On Supersingular Perturbations

Christoph Neuner

Abstract
This thesis consists of four papers and deals with supersingular rank one perturbations of self-adjoint operators and their models in Hilbert or Pontryagin spaces. Here, the term supersingular describes perturbation elements that are outside the underlying space but still obey a certain regularity conditions.

The first two papers study certain Sturm-Liouville differential expressions that can be realised as Schrödinger operators. In Paper I we show that for the potential consisting of the inverse square plus a comparatively well-behaved term we can employ an existing model due to Kurasov to describe these operators in a Hilbert space. In particular, this approach is in good agreement with ODE techniques.

In Paper II we study the inverse fourth power potential.While it is known that the ODE techniques still work, we show that the above model fails and thus that there are limits to the above operator theoretic approach.

In Paper III we concentrate on generalising Kurasov's model. The original formulation assumes that the self-adjoint operator is semi-bounded, whereas we drop this requirement. We give two models with a Hilbert and Pontryagin space structure, respectively, and study the connections between the resulting constructions.

Finally, in Paper IV, we consider the concrete case of the operator of multiplication by the independent variable, a self-adjoint operator whose spectrum covers the real line, and study its perturbations. This illustrates some of the formalism that was developed in the previous paper, and a number of more explicit results are obtained, especially regarding the spectra of the appearing perturbed operators.

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Sammanfattning

Denna avhandling består av fyra artiklar och behandlar supersingulära rang-ett-störningar av självadjungerade operatorer samt deras modeller i Hilbert-eller Pontryaginrum. Med supersingulära störningar avses här sådana störningselement som ligger utanför rummet där operatorn agerar men som ändå uppfyller vissa regularitetsvillkor.

De första två artiklarna handlar om speciella Sturm-Liouville differentialuttryck som kan realiseras som Schrödingeroperatorer. I den första artikeln studerar vi fallet där potentialen består av en inverterad kvadratisk term, samt en term som beter sig mindre singulärt vid origo. Vi visar att en modell skapad av Kurasov kan tillämpas för att beskriva dessa operatorer i ett Hilbertrum. Resultaten från denna metod är ekvivalenta med dem vi kan förvänta oss från ODE-tekniker.

I den andra artikeln undersöker vi fallet där potentialen är en inverterad kvartisk term. Det är känt att ODE-tekniker även fungerar här men vi visar att Kurasovs modell inte längre är applicerbar. Modellen har alltså vissa begränsningar i jämförelse med metoder från ODE-teorin.

I den tredje artikeln koncentrerar vi oss på att generalisera Kurasovs modell. I den ursprungliga formuleringen antas att den självadjungerade operatorn är begränsad nedåt, något som vi i denna artikel inte antar. Vi konstruerar två modeller som har antingen en Hilbert- eller Pontryaginrumsstruktur och undersöker relationen mellan dessa modeller.

I den sista artikeln studerar vi perturbationer av en specifik självadjungerad operator vars spektrum täcker hela den reella linjen, nämligen operatorn som multiplicerar en funktion med den oberoende variabeln. Detta exempel illustrerar delar av den formalism vi utvecklade i den tredje artikeln. Vi erhåller också en del konkreta resultat, speciellt angående spektrum av de störda operatorerna.

Zusammenfassung

Die vorliegende Arbeit besteht aus vier Artikeln und befasst sich mit supersingulären Rang-eins-Störungen selbstadjungierter Operatoren sowie deren Hilbert- oder Pontryaginraummodellen. Als supersingulär bezeichnen wir hier Störungsvektoren, die außerhalb jenes Raums, wo der gegebene Operator agiert, liegen, aber immer noch gewisse Regularitätsbedingungen erfüllen.

Die ersten beiden Artikel behandeln gewisse Sturm-Liouville-Differentialausdrücke, die sich als Schrödingeroperatoren realisieren lassen. Im ersten Artikel zeigen wir, dass für ein Potential, das aus einem invers quadratischen sowie einem vergleichsweise milderen Term besteht, ein bestehendes Modell von Kurasov angewandt werden kann, um die gestörten Operatoren zu beschreiben. Es zeigt sich, dass dieser Zugang vergleichbare Ergebnisse wie jene aus der Theorie gewöhnlicher Differentialgleichungen liefert.

Im zweiten Artikel untersuchen wir den Fall eines quartisch inversen Potentials. Hier ist zwar bekannt, dass der Differentialgleichungszugang weiterhin funktioniert, aber wir zeigen, dass das genannte Modell hier an seine Grenzen stößt und nicht mehr anwendbar ist.

