling constants $\varkappa$ are determined constructively in a unique way. Namely, the following formulae hold for $l = 1, 2, \dots, N$ and determine a_m, $m = 1, \dots, N$:*

$$\sum_{m: V_m \in \gamma_l} a_m = \lim_{\tau \to +\infty} \left\{ -\tau \Big(\sum_{V_m \in \gamma_l} \deg(V_m) - 2(N^{(l)} - 1) \Big) - \frac{1}{f_1^{(l)}(i\tau)} \right\},$$

where

$$f_1^{(l)}(\sqrt{z}) := \lim_{l^{(l)}_{N^{(l)}-1} \to 0} \dots \lim_{l_2^{(l)} \to 0} \lim_{l_1^{(l)} \to 0} f_1(\sqrt{z}), \tag{32}$$

where in the case $l = 1$ no limits are taken in (32).

4 Zero-range potentials with an internal structure

4.1 Zero-range models

In many models of mathematical physics, most notably in the analysis of Schrodinger operators, an explicit solution can be obtained in a very limited number of special cases (essentially, those that admit separation of variables and thus yield solutions in terms of special functions). This deficit of explicitly solvable models has led physicists, starting with E. Fermi in 1934, to the idea to replace potentials with some boundary condition at a point of three-dimensional space, i.e., a zero-range potential.

The rigorous mathematical treatment of this idea was initiated in [22]. It was shown that the corresponding model Hamiltonians are in fact self-adjoint extensions of a Laplacian which has been restricted to the set of $W^{2,2}$ functions vanishing in a vicinity of a fixed point x_0 in $\mathbb{R}^3$. These ideas were further developed in a vast series of papers and books, culminating in the monograph [4], which also contains an comprehensive list of references.

Physical applications of zero-range models have been treated in, e.g., [51]. It has been conjectured that zero-range models provide a good approximation of realistic physical systems in at least a far-away zone, where the concrete shape of the potential might be discarded, making them especially useful in the analysis of scattering problems. Here we also mention the celebrated Kronig-Penney model where a periodic array of zero-range potentials is used to model the atoms in a crystal lattice.

Despite the obvious success of the idea explained above, it still carries a number of serious drawbacks. In particular, it can be successfully applied to model spherically symmetric scatterers only. If one attempts to model a scatterer of a more involved structure, i.e., possessing a richer spectrum, by a finite set of zero-range potentials, the complexity of the model grows rapidly, essentially eliminating the main selling point of the model, i.e., its explicit solvability.

In 1980s, based in part on earlier physics papers by Shirokov et. al. where the idea was presented in an implicit form, B. S. Pavlov [111] rigorously introduced a model of zero-range potential with an internal structure. This idea was further developed by Pavlov and his students, see e.g. [3, 113] and references therein. In the mentioned works of Pavlov, one starts by considering the operator A_0 being a Laplacian restricted to the set of $W^{2,2}$ functions vanishing in a vicinity of a fixed point in $\mathbb{R}^3$, precisely as in [22]. Then, instead of considering von Neumann self-adjoint extensions of the latter, one passes over to the consideration of the so-called *out of space* extensions, i.e., extensions to self-adjoint operators in a larger Hilbert space. The theory of out-of-space extensions generalising that of J. von Neumann was constructed by M. A. Neumark in [100, 101] in the case of densely defined symmetric operators and by M. A. Krasnoselskii [78] and A. V. Strauss [128] in the case opposite, see also [129] for the connections with the theory of functional models.

In fact, Pavlov, being quite possibly unaware of these theoretical developments, has reinvented this technique in the following way. Alongside the original Hilbert space $H = L^2(\mathbb{R}^3)$, consider an auxiliary *internal* Hilbert space E (which can be in many important cases considered to be finite-dimensional) and a self-adjoint operator A with simple spectrum in it. Let ϕ be its generating vector and consider the restriction A_ϕ of A (non-densely defined) to the space

$$\operatorname{dom} A_\phi := \{(A - \mathrm{i})^{-1}\psi : \psi \in E, \langle \phi, \psi \rangle = 0\}.$$

This leads to the symmetric operator $\mathcal{A}_0$ on the Hilbert space $H \oplus E$, defined as $A_0 \oplus A_\phi$ on the domain

$$\operatorname{dom} \mathcal{A}_0 := \left\{ \begin{pmatrix} f \\ v \end{pmatrix} : f \in \operatorname{dom} A_0, v \in \operatorname{dom} A_\phi \right\},$$

where A_0 is the restricted Laplacian on H introduced above. The operator $\mathcal{A}_0$ is then a symmetric non-densely defined operator with equal deficiency indices, and one can consider its self-adjoint extensions $\mathcal{A}$. Among them, we will single out those which non-trivially couple the spaces H and E by feeding the boundary data at x_0 of a function $f \in W^{2,2}(\mathbb{R}^3)$ to the "part" of operator acting in E. The latter then serves as the operator of the "internal structure", which can be chosen arbitrarily complex. We elect not to dwell on the precise way in which the extensions $\mathcal{A}$ are constructed as an explicit examples of operators of this class will be presented below in the present section.

4.2 Connections with inhomogeneous media

Leaving the subject of zero-range models with an internal structure aside for a moment, let us briefly consider a number of physically motivated models giving rise to zero-range potentials in general. In particular, we will be interested in those models which lead to a distribution "potential" δ', where δ is the Dirac delta function. It is well-known, see, e.g., [4], that the question of relating an operator of the form $-\Delta + \alpha\delta'$ to one of self-adjoint von Neumann extensions of a properly selected symmetric restriction A_0 of $-\Delta$ is far from being trivial, as δ', unlike δ, is form-unbounded.

For the same reason, it is non-trivial to construct an explicit "regularisation" of a $\delta'-$perturbed Laplacian, i.e., a sequence of operators A_ε being either potential perturbations of the Laplacian or, in general, any perturbations of the latter which converge in some sense (say, in the sense of resolvent convergence) to the Laplacian with a δ' perturbation. In particular, we point out among many others the paper [39] where A_ε are chosen as first-order differential non-self-adjoint perturbations of the Laplacian of a special form and the paper [67] where the perturbation is assumed to admit the form $\varepsilon^{-2}v(x/\varepsilon)$.

It turns out that additive $\varepsilon-$dependant perturbations are not the most straightforward choice for the task described, as zero-range perturbations (and more precisely, zero-range perturbations with an internal structure) appear naturally in the asymptotic analysis of inhomogeneous media. In particular, in the paper [41] we studied the norm-resolvent asymptotics of differential operators A_ε with periodic coefficients with high contrast, defined by their resolvents $(A_\varepsilon - z)^{-1} : f \mapsto u$ as follows:

$$-\left(a^\varepsilon(x)u'\right)' - zu = f, \quad f \in L^2(\mathbb{R}), \quad \varepsilon > 0, \quad z \in \mathbb{C}, \tag{33}$$

where, for all $\varepsilon > 0$, the coefficient a^ε is 1-periodic and

$$a^\varepsilon(y) := \begin{cases} a\varepsilon^{-2}, & y \in [0, l_1), \\ 1, & y \in [l_1, l_1 + l_2), \\ a\varepsilon^{-2}, & y \in [l_1 + l_2, 1), \end{cases}$$

with $a > 0$, and $0 < l_1 < l_1 + l_2 < 1$. Here in (33) the "natural" matching conditions are imposed at the points of discontinuity of the symbol $a^\varepsilon(x)$, i.e., the continuity of both the function itself and of its conormal derivative, so that the operators A_ε can be thought as being defined by the form $\int a^\varepsilon(x)|u'(x)|^2 dx$. We remark that the operators A_ε are unitary equivalent to the operators of the double-porosity model of homogenisation theory in dimension one, see, e.g., [72].