Im dritten Artikel konzentrieren wir uns darauf, Kurasovs Modell zu verallgemeinern. In der ursprünglichen Formulierung waren die vorkommenden Operatoren als halbbeschränkt vorausgesetzt, was wir hier hingegen nicht mehr annehmen. Wir konstruieren zwei Modelle mit einer Hilbert- bzw. Pontryaginraumstruktur und studieren, wie diese zusammenhängen.

Im letzten Artikel betrachten wir einen konkreten selbstadjungierten Operator, dessen Spektrum die gesamte reelle Linie einnimmt, nämlich den Operator, der eine Funktion mit der unabhängigen Variablen multipliziert. Wir studieren seine Störungen und illustrieren so den Formalismus aus dem vorangegangenen Artikel. Außerdem können wir auf diese Weise explizite Aussagen über die vorkommenden gestörten Operatoren, besonders im Bezug auf ihr Spektrum, tätigen.

List of Papers

The following papers, referred to in the text by their Roman numerals, are included in this thesis.

PAPER I: **An Operator Theoretic Interpretation of the Generalized Titch-marsh-Weyl Function for Perturbed Spherical Schrödinger Operators**
Luger, A. & Neuner, C., *Complex Anal. Oper. Theory*, **9**, 1391-1410 (2015).
DOI: 10.1007/s11785-014-0425-8

PAPER II: **On the Weyl solution of the 1-dim Schrödinger operator with inverse fourth power potential**
Luger, A. & Neuner, C., *Monatsh Math*, **180**, 295-303 (2016).
DOI: 10.1007/s00605-015-0826-4

PAPER III: **On supersingular perturbations of not necessarily semibounded self-adjoint operators**
Kurasov, P., Luger, A. & Neuner, C., *submitted* (2017).

PAPER IV: **Some supersingular perturbations of a multiplication operator**
Neuner, C., *manuscript* (2017).

Contents

Acknowledgements

Introduction

This thesis consists of four papers. The research contained therein is concerned with topics in mathematical analysis. It uses and develops the technique of supersingular perturbations of self-adjoint operators and touches, in particular, on the following three areas: extension theory of symmetric operators, Sturm-Liouville problems with strongly singular potentials, and — naturally appearing every now and then — Nevanlinna functions. We shall therefore introduce these subjects in the following. In the end of this introduction we shall give a short summary of the papers included in this thesis.

We also already point out here in the beginning that the second half of this introduction, entitled Sturm-Liouville problems, was adapted from the licentiate thesis [30]. By this we mean that some parts have been shortened as well as that notation and examples have been unified. Furthermore, Papers I and II were also included in the licentiate.

1 Supersingular Perturbations of Self-adjoint Operators

Let us start with some perturbation theory for self-adjoint operators. In the end we would like to understand formal sums like

$$A + \alpha \langle \varphi, \cdot \rangle \varphi$$

for a self-adjoint operator A in a Hilbert space $\mathcal{H}$, numbers $\alpha \in \mathbb{R} \cup \{\infty\}$ and a perturbation element φ. It should already be noted here that we do not demand φ to be a vector from the Hilbert space.

1.1. Self-adjoint and Symmetric Operators A (complex) Hilbert space $\mathcal{H}$ is a vector space (over the base field $\mathbb{C}$) with an inner product $\langle \cdot, \cdot \rangle$ that is also complete in the norm $\| \cdot \| := \sqrt{\langle \cdot, \cdot \rangle}$ induced by the scalar product. We will, unless specifically stated otherwise, always consider the scalar product to be linear in the second entry.

If one sticks to finite dimensions and considers $\mathbb{C}^n$ for $1 < n < \infty$ one can study linear mappings in this space, i.e., $n \times n$-matrices. An especially nice class of such mappings are self-adjoint matrices, that is $A \in \mathbb{C}^{n \times n}$ satisfying

$$\langle Ax, y \rangle = \langle x, Ay \rangle \qquad \forall x, y \in \mathbb{C}^n \tag{1.1}$$

or, equivalently,

$$A = A^* := A^H \tag{1.2}$$

where A^H is the Hermitian (conjugate transpose) of A. Remember the eigenvalue equation $Ax = \lambda x$ with $\lambda \in \mathbb{C}$ and $x \in \mathbb{C}^n$, where the nonzero vectors x solving the equation are referred to as eigenvectors and the accompanying λ as eigenvalue. In the case of a self-adjoint matrix A, all eigenvalues turn out to be real and it is possible to choose an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors of A. Furthermore, self-adjoint matrices allow for a spectral theorem.

Theorem 1.1. *Let $A = A^* \in \mathbb{C}^{n \times n}$. Let $\lambda_1, \ldots, \lambda_n$ be the eigenvalues of A counted with multiplicities, and $x_1, \ldots, x_n$ a set of corresponding orthogonal eigenvectors of A. If P_j is the orthogonal projection onto x_j for $j = 1, \ldots, n$ then*

$$A = \sum_{j=1}^{n} \lambda_j P_j.$$

However, there are also Hilbert spaces $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ of infinite dimensions and the study of linear mappings therein. In this setting, one works with operators $T : \operatorname{dom} T \to \mathcal{H}$ that are no longer necessarily defined everywhere in the Hilbert space but instead on $\operatorname{dom} T \subseteq \mathcal{H}$. The set $\operatorname{dom} T$ is called the domain of T and we call T densely defined if $\operatorname{dom} T$ is a dense subset of $\mathcal{H}$. Also in this setting there is a notion of self-adjointness. In finite dimensions, the defining features (1.1) and (1.2) both lead to the same class of matrices. In infinite dimensions, they describe different classes of operators.

Definition 1.2. Let $T : \operatorname{dom} T \to \mathcal{H}$ be densely defined. Then its adjoint T^* is given by the operator

$$\operatorname{dom} T^* := \{ x \in \mathcal{H} : \exists! \, h_x \in \mathcal{H} \text{ such that } \langle x, Ty \rangle = \langle h_x, y \rangle \, \forall y \in \operatorname{dom} T \}$$
$$T^* x := h_x$$

With this notion the generalisation of (1.2) is immediate.

Definition 1.3. A densely defined operator $A : \operatorname{dom} A \to \mathcal{H}$ is called self-adjoint if $A = A^*$.

If S, T are two operators in $\mathcal{H}$ then writing $S \subset T$ means that $\operatorname{dom} S \subset \operatorname{dom} T$ and $Sx = Tx$ for all x belonging to the smaller set $\operatorname{dom} S$. With this in mind, it turns out that requiring something like (1.1) to hold at least for all vectors from the domain of some operator S gives only that $S \subseteq S^*$. Hence, we arrive at a second, larger class of operators.

Definition 1.4. A densely defined operator $S : \operatorname{dom} S \to \mathcal{H}$ is called symmetric if $\langle Sx, y \rangle = \langle x, Sy \rangle$ holds for all $x, y \in \operatorname{dom} S$.

For self-adjoint operators in infinite dimensional Hilbert spaces there is a spectral theorem again and it remains true that self-adjoint operators have only real spectrum. The spectrum $\sigma(T)$ is the set of those $\lambda \in \mathbb{C}$ for which $T - \lambda$ is not bijective; its complement is called the resolvent set $\rho(T)$. It is known from elementary operator theory that the spectrum of an operator contains the set of eigenvalues, i.e., when the kernel $\ker(T - \lambda)$ is nontrivial, just as in the finite-dimensional setting. We mention, however, that the spectrum can contain also other points that are no eigenvalues as in the infinite-dimensional setting $T - \lambda$ can be injective but fail to be surjective.

Theorem 1.5. *Let $A = A^*$ be a densely defined self-adjoint operator in a Hilbert space $\mathcal{H}$. Then there exists a unique resolution of the identity $E_\lambda(\cdot)$ that is concentrated on the spectrum $\sigma(A) \subseteq \mathbb{R}$ of A and such that*

$$A = \int_{\sigma(A)} t \, dE(t).$$

We point out that this also means that self-adjoint operators are unitarily equivalent to multiplication operators, that is, they can in a certain sense be diagonalized.
Self-adjoint operators also play a big role in mathematical physics where they for example appear as observables in formulations of quantum mechanics.

1.2. Extension Theory of Symmetric Operators An operator being self-adjoint implies also that it is symmetric but not the other way round. Considering the notations $A = A^*$ versus $S \subseteq S^*$ it is not just a question of how an operator acts but rather where it is defined that gives information about symmetry or self-adjointness. For operators $R \subseteq T$ going to adjoints yields $T^* \subseteq R^*$. So, informally speaking, given a symmetric operator $S \subseteq S^*$ it begs the question if it is possible to somehow extend S — or equivalently restrict S^* — to a self-adjoint operator. In other words, does there exist a self-adjoint operator A such that

$$S \subseteq A = A^* \subseteq S^*$$

is satisfied? And if yes, how many such extensions are there? This classical question is investigated in the extension theory of symmetric operators, cf. for example [31].