The main result of the named paper can be reformulated as follows.

Theorem 4.1. *The norm-resolvent limit of the sequence A_ε is unitarily equivalent to the operator A_{hom} in $L^2(\mathbb{R})$ given by the differential expression $-l_2^{-2} d^2/dx^2$ on*

$$\begin{aligned} &\text{dom}(A_{\text{hom}}) \\ &= \big\{U : \forall n \in \mathbb{Z}\ \ U \in W^{2,2}(n, n{+}1),\ \ U' \in C(\mathbb{R}),\ \forall n \in \mathbb{Z}\ \ U(n{+}0) - U(n{-}0) = l_2^{-1}(l_1{+}l_3)U'(n)\big\}, \end{aligned}$$

where $l_3 := 1 - (l_1 + l_2)$. Moreover, for all z in a compact set K_σ such that the distance of the latter from the positive real line is not less than a fixed $\sigma > 0$, this norm resolvent convergence is uniform, with the (uniform) error bound $O(\varepsilon^2)$.

By inspection, the operator A_{hom} defined above corresponds to the formal differential expression

$$-l_2^{-2} \frac{d^2}{dx^2} + \frac{(l_1 + l_3)}{l_2} \sum_{n \in \mathbb{Z}} \delta'(x - n),$$

i.e., it is the operator of the Kronig-Penney dipole-type model on the real line. It is also quite clear that the periodicity of the model considered has nothing to do with the fact that the effective operator acquires the δ'-type potential perturbation. Thus it leads to the understanding that strong inhomogeneities in the media in generic (i.e., not necessarily periodic) case naturally give rise to zero-range potentials of δ'-type.

In order to relate this exposition to our subject of zero-range potentials with an internal structure, let us describe the main ingredient leading to the result formulated above. As usual in dealing with periodic problems, we apply the Gelfand transform

$$\hat{U}(y, \tau) = (2\pi)^{-d/2} \sum_{n \in \mathbb{Z}^d} U(y + n) \exp\big(-\mathrm{i}\tau \cdot (y + n)\big), \quad y \in [0, 1],\ \tau \in [-\pi, \pi), \tag{34}$$

to the operator family A_ε, which yields the operator family $A_\varepsilon^{(\tau)}$ corresponding to the differential expression

$$-\left(\frac{d}{dx} + \mathrm{i}\tau\right) a^\varepsilon(x) \left(\frac{d}{dx} + \mathrm{i}\tau\right)$$

on the interval $[0, 1]$ with periodic boundary conditions at the endpoints. Here $\tau \in [-\pi, \pi)$ is the quasimomentum. As above, the matching conditions at the points of discontinuity of the symbol $a^\varepsilon(x)$ are assumed to be natural.

The asymptotic analysis of the operator family $A_\varepsilon^{(\tau)}$, as shown in [41, 44], yields the following operator as its norm-resolvent asymptotics. Let $H_{\rm hom} = H_{\rm soft} \oplus \mathbb{C}^1$. For all values $\tau \in [-\pi, \pi)$, consider a self-adjoint operator $\mathcal{A}_{\rm hom}^{(\tau)}$ on the space $H_{\rm hom}$, defined as follows. Let the domain $\operatorname{dom} \mathcal{A}_{\rm hom}^{(\tau)}$ be defined as

$$\operatorname{dom} \mathcal{A}_{\rm hom}^{(\tau)} = \Big\{ (u, \beta)^\top \in H_{\rm hom}: \ u \in W^{2,2}(0, l_2), u(0) = \overline{\xi^{(\tau)}} u(l_2) = \beta / \sqrt{l_1 + l_3} \Big\}.$$

On $\operatorname{dom} \mathcal{A}_{\rm hom}^{(\tau)}$ the action of the operator is set by

$$\mathcal{A}_{\rm hom}^{(\tau)} \begin{pmatrix} u \\ \beta \end{pmatrix} = \left(\begin{array}{c} \left(\dfrac{1}{\mathrm{i}} \dfrac{d}{dx} + \tau \right)^2 \\ -\dfrac{1}{\sqrt{l_1 + l_3}} \big(\partial^{(\tau)} u \big|_0 - \overline{\xi^{(\tau)}} \partial^{(\tau)} u \big|_{l_2} \big) \end{array} \right).$$

Here

$$\xi^{(\tau)} := \exp\big(\mathrm{i}(l_1 + l_3)\tau \big), \qquad \partial^{(\tau)} u := \left(\frac{d}{dx} + \mathrm{i}\tau \right) u.$$

Theorem 4.2. *The resolvent* $(A_\varepsilon^{(\tau)} - z)^{-1}$ *admits the following estimate in the uniform operator norm topology:*

$$(A_\varepsilon^{(\tau)} - z)^{-1} - \Psi^* (\mathcal{A}_{\rm hom}^{(\tau)} - z)^{-1} \Psi = O(\varepsilon^2),$$

where Ψ *is a partial isometry from* $H = L^2(0, 1)$ *to* $H_{\rm hom}$*. This estimate is uniform in* $\tau \in [-\pi, \pi)$ *and* $z \in K_\sigma$*.*

It is clear now that the operator $\mathcal{A}_{\rm hom}^{(\tau)}$ is nothing but the simplest possible example of Pavlov's zero-range perturbations with an internal structure, corresponding to the case where the dimension of the internal space E is equal to one. The definition of $\mathcal{A}_{\rm hom}^{(\tau)}$ implies that the support of the zero-range potential here is located at the point $x_0 = 0$, which is identified due to quasi-periodic (of Datta–Das Sarma type) boundary conditions with the point $x = l_2$.

Next it is shown (see [41] for details) that under an explicit unitary transform the operator family $\mathcal{A}_{\rm hom}^{(\tau)}$ is unitary equivalent to the family $\mathcal{A}'_{\rm hom}(\tau')$ at the quasimomentum point $\tau' = \tau + \pi (\bmod\ 2\pi)$. Here $\mathcal{A}'_{\rm hom}(\tau')$ acts in the space $L^2[0, l_2]$ and is defined by the same differential expression as $\mathcal{A}_{\rm hom}^{(\tau)}$, with the parameter τ replaced by τ' :

$$\left(\frac{1}{\mathrm{i}} \frac{d}{dx} + \tau' \right)^2,$$

on the domain described by the conditions

$$u(0) + \mathrm{e}^{-\mathrm{i}(l_1 + l_3)\tau'} u(l_2) = (l_1 + l_3) \partial^{(\tau')} u \big|_0,$$
$$\partial^{(\tau')} u \big|_0 = -\mathrm{e}^{-\mathrm{i}(l_1 + l_3)\tau'} \partial^{(\tau')} u \big|_{l_2}.$$

An application of the inverse Gelfand transform then yields Theorem 4.1. This shows that the operator $\mathcal{A}_{\rm hom}^{(\tau)}$ which is an operator of a zero-range model with the internal space E of dimension one is in fact a differential operator with a δ'−potential, up to a unitary transformation. In view of [85, 123] it is plausible that by a similar argument it could be shown, that an operator with a $\delta^{(n)}-$potential can be realized as a zero-range model with $\dim E = n$, for any natural n.