An operator is called closed if its graph is closed. It is called closable if it can be extended to a closed operator. Symmetric operators are closable, so it is no loss of generality to only deal with closed symmetric operators from now on.

We will come back to the following example at different places in this introduction to illustrate some of the appearing concepts.

Example (Part I)**.** Let $\mathcal{H} := L^2(0,\infty)$ and consider the differential expression $\tau := -\frac{d^2}{dx^2}$, the formal operation of taking the negative second derivative. Let

$$\mathcal{D}_{\max} := \left\{ f \in \mathcal{H} : f, f' \in AC_{loc}(0,\infty), f'' \in L^2(0,\infty) \right\},$$

i.e., all functions that are locally absolutely continuous, that have derivatives with the same property and square integrable second derivatives. We define an operator $L_{\max}$ on $\operatorname{dom} L_{\max} := \mathcal{D}_{\max}$ and with action $L_{\max} f := \tau f = -f''$, which will be called the maximal operator as it is defined on the largest possible set in $\mathcal{H}$. If we consider the domain

$$\mathcal{D}_{\min} := \left\{ f \in \mathcal{D}_{\max} : f(0) = f'(0) = 0 \right\},$$

and set $L_{\min} := L_{\max}|_{\mathcal{D}_{\min}}$ then the so-called minimal operator $L_{\min}$ is symmetric and its adjoint turns out to be just $L_{\max}$. An example for a self-adjoint operator is $L_0 := L_{\max}|_{\mathcal{D}_0}$ with the set

$$\mathcal{D}_0 := \left\{ f \in \mathcal{D}_{\max} : f(0) = 0 \right\}.$$

It is clear from the description that in this case

$$L_{\min} \subseteq L_0 = L_0^* \subseteq L_{\max} = L_{\min}^*$$

holds.   ◇

Von Neumann's Approach   The following well-known concepts can be found with more details for example in [12] or [31]. Recall that for elements λ from the resolvent set $\rho(T)$ of an operator the expression $T - \lambda$ is bijective. The inverse $(T - \lambda)^{-1}$ is called the resolvent and it is a bounded, i.e., continuous, operator that is defined everywhere. We also mention here the important resolvent identity

$$(T - \lambda)^{-1} - (T - \mu)^{-1} = (\lambda - \mu)(T - \lambda)^{-1}(T - \mu)^{-1} \qquad \lambda \neq \mu. \qquad (1.3)$$

Dropping the requirement that the resolvent be defined everywhere characterizes the so-called points of regular type $r(T)$. Clearly, they encompass the resolvent set. For a symmetric operator it turns out that there are at most two connected components, containing the upper and lower half-planes $\mathbb{C}^\pm$. Furthermore, it is in general true that on each component of $r(T)$ the dimension of the orthogonal complement of $\mathrm{ran}(T-\lambda)$ is constant.

Definition 1.6. Let $S \subseteq S^*$ be a densely defined closed symmetric operator. Then

$$\mathfrak{N}_\lambda := (\mathrm{ran}(S-\overline{\lambda}))^\perp = \ker(S^*-\lambda)$$

for $\lambda \in \mathbb{C}\backslash\mathbb{R}$ are called defect spaces and

$$n_\pm := \dim \mathfrak{N}_\lambda \qquad \lambda \in \mathbb{C}^\pm$$

are called the defect indices of S.

Given the defect spaces one can show von Neumann's first formula.

Theorem 1.7. *Let $S \subseteq S^*$ be a closed densely defined symmetric operator and $\lambda \neq \overline{\lambda}$. Then*

$$\mathrm{dom}\, S^* = \mathrm{dom}\, S \dotplus \mathfrak{N}_\lambda \dotplus \mathfrak{N}_{\overline{\lambda}}.$$

It then immediately follows that a symmetric operator is self-adjoint iff its defect indices are $(n_+, n_-) = (0,0)$. If the defect indices are not trivial, the question arises when there are self-adjoint extensions A of S, i.e., operators that fit

$$S \subseteq A = A^* \subseteq S^*.$$

An answer can again be given in terms of the defect indices.

Theorem 1.8. *A closed densely defined symmetric operator $S \subseteq S^*$ has self-adjoint extensions in $\mathcal{H}$ iff $n_+ = n_-$.*

The proof of this usually proceeds as follows: translate the problem to investigating when a partial isometry T, i.e., it satisfies $\langle Tx, Ty\rangle = \langle x, y\rangle$ for $x, y \in \mathrm{dom}\, T$, can be extended to a unitary operator, i.e., an isometry that is defined everywhere. This is achieved via the Cayley transform, i.e., one considers $T := \mathcal{C}(S) = (S+i)(S-i)^{-1}$. This T is then a partial isometry and has the property that it maps $\mathrm{ran}(S-i) = \mathfrak{N}_i^\perp$ into $\mathrm{ran}(S+i) = \mathfrak{N}_i^\perp$. Hence, we are in the following situation:

$$
\left\{
\begin{array}{ccc}
T: & \mathfrak{N}_{\overline{i}}^\perp & \longrightarrow & \mathfrak{N}_i^\perp \\
& \oplus & & \oplus \\
& \mathfrak{N}_{\overline{i}} & \overset{?}{\dashrightarrow} & \mathfrak{N}_i
\end{array}
\right.
$$

So extending T to a unitary operator U in $\mathcal{H}$ boils down to requiring the dimensions of $\mathfrak{N}_{\bar{i}}$ and $\mathfrak{N}_i$ to be the same. Going back via the inverse Cayley transform, one sees that $A := \mathcal{C}^{-1}(U)$ is a self-adjoint extension of S. Moreover, one sees from this how von Neumann's second formula parametrises all self-adjoint extensions of a given symmetry.

Theorem 1.9. *Every self-adjoint extension A^V of a closed densely defined symmetric operator $S \subseteq S^*$ with equal defect indices $n_+ = n_-$ is given by*

$$\operatorname{dom} A^V = \operatorname{dom} S \dotplus (V + I)\mathfrak{N}_i$$

where $V : \mathfrak{N}_\lambda \to \mathfrak{N}_{\bar{\lambda}}$ is unitary.

Remark 1.10. One can also just parametrise symmetric extensions $\tilde{S}$ of S, i.e. one has $S \subseteq \tilde{S} \subsetneq \tilde{S}^* \subseteq S^*$, by using $\tilde{V}$ which maps a subspace of $\mathfrak{N}_\lambda$ unitarily into an equally dimensioned subspace of $\mathfrak{N}_{\bar{\lambda}}$. $\diamond$

Thus, von Neumann's theory gives a complete picture of when self-adjoint extensions exist and what they look like.

Example (Part II). Let us continue with the previous example and the operators $L_{\min} \subseteq L_0 \subseteq L_{\max}$. We see that the defect spaces for the symmetry $L_{\min}$ is one-dimensional as $\mathfrak{N}_\lambda = \ker(L_{\max} - \lambda) = \operatorname{span}\left\{ e^{-\sqrt{-\lambda}x} \right\}$ when λ is nonreal and where we take the branch cut of the square root along the negative real axis. Hence, $L_{\min}$ has defect indices $(1,1)$. In contrast to this, note that $\ker(L_0 - \lambda) = \{0\}$ for all nonreal λ so that L_0 has indeed defect indices $(0,0)$. By von Neumann's first formula, we can thus write

$$\mathcal{D}_{\max} = \mathcal{D}_{\min} \dotplus \operatorname{span}\left\{ e^{-\sqrt{-\lambda}x} \right\} \dotplus \operatorname{span}\left\{ e^{-\sqrt{-\bar{\lambda}}x} \right\}.$$

If V_θ with $\theta \in [0, 2\pi)$ is defined from $e^{-\sqrt{-\lambda}x} \mapsto e^{i\theta} e^{-\sqrt{-\bar{\lambda}}x}$ then the domain of a self-adjoint extension L^V of $L_{\min}$ is given by

$$\operatorname{dom} L^{V_\theta} = \mathcal{D}_{\min} \dotplus (V_\theta + I) \operatorname{span}\left\{ e^{-\sqrt{-\lambda}x} \right\}.$$

In terms of boundary values at the origin, it can be deduced that a function belongs to this domain if it satisfies a condition of the form

$$f(0) = \frac{e^{-i\theta/2} + e^{i\theta/2}}{-\sqrt{-\lambda}e^{-i\theta/2} - \sqrt{-\bar{\lambda}}e^{i\theta/2}} f'(0) =: s_\lambda(\theta) f'(0)$$

with the parameter $s_\lambda(\theta) \in \mathbb{R} \cup \{\infty\}$ depending on the chosen unitary operator V_θ, i.e., it also holds that

$$\operatorname{dom} L^{V_\theta} = \left\{ f \in \mathcal{D}_{\max} : f(0) = s_\lambda(\theta) f'(0) \right\}.$$

In particular, for $\theta = \pi$ one gets $s(\pi) = 0$ and thus $L^{V_\pi} = L_0$. $\diamond$

1.3. Nevanlinna Functions We give a brief survey of Nevanlinna functions at this point as they will appear naturally in the following sections.