It is interesting to note that an operator admitting the same form as $\mathcal{A}_{\text{hom}}^{(\tau)}$ (with $\tau = 0$) appears naturally in the setting of [57,81,82], who discuss the behaviour of the spectra of operator sequences associated with domains "shrinking" as $\varepsilon \to 0$ to a metric graph embedded into $\mathbb{R}^d$. Here the rate of shrinking of the "edge" parts is assumed to be related to the rate of shrinking of the "vertex" parts of the domain via

$$\frac{\text{vol}(V_{\text{vertex}}^{\varepsilon})}{\text{vol}(V_{\text{edge}}^{\varepsilon})} \to \alpha > 0, \quad \varepsilon \to 0. \tag{35}$$

It is shown in the above works that the spectra of the corresponding Laplacian operators with Neumann boundary conditions converge to the spectrum of a quantum graph associated with a Laplacian on the metric graph obtained as the limit of the domain as $\varepsilon \to 0$. The "weight" $l_1 + l_3$ in $\mathcal{A}_{\text{hom}}^{(\tau)}$ plays the rôle of the constant α in (35).

By a similar argument to the one presented above one can show, that in the case of domains shrinking to a graph under the "resonant" condition (35) one obtains, under a suitable unitary transform, the matching condition of δ' type at the internal graph vertices, with the corresponding coupling constant equal to α.

4.3 A PDE model: BVPs with a large coupling

4.3.1 Problem setup

In [76], we studied a prototype large-coupling transmission problem, posed on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$, see Fig. 1, containing a "low-index" (equivalently, "high propagation speed") inclusion Ω_-, located at a positive distance to the boundary $\partial\Omega$. Mathematically, this is modelled by a "weighted" Laplacian $-a_{\pm}\Delta$, where $a_+ = 1$ (the weight on the domain $\Omega_+ := \Omega \setminus \overline{\Omega_-}$), and $a_- \equiv a$ (the weight on the domain Ω_-) is assumed to be large, $a_- \gg 1$. This is supplemented by the Neumann boundary condition $\partial u / \partial n = 0$ on the outer boundary $\partial\Omega$, where n is the exterior normal to $\partial\Omega$, and "natural" continuity conditions on the "interface" $\Gamma := \partial\Omega_-$. For each a, we consider time-harmonic vibrations of the physical domain represented by Ω, described by the eigenvalue problem for an appropriate operator in $L^2(\Omega)$. It is easily seen that eigenfunction sequences for

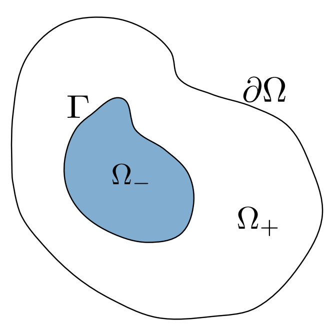

Figure 1: Domain with a "stiff" inclusion.

these eigenvalue problems converge, as $a \to \infty$, to either a constant or a function of the form

$$v - \frac{1}{|\Omega|}\int_{\Omega_+} v,$$

where v satisfies the spectral boundary-value problem (BVP)

$$-\Delta v = z\left(v - \frac{1}{|\Omega|}\int_{\Omega_+} v\right) \quad \text{in } \Omega_+, \qquad v|_\Gamma = 0, \qquad \left.\frac{\partial v}{\partial n}\right|_{\partial\Omega} = 0. \tag{36}$$

Here the spectral parameter z represents the ratio of the size of the original physical domain to the wavelength in its part represented by Ω_+.

The problem (36) is isospectral to the so-called "electrostatic problem" discussed in [138, Lemma 3.4], see also [9] and references therein, namely the eigenvalue problem for the self-adjoint operator Q defined by the quadratic form

$$q(u,u) = \int_{\Omega_+} \nabla v \cdot \overline{\nabla v}, \qquad u = v + c, \quad v \in H^1_{0,\Gamma} := \{v \in H^1(\Omega_+),\ v|_\Gamma = 0\}, \quad c \in \mathbb{C}$$

on the Hilbert space $L^2(\Omega_+) \dotplus \mathbb{C}$, treated as a subspace of $L^2(\Omega)$.

Denote by A_0^+ the Laplacian $-\Delta$ on Ω_+, subject to the Dirichlet condition on Γ and the Neumann boundary condition on $\partial\Omega$ and let λ_j^+, ϕ_j^+, $j = 1, 2, \dots,$ be the eigenvalues and the corresponding orthonormal eigenfunctions, respectively, of A_0^+.

It is then easily shown, that the spectrum of the electrostatic problem is the union of two sets: a) the set of z solving the equation

$$z\left[|\Omega| + z\sum_{j=1}^{\infty}(\lambda_j^+ - z)^{-1}\left|\int_{\Omega_+} \phi_j^+\right|^2\right] = 0.$$

and b) the set of those eigenvalues λ_j^+ for which the corresponding eigenfunction ϕ_j^+ has zero mean over Ω_+.

4.3.2 Norm-resolvent convergence to a zero-range model with an internal structure

Suppose that Ω is a bounded $C^{1,1}$ domain, and $\Gamma \subset \Omega$ is a closed $C^{1,1}$ curve, so that $\Gamma = \partial\Omega_-$ is the common boundary of domains Ω_+ and Ω_-, where Ω_- is strictly contained in Ω, such that $\overline{\Omega}_+ \cup \overline{\Omega}_- = \overline{\Omega}$, see Fig. 1.

For $a > 0$, $z \in \mathbb{C}$ we consider the "transmission" eigenvalue problem (*cf.* [121])

$$\begin{cases} -\Delta u_+ = z u_+ \ \text{ in } \Omega_+, \\ -a\Delta u_- = z u_- \ \text{ in } \Omega_-, \\ u_+ = u_-, \quad \dfrac{\partial u_+}{\partial n_+} + a\dfrac{\partial u_-}{\partial n_-} = 0 \ \text{ on } \Gamma, \\ \dfrac{\partial u_+}{\partial n_+} = 0 \quad \text{on } \partial\Omega, \end{cases} \tag{37}$$

where $n_\pm$ denotes the exterior normal (defined a.e.) to the corresponding part of the boundary. The above problem is understood in the strong sense, i.e. $u_\pm \in H^2(\Omega_\pm)$, the Laplacian differential expression Δ is the corresponding combination of second-order weak derivatives, and the boundary values of $u_\pm$ and their normal derivatives are understood in the sense of traces according to the embeddings of $H^2(\Omega_\pm)$ into $H^s(\Gamma)$, $H^s(\partial\Omega)$, where $s = 3/2$ or $s = 1/2$.