Definition 1.11. An analytic function $q : \mathbb{C}\backslash\mathbb{R} \to \mathbb{C}$ satisfying $q(\overline{z}) = \overline{q(z)}$ for $z \in \mathbb{C}\backslash\mathbb{R}$ and such that $\mathfrak{Im}\,z > 0$ implies $\mathfrak{Im}\,q(z) \geq 0$ is called a Nevanlinna function. In this case we write $q \in \mathcal{N}$.

This concept of analytic functions mapping the open upper halfplane $\mathbb{C}^+$ into the closed upper halfplane $\mathbb{C}^+ \cup \mathbb{R}$ can be generalized into several directions. First, however, let us remember a classical theorem characterizing Nevanlinna functions, cf. for example [1], Section 59 for (ii) and [27] for (iii).

Theorem 1.12. *The following are equivalent:*

(i) $q \in \mathcal{N}$

(ii) There exists a Borel measure μ, satisfying $\int_{\mathbb{R}} \frac{1}{1+t^2}\,d\mu(t) < \infty$, as well as constants $a \in \mathbb{R}$ and $b \geq 0$ such that

$$q(z) = a + bz + \int_{\mathbb{R}} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) d\mu(t). \qquad (1.4)$$

(iii) There exists a Hilbert space $(\mathcal{H}, \langle \cdot, \cdot \rangle)$, a self-adjoint linear relation $A = A^*$ (cf. Remark 1.14), an element $v \in \mathcal{H}$ and $z_0 \in \mathbb{C}^+$ such that

$$q(z) = \overline{q(z_0)} + (z - \overline{z_0})\langle (I + (z - z_0)(A - z)^{-1})v, v \rangle, \qquad (1.5)$$

where I is the identity in $\mathcal{H}$.

This theorem thus opens up the possibility to study a Nevanlinna function q in terms of the associated measure μ or via a Hilbert space model involving a self-adjoint linear relation A. We will in the following often encounter Nevanlinna functions of the form $z \mapsto \langle f, (A - z)^{-1} f \rangle$ with a self-adjoint operator A and a certain element f in a given Hilbert space.

Remark 1.13. We note that the measure μ appearing in Theorem 1.12 (ii) can be calculated from q by way of the Stieltjes inversion formula

$$\frac{1}{2}\left(\mu((\alpha, \beta)) + \mu([\alpha, \beta]) \right) = \lim_{\varepsilon \searrow 0} \frac{1}{\pi} \int_{\alpha}^{\beta} \mathfrak{Im}\,q(t + i\varepsilon)\,dt, \qquad (1.6)$$

where $[\alpha, \beta] \subset \mathbb{R}$. $\diamond$

Remark 1.14. Linear relations essentially generalize the notion of linear operators. More concretely, if $\mathcal{H}$ is a Hilbert space then one considers linear subspaces of $\mathcal{H} \times \mathcal{H}$. Every linear operator is also a linear relation when identifying the operator with its graph. Basic operations such as the sum

or multiplication of two linear relations is defined purely algebraically. Furthermore, concepts such as kernel, range and domain carry over easily to linear relations. For operators all the above boils down to the usual definitions. We draw attention to the following two points:

First, a linear relation T is an operator if and only if the multi-valued part

$$\operatorname{mul} T := \{g \in \mathcal{H} : (0; g) \in T\}$$

is trivial. Hence, linear relations can be thought of as multi-valued linear operators.

Second, the adjoint relation T^* of a linear relation T is defined as the subspace

$$T^* := \{(f; g) \in \mathcal{H} \times \mathcal{H} : \langle f, v \rangle = \langle g, u \rangle \text{ for all } (u; v) \in T\}.$$

This coincides again with the usual definition of an adjoint in the case of an operator. With this in mind the definition of symmetric and self-adjoint linear relations is straightforward.