Denote by A_a the operator of the above boundary value problem. Its precise definition is given on the basis of the boundary triples theory in the form of [120].

Consider the space $H_{\text{eff}} = L^2(\Omega_+) \oplus \mathbb{C}$ and the following linear subset of $L^2(\Omega)$:

$$\operatorname{dom} \mathcal{A}_{\text{eff}} = \left\{ \begin{pmatrix} u_+ \\ \eta \end{pmatrix} \in H_{\text{eff}} : \ u_+ \in H^2(\Omega_+), \quad u_+|_\Gamma = \frac{\eta}{\sqrt{|\Omega_-|}} \mathbb{1}_\Gamma, \quad \left.\frac{\partial u_+}{\partial n_+}\right|_{\partial\Omega} = 0 \right\},$$

where $u|_\Gamma$ is the trace of the function u and $\mathbb{1}_\Gamma$ is the unity function on Γ. On $\operatorname{dom} \mathcal{A}_{\text{eff}}$ we set the action of the operator $\mathcal{A}_{\text{eff}}$ by the formula

$$\mathcal{A}_{\text{eff}} \begin{pmatrix} u_+ \\ \eta \end{pmatrix} = \begin{pmatrix} -\Delta u_+ \\ \dfrac{1}{\sqrt{|\Omega_-|}} \int_\Gamma \dfrac{\partial u_+}{\partial n_+} \end{pmatrix}. \tag{38}$$

Theorem 4.3. *The operator $\mathcal{A}_{\text{eff}}$ is the norm-resolvent limit of the operator family A_a. This convergence is uniform for $z \in K_\sigma$, with an error estimate by $O(a^{-1})$.*

This theorem yields in particular the convergence (in the sense of Hausdorff) of the spectra of A_a to that of $\mathcal{A}_{\text{eff}}$. This convergence is uniform in K_σ, and its rate is estimated as $O(a^{-1})$. Moreover, it is shown that the spectrum of $\mathcal{A}_{\text{eff}}$ coincides with the spectrum of the electrostatic problem (36).

Note that the form of $\mathcal{A}_{\text{eff}}$ is once again identical to that of a zero-range model with an internal structure in the case when the internal space E is one-dimensional. The obvious difference is that here the effective model of the medium is no longer "zero-range" per se; rather it pertains to a singular perturbation supported by the boundary Γ. Therefore, the result described above allows one to extend the notion of internal structure to the case of distributional perturbations supported by a curve, see also [86] where this idea was first suggested, although unlike above no asymptotic regularisation procedure was considered. Moreover, well in line with the narrative of preceding sections, the internal structure appears owing exclusively to the strong inhomogeneity of the medium considered.

We remark that a "classical" zero-range perturbation with an internal structure can still be obtained by a rather simple modification of the problem considered. Namely, let a be fixed, and let the *volume* of the inclusion Ω_- now wane to zero as the new parameter $\varepsilon \to 0$. This represents a model that has been studied in detail, see, e.g., [8] and references therein. In this modified setup, a virtually unchanged argument leads to the inclusion being asymptotically modelled by a zero-range potential with an internal structure. Moreover, the dimension of the internal space E is again equal to one, provided that a uniform norm-resolvent convergence is sought for the spectral parameter belonging to the compact K_σ.

4.3.3 Internal structure with higher dimensions of internal space E

A natural question must therefore be posed: can strongly inhomogeneous media only give rise to simplest possible zero-range models with an internal structure, pertaining to the case of $\dim E = 1$, or is it possible to obtain effective models with more involved internal structures? It turns out that the second mentioned possibility is realised, which we will demonstrate briefly using the material of the preceding section.

Recall that in all the results formulated above the uniform convergence was claimed under the additional assumption that the spectral parameter belongs to a fixed compact. If one drops this assumption, within the setup of the previous section one has the following statement.

Theorem 4.4. *Up to a unitary equivalence, for and $k \in \mathbb{N}$ there exists a self-adjoint operator $\mathcal{A}_{\text{eff}}$ of a zero-range model with an internal structure on the space $H_{\text{eff}} := L^2(\Omega_+) \oplus \mathbb{C}^k$ such that*

$$(A_a - z)^{-1} \simeq \mathfrak{P}(\mathcal{A}_{\text{eff}} - z)^{-1}\mathfrak{P} + O\big(\max\{a^{-1}, |z|^{k+1}a^{-k}\}\big) \tag{39}$$

in the uniform operator norm topology. Here $\mathfrak{P}$ is the orthogonal projection of H_{eff} onto $L^2(\Omega_+) \oplus \mathbb{C}$ (i.e., the space H_{eff} of the previous section).

Note that unlike the results pertaining to the situation of the spectral parameter contained in a compact, here the leading-order term of the asymptotic expansion of the resolvent of the original operator A_a is not the resolvent of some self-adjoint operator (unless $k = 1$), but rather a generalised resolvent. It is also obvious that the concrete choice of k to be used in the last theorem depends on the concrete relationship between z and a and on the error estimate sought: the error estimate of the theorem becomes tighter at k increases. In essence, this brings about the understanding that despite the fact that on the face of it the problem at hand is one-parametric, it must be treated as having two parameters, z and a.

The operator $\mathcal{A}_{\text{eff}}$ of the last Theorem admits an explicit description for any $k \in \mathbb{N}$, but this description is rather involved. In view of better readability of the paper, we only present its explicit form in the case $k = 2$:

$$\mathcal{A}_{\text{eff}} \begin{pmatrix} u_+ \\ \eta_1 \\ \eta_2 \end{pmatrix} := \begin{pmatrix} -\Delta u_+ \\ \dfrac{1}{\kappa} \int_\Gamma \dfrac{\partial u_+}{\partial n_+} + a(B^2 D^{-1}\eta_1 + B\eta_2) \\ a(B\eta_1 + D\eta_2) \end{pmatrix}.$$

Here B, D and κ are real parameters, which are explicitly computed.

It should be noted that similar results can be obtained in the homogenisation-related setup of the previous section, see also Section 5.

We can therefore conclude that zero-range models with an internal structure appear naturally in the asymptotic analysis of highly inhomogeneous media. Moreover, in the generic case they appear as Neumark-Strauss dilations (see [101,102,126,129]) of main order terms in the asymptotic expansions of the resolvents of problems considered. The complexity of the internal structure can be arbitrarily high (i.e., the dimension of the internal space E can be made as high as required), provided that the spectral parameter z is allowed to grow with the parameter $a \to \infty$ (or $\varepsilon \to 0$). Further, owing to the remark made above that an operator with a $\delta^{(n)}$-potential could be realized as a zero-range model with $\dim E = n$ for any natural n, we expect models with strong inhomogeneities to admit the role of the tool of choice in the regularisation of singular and super-singular perturbations, beyond the form-bounded case and including the case of singular perturbations supported by a curve or a surface.

4.4 The rôle of generalised resolvents

We close this section with a brief exposition of how precisely the asymptotic results formulated above are obtained. The analysis starts with the family of resolvents, say (in the case of Section 4.2) $(A_\varepsilon - z)^{-1}$, describing the inhomogeneous medium at hand. One then passes over to the generalised resolvent $R_\varepsilon(z) := P(A_\varepsilon - z)^{-1}P^*$, where P denotes the orthogonal projection onto the "part" of the medium which is obtained by removing the inhomogeneities. Note that the generalised resolvent thus defined is a solution operator of a BVP pertaining to homogeneous medium, albeit subject to non-local $z-$dependant boundary conditions. The problem considered therefore reduces to the asymptotic analysis of the operator $B_\varepsilon(z)$, parameterising these conditions. As such, it becomes a classical problem of perturbation theory.

Assuming now, for the sake of argument, that $R_\varepsilon(z)$ has a limit, as $\varepsilon \to 0$, in the uniform operator topology for z in a domain $D \subset \mathbb{C}$, and, further, that the resolvent $(A_\varepsilon - z)^{-1}$ also admits such limit, one clearly has

$$P\big(A_{\text{eff}} - z\big)^{-1}P^* = R_0(z), \quad z \in D \subset \mathbb{C}, \tag{40}$$

where R_0 and A_{eff} are the limits introduced above. The idea of simplifying the required analysis by passing to the resolvent "sandwiched" by orthogonal projections onto a carefully chosen subspace is in fact the same as in [87], where the resulting sandwiched operator is shown to be the resolvent of a dissipative operator.

The function R_0 defined by (40) is a generalised resolvent, whereas A_{eff} is its out-of-space self-adjoint extension (or *Neumark-Strauss dilation* [126]). By a theorem of Neumark [101] (see Section 2.5 of the present paper) this dilation is defined uniquely up to a unitary transformation of a special form, provided that the minimality condition holds. The latter can be reformulated along the following lines: one has minimality, provided that there are no eigenmodes in the effective media modelled by the operator A_ε, and therefore in the medium modelled by the operator A_{eff} as well, such that they "never enter" the part of the medium without inhomogeneities. A quick glance at the setup of our models helps one immediately convince oneself that this must be true. It then follows that the effective medium is completely determined, up to a unitary transformation, by $R_0(z)$. Once this is established, it is tempting to construct its Neumark-Strauss dilation and conjecture, that it is precisely this dilation that the original operator family converges to in the norm-resolvent sense (of course, up to a unitary transformation).

This conjecture in fact holds true, although it is impossible to prove it on the abstract level: taking into account no specifics of problems at hand, one can claim weak convergence at best. Still, the approach suggested seems to be very transparent in allowing to grasp the substance of the problem and to almost immediately "guess" correctly the operator modelling the effective medium.

5 Applications to continuum mechanics and wave propagation

Parameter-dependent problems for differential equations have traditionally attracted much interest within applied mathematics, by virtue of their potential for replacing complicated formulations with more straightforward, and often explicitly solvable, ones. This drive has led to a plethora of asymptotic techniques, from perturbation theory to multi-scale analysis, covering a variety of applications to physics, engineering, and materials science. While this subject area can be viewed as "classical", problems that require new ideas continue emerging, often motivated by novel wave phenomena. One of the recent application areas of this kind is provided by composites and structures involving components with highly contrasting material properties (stiffness, density, refractive index). Mathematically, such problems lead to boundary-value formulations for differential operators with parameter-dependent coefficients. For example, problems of this kind have arisen in the study of periodic composite media with "high contrast" (or "large coupling") between the material properties of the components, see [43, 72, 137].

In what follows, we outline how the contrast parameter emerges as a result of dimensional analysis, using a scalar elliptic equation of second order with periodic coefficients as a prototype example.

5.1 Scaling regimes for high-contrast setups

We will consider the physical context of elastic waves propagating through a medium with whose elastic moduli vary periodically in a chosen plane (say (x_1, x_2)-plane) and are constant in the third, orthogonal, direction (say, the x_3 direction). For example, one could think of a periodic arrangement of parallel fibres of a homogeneous elastic material within a "matrix" of another homogeneous elastic material. We will look at the "polarised" anti-plane shear waves, which can be described completely by a scalar function representing the displacement of the medium in the x_3 direction. In the case of the fibre geometry mentioned above, the relevant elastic moduli G then have the form

$$G(y) = \begin{cases} G_0, & y \in Q_0, \\ G_1, & y \in Q_1, \end{cases} =: \left\{ \begin{array}{c} G_0 \\ G_1 \end{array} \right\}(y).$$

where Q_0, Q_1 are the mutually complementary cross-sections of the fibre and matrix components, respectively, so that $\overline{Q}_0 \cup \overline{Q}_1 = [0,1]^2$. the mass density of the described composite medium is assumed to be constant. (The constants G_0, G_1 are the so-called shear moduli of the materials occupying Q_0, Q_1.) This physical setup was considered in [94, 114].

Denote by d the period of the original "physical" medium and consider time-harmonic wave motions, i.e. solutions of the wave equation that have the form

$$U(x,t) = \mathrm{e}^{\mathrm{i}\omega t} u(x), \qquad x \in \mathbb{R}^2, \quad t \geq 0, \tag{41}$$

where ω is a fixed frequency. In the setting of time-harmonic waves, see (41), the function $u = u(x)$ satisfies the following equation, written in terms of the original physical units:

$$-\nabla_x \cdot \left\{ \begin{array}{c} G_0 \\ G_1 \end{array} \right\}(x/d) \nabla_x u = \rho \omega^2 u, \tag{42}$$

Multiply both sides by G_1^{-1} and denote $\delta := G_0/G_1$. the parameter δ represents the "inverse contrast", which will be assumed "small" later, and corresponds to the value a^{-1} of the "large" parameter of Sections 4.3.2, 4.3.3. The equation (42) takes the form

$$-\nabla_x \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\}(x/d) \nabla_x u = \frac{\rho}{G_1} \omega^2 u$$

Note that

$$\omega = \frac{2\pi c_1}{\lambda_1} = \frac{2\pi c_0}{\lambda_0}, \tag{43}$$

where c_j, λ_j are the wave speed and wavelength in the relevant media ($j = 0, 1$).

Introduce a non-dimensional spatial variable $\tilde{x} = 2\pi x/\lambda_1$:

$$-\frac{4\pi^2}{\lambda_1^2}\nabla_{\tilde{x}} \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} \left(\frac{\tilde{x}}{2\pi d/\lambda_1}\right)\nabla_{\tilde{x}} u = \frac{\rho}{G_1}\omega^2 u,$$

equivalently, with $\varepsilon := 2\pi d/\lambda_1$:

$$-\nabla_{\tilde{x}} \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (\tilde{x}/\varepsilon)\nabla_{\tilde{x}} u = \frac{\rho}{G_1}c_1^2 u,$$

where we have used (43). Note that $c_1\sqrt{\rho/G_1} = 1$ and relabel $\tilde{x}$ by x :

$$-\nabla_x \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (x/\varepsilon)\nabla_x u = u,$$

Let us "scale to the period one" i.e. consider the change of variable $y = \tilde{x}/\varepsilon = x/d$:

$$-\varepsilon^{-2}\nabla_y \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (y)\nabla_y u = u,$$

or

$$-\nabla_y \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (y)\nabla_y u = \left(\frac{2\pi d}{\lambda_1}\right)^2 u.$$