For further details, see for example [2; 6–8; 27]. ◇

Note that the implication

$$\mathfrak{Im}\, z > 0 \quad \Rightarrow \quad \mathfrak{Im}\, q(z) \geq 0$$

in Definition 1.11 for a given function q can be substituted by the requirement that the associated Nevanlinna kernel

$$\mathcal{K}_q(z, w) := \frac{q(z) - \overline{q(w)}}{z - \overline{w}}, \tag{1.7}$$

is positive definite, i.e., that for any $N \in \mathbb{N}$ and $z_1, \ldots, z_N \in \mathbb{C}^+$ the Hermitian matrix $(\mathcal{K}_q(z_i, z_j))_{i,j=1}^N$ has this property. With this it is now easy to see two principal ways how to broaden the definition of Nevanlinna functions: On the one hand, one can consider matrix- or operator-valued functions. On the other hand, the condition (1.7) can in a sense be relaxed. It goes without saying that both of these possibilities can then also be combined.

The first case is straighforward. For the sake of simplicity we only consider matrix-valued functions as only those will (on occasion) appear in the following.

Definition 1.15. Let $n \geq 1$. An analytic function $Q : \mathbb{C} \backslash \mathbb{R} \to \mathbb{C}^{n \times n}$ is called an $(n \times n)$-matrix-valued Nevanlinna function if it obeys the symmetry condition $Q(\overline{z}) = Q(z)^*$ and it satisfies that $\frac{Q(z) - Q(z)^*}{z - \overline{z}} \geq 0$, i.e., that all these matrices are positive semidefinite. In this case one writes $Q \in \mathcal{N}^{n \times n}$.

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For the second case, let us first recall that $\mathcal{K}_q(\cdot, \cdot)$ having $\kappa \geq 0$ negative squares means that for any $N \in \mathbb{N}$ and $z_1, \ldots, z_N \in \mathbb{C}^+$ the Hermitian matrix $(\mathcal{K}_q(z_i, z_j))_{i,j=1}^N$ has at most κ negative eigenvalues and κ is minimal regarding this property.

Definition 1.16. A meromorphic function $q : \mathbb{C}\backslash\mathbb{R} \to \mathbb{C}$ satisfying $q(\overline{z}) = \overline{q(z)}$ and whose associated Nevanlinna kernel $\mathcal{K}_q(\cdot, \cdot)$ has κ negative squares is called a generalized Nevanlinna function. In this case one writes $q \in \mathcal{N}_\kappa$.

The case where $\mathcal{K}_q(\cdot, \cdot)$ has $\kappa = 0$ negative squares is exactly (1.7) so that one reverts back to $\mathcal{N}_0 = \mathcal{N}$.

As is the case with the scalar setting, also matrix- and operator-valued Nevanlinna functions can be generalized that way. As before, the condition of $\frac{Q(z)-Q(\overline{z})}{z-\overline{z}} \geq 0$ is replaced by considering a Nevanlinna kernel $\mathcal{K}_Q(\cdot, \cdot)$ defined as above and requiring this kernel to have κ negative squares.

Regarding Theorem 1.12, let us only mention that similar characterizations exist. The integral representation becomes more involved whereas the operator representation still looks the same. However, in the case of generalized Nevanlinna functions, these models will no longer involve a Hilbert space but a Pontryagin space (cf. Definition 1.20), reflecting the negative squares present in the Nevanlinna kernel.

For further information, especially on the generalized setting, see also the survey article [29] and the references therein.

1.4. Parametrization of Self-adjoint Extensions via Krein's Formula As we have seen, the question of when self-adjoint extensions of a symmetry exist has been answered in terms of equality of defect indices and these extensions can furthermore all be described in von Neumann's theory. However, there are other possibilities to parametrise them, cf. for example [1] or the more recent [3] and the references therein.

Take again a closed, densely defined symmetric operator $S \subseteq S^*$ with equal and, for the sake of simplicity, finite defect indices $n := n_+ = n_- < \infty$. Furthermore, fix a self-adjoint extension $A_0 = A_0^*$ and a nonreal number z_0. Choose also an n-dimensional auxiliary Hilbert space $\mathcal{G}$ and a bijective map $\gamma_{z_0} : \mathcal{G} \to \mathfrak{N}_{z_0}$. This gives rise to the so-called Gamma-field

$$\gamma_z := (A_0 - z_0)(A_0 - z)^{-1}\gamma_{z_0} : \mathcal{G} \to \mathfrak{N}_z \qquad z \in \mathbb{C}\backslash\mathbb{R} \tag{1.8}$$

with adjoint $\gamma_z^* : \mathfrak{N}_z \to \mathcal{G}$. This in turn lets us define the so-called Q-function

$$Q(z) := Q_0^* + (z - \overline{z_0})\gamma_{z_0}^*\gamma_z \qquad z \in \mathbb{C}\backslash\mathbb{R}$$

where Q_0 satisfies

$$\frac{Q_0 - Q_0^*}{z_0 - \overline{z_0}} = \gamma_{z_0}^* \gamma_{z_0}.$$

It turns out that Q is a Nevanlinna ($n \times n$-matrix) function, cf. the above Definition 1.15.