The different scaling regimes, ranging from what we know as "finite frequency, high contrast" to "high frequency, high contrast", are described by setting

$$\varepsilon^2 = \delta^\nu \widetilde{z}, \tag{44}$$

where $\widetilde{z}$ is obviously dimensionless is assumed to vary over the compact K_σ, and $0 \le \nu \le 1$. Note that $\widetilde{z}$ can be alternatively expressed as

$$\widetilde{z} = \delta^{-\nu}\rho G_1^{-1}(d\omega)^2. \tag{45}$$

In particular, the setup analysed in the paper [43] corresponds to the case $\nu = 1$:

$$-\,\delta^{-1}\nabla_y \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (y)\nabla_y u = zu. \tag{46}$$

In terms of the original spatial variable x the equation (46) takes the form

$$-d^2\delta^{-1}\nabla_x \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (x)\nabla_x u = zu,$$

or

$$-\nabla_x \cdot \left\{ \begin{array}{c} \delta \\ 1 \end{array} \right\} (x)\nabla_x u = k^2 u,$$

where the wavenumber (i.e. "spatial frequency") is given by $k := d^{-1}\sqrt{\delta z}$, so that

$$(kd)^2 = \frac{z}{n^2},$$

where $n^2 = \delta^{-1} = G_0/G_1$ is the shear modulus of the material occupying Q_0 relative to the material occupying Q_1.

The setup (46) is the "periodic" version of the formulation discussed in Section 4.3, see also Section 4.2 for the one-dimensional version of a high-contrast homogenisation problem that gives rise to the same formulation. Similarly, choosing the values $\nu = 2/(k+1)$, $k = 2, 3, \dots$, in (44) gives rise to "high-frequency large-coupling" formulations, which in turn lead, in the limit as $\delta \to 0$, to effective operators with an "internal space" of dimension k, see Section 4.3.3. The parameter $\widetilde{z}$ is the related to the spectral parameter z in (39) via

$$z = \widetilde{z}\delta^{1-\nu} = \widetilde{z}\delta^{\frac{k-1}{k+1}} = \widetilde{z}a^{\frac{k+1}{k-1}}, \qquad k = 2, 3, \dots,$$

so that the error estimate in (39) is optimal for $\widetilde{z} \in K_\sigma$, in the sense that for such $\widetilde{z}$ it yields an error of order $a^{-1} \sim |z|^{k+1}a^{-k}$ for large a.

5.2 Homogenisation of composite media with resonant components

5.2.1 Physical motivation

The mathematical theory of homogenisation (see *e.g.* [15, 21, 74]) aims at characterising limiting, or "effective", properties of small-period composites. Following an appropriate non-dimensionalisation procedure, a typical problem here is to study the asymptotic behaviour of solutions to equations of the type

$$-\operatorname{div}\big(A^\varepsilon(\cdot/\varepsilon)\nabla u_\varepsilon\big) - \widetilde{\omega}^2 u_\varepsilon = f, \quad f \in L^2(\mathbb{R}^d), \quad d \geq 2, \qquad \widetilde{\omega}^2 \notin \mathbb{R}_+, \tag{47}$$

where for all $\varepsilon > 0$ the matrix A^ε is Q-periodic, $Q := [0,1)^d$, non-negative, bounded, and symmetric. The parameter $\widetilde{\omega}$ here represents a "non-dimensional frequency": $\widetilde{\omega}^2 = \widetilde{z}$, where $\widetilde{z}$ is the spectral parameter introduced in (44), so for example for $\nu = 1$ one can set $\widetilde{\omega} = d\sqrt{\rho/G_0}\,\omega$, see (45).

One proves (see [28, 136] and references therein) that when A is uniformly elliptic, there exists a constant matrix A^{hom} such that solutions u_ε to (47) converge to u_{hom} satisfying

$$-\operatorname{div}\big(A^{\text{hom}}\nabla u_{\text{hom}}\big) - \widetilde{\omega}^2 u_{\text{hom}} = f. \tag{48}$$

In what follows we write ω, z in place of $\widetilde{\omega}$, $\widetilde{z}$, implying that either the dimensional or non-dimensional version of the equation is chosen.

In recent years, the subject of modelling and engineering a class of composite media with "unusual" wave properties (such as negative refraction) has been brought to the forefront of materials science. Such media are generically referred to as metamaterials, see *e.g.* [38]. In the context of homogenisation, the result sought (*i.e.*, the "metamaterial" behaviour in the limit of vanishing ε) belongs to the domain of the so-called time-dispersive media (see, *e.g.*, [59, 60, 131, 132]). For such media, in the frequency domain one faces equations of the form

$$-\operatorname{div}\big(A\nabla u\big) + \mathfrak{B}(\omega^2)u = f, \quad f \in L^2(\mathbb{R}^d), \tag{49}$$

where A is a constant matrix and $\mathfrak{B}(\omega^2)$ is a frequency-dependent operator in $L^2(\mathbb{R}^d)$ taking the place of $-\omega^2$ in (47), if, for the sake of argument, in the time domain we started with an equation of second order in time. If, in addition, the matrix function $\mathfrak{B}$ is scalar, *i.e.*, $\mathfrak{B}(\omega^2) = \beta(\omega^2)I$ with a scalar function β, the problem of the type

$$-\operatorname{div}\big(A^{\text{hom}}(\omega^2)\nabla u\big) = \omega^2 u \tag{50}$$

appears in place of the spectral problem after a formal division by $-\beta(\omega^2)/\omega^2$, with frequency-dependent (but independent of the spatial variable) matrix $A^{\rm hom}(\omega^2)$.

In the equation (50), in contrast to (48), the matrix elements of $A^{\rm hom}$, interpreted as material parameters of the medium, acquire a non-trivial dependence on the frequency, which may lead to their taking negative values in some frequency intervals. The possibility of electromagnetic media exhibiting negative refraction was envisaged in an early work [134], who showed theoretically that the material properties of such media must be frequency-dependent, and the last two decades have seen a steady advance towards realising such media experimentally. One may hope that upon relaxing the condition of uniform ellipticity on A^ε one may be able to achieve a metamaterial-type response to wave propagation for sufficiently small values of ε. It is therefore important to understand how inhomogeneity in the spatial variable in (47) can lead, in the limit $\varepsilon \to 0$, to frequency dispersion as in (49).

5.2.2 Operator-theoretic motivation

Already in the setting of finite-dimensional matrix algebra equations of the form (see (49))

$$Au + \mathfrak{B}(z)u = f, \qquad u \in \mathbb{C}^d, \tag{51}$$

where $A = A^* \in \mathbb{C}^{d\times d}$, $f \in \mathbb{C}^d$, $\mathfrak{B}$ is a Herglotz function with values in $\mathbb{C}^{d\times d}$, emerge when one seeks solutions to the standard resolvent equation for a block matrix:

$$\begin{pmatrix} A & B \\ B^* & C \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} - z\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} u \\ v \end{pmatrix} \in \mathbb{C}^{d+k}. \tag{52}$$

where $B \in \mathbb{C}^{k\times d}$, $C = C^* \in \mathbb{C}^{k\times k}$.

Indeed, it is the result of a straightforward calculation that (52) implies

$$Au - (B(C-z)^{-1}B^* + zI)u = f,$$

whenever $-z$ is not an eigenvalues of C, so (52) implies (51) with $\mathfrak{B}(z) = -B(C-z)^{-1}B^* - zI$. Another consequence of the above calculation is that for any vector $(f, g)^\top \in \mathbb{C}^{d+k}$ one has

$$u = P\left\{\begin{pmatrix} A & B \\ B^* & C \end{pmatrix} + zI\right\}^{-1} P * \begin{pmatrix} f \\ g \end{pmatrix},$$

where P is the orthogonal projection of $\mathbb{C}^{d+k}$ onto $\mathbb{C}^k$ and P^* is interpreted as a restriction to the k-dimensional subspace of vectors of the form $(f, 0)^\top$, $f \in \mathbb{C}^k$.

The above argument, in the more general setting of block operator matrices in a Hilbert space, likely appeared for the first time in [59]. "Generalised resolvents", i.e. objects of the form

$$P(\mathcal{A} - z)^{-1}P^*, \tag{53}$$

where $\mathcal{A}$ is an operator in a Hilbert space $\mathcal{H}$ and P is an orthogonal projection of $\mathcal{H}$ onto its subspace H have already been discussed in the present survey, see Sections 2.5, 4.4. As discussed in Section 2.5, abstract results of Neumark and Strauss [101, 126] establish that solution operators for formulations (51), where A is a self-adjoint operator in a Hilbert space H can be written in the form (53) for a suitable "out-of-space" extension $\mathcal{A}$. Therefore, a natural question is whether formulations (49) can be viewed as generalised resolvents obtained by an asymptotic analysis of some parameter-dependent operator family describing a heterogeneous medium. One piece of evidence pointing at the validity of such a conjecture is the result of Section 4.3.2, where the role of the operator $\mathcal{A}$ in (53) is played by $\mathcal{A}_{\text{eff}}$, see (38).

In [41,42,44] a model of a high-contrast graph periodic along a single direction was considered. A unified treatment of critical-contrast homogenisation was proposed and carried out in three distinct cases: (i) where neither the soft nor the stiff component of the medium is connected; (ii) where the stiff component of the medium is connected; (iii) where the soft component of the medium is connected. The analytical toolbox presented in these works was then amplified to the PDE setting in [43]. In the wider context of operator theory and its applications, this provides a route towards: constructing explicit spectral representations and functional models for both homogenisation limits of critical-contrast composites and the related time-dispersive models, as well as solving the related direct and inverse scattering problems.

5.2.3 Prototype problem setups in the PDE context

Consider the problem (47) under the following assumptions:

$$A^{\varepsilon}(y) = \begin{cases} aI, & y \in Q_{\text{stiff}}, \\ \varepsilon^2 I, & y \in Q_{\text{soft}}, \end{cases}$$

where Q_{soft} (Q_{stiff}) is the soft (respectively, stiff) component of the unit cube $Q = [0,1)^d \subset \mathbb{R}^d$, so that $\overline{Q} = \overline{Q}_{\text{soft}} \cup \overline{Q}_{\text{stiff}}$, and $a > 0$.

Two distinct setups were studied in [43]. For one of them ("Model I"), which is unitary equivalent to the model of [62, 72], the component $Q_{\text{soft}} \subset Q$ is simply connected and and its distance to ∂Q is positive, *cf.* [40, 137]. For the other one ("Model II") the component Q_{stiff} has the described properties. It is assumed that the Dirichlet-to-Neumann maps for Q_{soft} and Q_{stiff}, which map the boundary traces of harmonic functions in Q_{soft} and Q_{stiff} to their boundary normal derivatives, are well-defined as pseudo-differential operators of order one in the L^2 space on the boundary [1, 10, 61, 73].

For both above setups, [43] deals with the resolvent $(A_\varepsilon - z)^{-1}$ of a self-adjoint operator in $L^2(\mathbb{R}^d)$ corresponding to the problem (47), so that its solutions are expressed as $u_\varepsilon = (A_\varepsilon - z)^{-1} f$ with $z = \omega^2$. For each $\varepsilon > 0$, the operator A_ε is defined by the forms

$$\int_{\mathbb{R}^d} A^{\varepsilon}(\cdot/\varepsilon)\nabla u \cdot \overline{\nabla u}, \qquad u, v \in H^1(\mathbb{R}^d).$$

It is assumed that $z \in \mathbb{C}$ is separated from the spectrum of the original operator family, in particular $z \in K_\sigma$, where K_σ is defined in Theorem 4.1.

In order to deal with operators having compact resolvents, it is customary to apply Gelfand transform [64], which we review next.

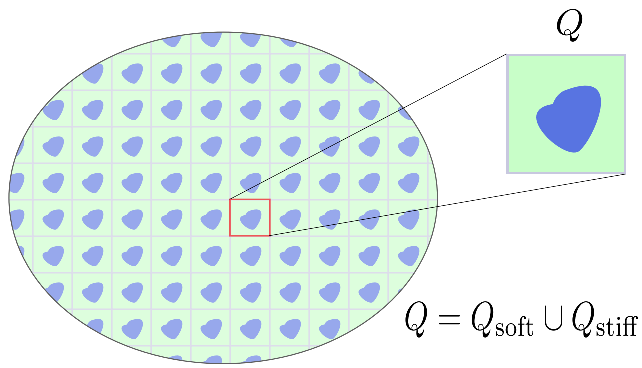

Figure 2: Model setups. Model I: soft component Q_{soft} in blue, stiff component Q_{stiff} in green. Model II: soft component Q_{soft} in green, stiff component Q_{stiff} in blue.

5.2.4 Gelfand transform and direct integral

The version of the Gelfand transform convenient for the analysis of the operators A_ε is defined on functions $u \in L^2(\mathbb{R}^d)$ by the formula[4] (*cf.* (34))

$$G_\varepsilon u(y,t) := \left(\frac{\varepsilon^2}{2\pi}\right)^{d/2} \sum_{n\in\mathbb{Z}^d} u\big(\varepsilon(y+n)\big)\exp\big(-\mathrm{i}\tau\cdot(y+n)\big), \quad y\in Q, \quad \tau \in Q' := [-\pi,\pi)^d,$$

This yields a unitary operator $G_\varepsilon : L^2(\mathbb{R}^d) \longrightarrow L^2(Q\times Q')$, and the inverse with the inverse mapping given by

$$u(x) = (2\pi)^{-d/2}\int_{Q'} G_\varepsilon u\left(\frac{x}{\varepsilon},\tau\right)\exp\left(\mathrm{i}\tau\cdot\frac{x}{\varepsilon}\right)d\tau, \qquad x\in\mathbb{R}^d,$$

where $G_\varepsilon u$ is extended to $\mathbb{R}^d \times Q'$ by Q-periodicity in the spatial variable.

As in [28], an application of the Gelfand transform G to the operator family A_ε corresponding to the problem (47) yields the two-parametric family $A_\varepsilon^{(\tau)}$ of operators in $L^2(Q)$ given by the differential expression

$$-(\nabla + \mathrm{i}\tau)A^\varepsilon(x/\varepsilon)(\nabla+\mathrm{i}\tau), \qquad \varepsilon>0, \quad \tau\in Q',$$

subject to periodic boundary conditions $\partial(\varepsilon Q)$ and defined by the corresponding closed coercive sesquilinear form. For each $\varepsilon > 0$, the operator A_ε is then unitary equivalent to the von Neumann integral (see *e.g.* [27, Chapter 7]) of $A_\varepsilon^{(\tau)}$:

$$A_\varepsilon = G_\varepsilon^*\left(\oplus\int_{Q'} A_\varepsilon^{(\tau)} d\tau\right)G_\varepsilon.$$

Similar to [62] and facilitated by the abstract framework of [120], the operator $A_\varepsilon^{(\tau)}$ can be associated to transmission problems [121], akin to those considered in Section 4.3.2. To this end,

[4] The formula (34) is first applied to continuous functions U with compact support, and then extended to the whole of $L^2(\mathbb{R}^d)$ by continuity.

consider Q as a torus with the opposite parts of ∂Q identified, and view $Q_{\rm soft}$ and $Q_{\rm stiff}$ as subsets of this torus. Furthermore, in line with the notation of Section 4.3.2, denote by Γ the interface between $Q_{\rm soft}$ and $Q_{\rm stiff}$. For each ε, τ, $f \in L^2(Q)$, the transmission problem is formulated as finding a function $u \in L^2(Q)$ such that $u|_{Q_{\rm soft}} \in H^1(Q_{\rm soft})$, $u|_{Q_{\rm stiff}} \in H^1(Q_{\rm stiff})$, that solves, in the weak sense, the boundary-value problem (*cf.* (37))

$$\begin{cases} -\varepsilon^{-2}(\nabla + {\rm i}\tau)^2 u_+ - z u_+ = f \quad \text{in} \;\; Q_{\rm stiff}, \\ -(\nabla + {\rm i}\tau)^2 u_- - z u_- = f \quad \text{in} \;\; Q_{\rm soft}, \\ u_+ = u_-, \qquad \Big(\dfrac{\partial}{\partial n_+} + {\rm i}\tau\cdot n_+\Big) u_+ + \varepsilon^{-2}\Big(\dfrac{\partial}{\partial n_-} + {\rm i}\tau\cdot n_-\Big) u_- = 0, \quad \text{on} \;\; \Gamma. \end{cases}$$

where n_+ and $n_- = -n_+$ are the outward normals to Γ with respect to $Q_{\rm soft}$ and $Q_{\rm stiff}$. By a classical argument the weak solution of the above problem is shown to coincide with $(A_\varepsilon^{(\tau)} - z)^{-1} f$.

5.2.5 Homogenised operators and convergence estimates

Throughout this section, $H_{\rm hom} := L^2(Q_{\rm soft}) \oplus \mathbb{C}^1$, $\mathcal{H} := L^2(\Gamma)$, and $\partial_n^\tau u := -(\partial u/\partial n + {\rm i}\tau\cdot n u)|_\Gamma$ is the co-normal boundary derivative for $Q_{\rm soft}$.

Model I. Set

$$\operatorname{dom}\mathcal{A}_{\rm hom}^{(\tau)} = \Big\{(u,\beta)^\top \in H_{\rm hom}: \; u \in H^2(Q_{\rm soft}), u|_\Gamma = \langle u|_\Gamma, \psi_0\rangle_{\mathcal{H}}\psi_0 \text{ and } \beta = \kappa\langle u|_\Gamma, \psi_0\rangle_{\mathcal{H}}\Big\},$$

where $\kappa := |Q_{\rm stiff}|^{1/2}/|\Gamma|^{1/2}$, $\psi_0(x) = |\Gamma|^{-1/2}$, $x \in \Gamma$, and define

$$\mathcal{A}_{\rm hom}^{(\tau)}\begin{pmatrix} u \\ \beta\end{pmatrix} = \begin{pmatrix} -(\nabla + {\rm i}\tau)^2 u \\ -\kappa^{-1}\langle \partial_n^\tau u|_\Gamma, \psi_0\rangle_{\mathcal{H}} - \kappa^{-2}\varepsilon^{-2}(\mu_*\tau\cdot\tau)\beta \end{pmatrix}, \qquad \begin{pmatrix} u \\ \beta\end{pmatrix} \in \operatorname{dom}\mathcal{A}_{\rm hom}^{(\tau)},$$

where $\mu_*\tau\cdot\tau$ is the leading-order term (for small τ) of the first Steklov eigenvalue for $-(\nabla + {\rm i}\tau)^2$ on $Q_{\rm soft}$.

Model II. Set

$$\operatorname{dom}\mathcal{A}_{\rm hom}^{(\tau)} = \Big\{(u,\beta)^\top \in H_{\rm hom}: \; u \in H^2(Q_{\rm soft}), u|_\Gamma = \langle u|_\Gamma, \psi_\tau\rangle_{\mathcal{H}}\psi_\tau \text{ and } \beta = \kappa\langle u|_\Gamma, \psi_\tau\rangle_{\mathcal{H}}\Big\},$$

where κ is as above and $\psi_\tau(x) = |\Gamma|^{-1/2}\exp(-{\rm i}\tau\cdot x)|_\Gamma$, $x \in \Gamma$. The action of the operator is set by

$$\mathcal{A}_{\rm hom}^{(\tau)}\begin{pmatrix} u \\ \beta\end{pmatrix} = \begin{pmatrix} -(\nabla + {\rm i}\tau)^2 u \\ -\kappa^{-1}\langle \partial_n^\tau u|_\Gamma, \psi_\tau\rangle_{\mathcal{H}} \end{pmatrix}, \qquad \begin{pmatrix} u \\ \beta\end{pmatrix} \in \operatorname{dom}\mathcal{A}_{\rm hom}^{(\tau)}.$$

Convergence estimate. Set $\gamma = 2/3$ for the case of Model I and $\gamma = 2$ for the case of Model II. The resolvent $(A_\varepsilon^{(\tau)} - z)^{-1}$ admits the following estimate in the uniform operator-norm topology:

$$\big(A_\varepsilon^{(\tau)} - z\big)^{-1} - \Theta^*\big(\mathcal{A}_{\rm hom}^{(\tau)} - z\big)^{-1}\Theta = O(\varepsilon^\gamma), \tag{54}$$

where Θ is a partial isometry from $L^2(Q)$ onto $H_{\rm hom}$: on the subspace $L^2(Q_{\rm soft})$ it coincides with the identity, and each function from $L^2(Q_{\rm stiff})$ represented as an orthogonal sum

$$c_\tau\|\Pi_{\rm stiff}\psi_\tau\|^{-1}\Pi_{\rm stiff}\psi_\tau \oplus \xi_\tau, \qquad c_\tau \in \mathbb{C}^1,$$

is mapped to c_τ unitarily. Here $\Pi_{\rm stiff}$ maps φ on Γ to the solution u_φ of $-(\nabla + {\rm i}\tau)^2 u_\varphi = 0$ in $Q_{\rm soft}$, $u_\varphi|_\Gamma = \varphi$. The estimate (54) is uniform in $\tau \in Q'$ and $z \in K_\sigma$.

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