With these notions in mind one then arrives at a parametrisation of all self-adjoint extensions. In particular, this is achieved by the following formula involving resolvents.

Theorem 1.17 (Krein's formula)**.** *Let $S \subseteq S^*$ be a densely defined closed symmetric operator with deficiency index (n, n). Choose a fixed self-adjoint extension A_0, a Gamma-field γ_z and let Q be given as above. Then*

$$(A_T - z)^{-1} = (A_0 - z)^{-1} - \gamma_z (T + Q(z))^{-1} \gamma_{\overline{z}}^* \tag{1.9}$$

establishes a one-to-one correspondence between all resolvents of self-adjoint extensions A_T of S and all self-adjoint linear relations $T = T^*$ in $\mathcal{G} \times \mathcal{G}$.

Remark 1.18. The case $n = 1$ is especially important for us in the following. Here, the auxiliary Hilbert space $\mathcal{G}$ is just $\mathbb{C}$. The set of all self-adjoint linear relations in $\mathbb{C} \times \mathbb{C}$ is then made up of $\mathbb{R}$ together with the formal element $\{\infty\}$. ◇

Remark 1.19. Krein's formula can be also used to to parametrise self-adjoint extensions of a symmetric operator that are defined in a larger Hilbert space properly containing the original one. These extensions with exit, and Krein's formula involving so-called generalized resolvents and Nevanlinna families, do not play a role in the following and shall thus only be mentioned here. More details can be found in the references given in the beginning of this section. ◇

Example (Part III)**.** We continue with the closed densely defined symmetric $L_{\min} \subseteq L_{\max}$ with defect indices $(1, 1)$. Then L_0 is the obvious fixed self-adjoint extension. The bijection $\gamma_i : \mathbb{C} \to \mathfrak{N}_i$ acting as $\omega \mapsto \omega e^{-\sqrt{-i}x}$ can be extended to a Gamma-field by (1.8), i.e., $\gamma_z : \omega \mapsto \omega e^{-\sqrt{-z}x}$ with transpose $\gamma_z^* : f \mapsto \langle e^{-\sqrt{-z}x}, f \rangle$. A Q-function can be calculated as

$$q(z) = \int_0^\infty \overline{e^{-\sqrt{-i}x}} \left((z + i) e^{-\sqrt{-z}x} - i e^{-\sqrt{-i}x} \right) dx$$

$$= (z + i) \int_0^\infty e^{-(\sqrt{i} + \sqrt{-z})x} dx - i \int_0^\infty e^{-(\sqrt{i} + \sqrt{-i})x} dx$$

$$= \frac{z + i}{\sqrt{i} + \sqrt{-z}} - i \frac{1}{\sqrt{2}} = -\sqrt{-z} + \sqrt{i} - \frac{i}{\sqrt{2}} = -\sqrt{-z} + C$$

with $C \in \mathbb{R}$. Given these ingredients, Krein's formula then describes all canonical extensions via

$$(L_t - z)^{-1} = (L_0 - z)^{-1} - \frac{\langle e^{-\sqrt{-\bar{z}}\cdot}, \cdot \rangle}{q(z) + \frac{1}{t}} e^{-\sqrt{-z}\cdot} \tag{1.10}$$

The constant $\frac{1}{t}$ is chosen such that if $t = 0$ then the denominator on the right side is infinite and so one gets back the original extension L_0.

1.5. Extensions in Pontryagin spaces

Definition 1.20. Let V be a vector space endowed with an indefinite inner product $[\cdot, \cdot]$. Then V is called a Pontryagin space if there is a decomposition $V = V_+ \oplus V_-$ with respect to the inner product such that $\dim V_- < \infty$, the inner product is negative definite on V_- and $(V_+, [\cdot, \cdot])$ is a Hilbert space. In this case, one often writes $V = \Pi_\kappa$ where κ is the dimension of the negative definite space.

In other words, a Pontryagin space is a Hilbert space up to a finite dimensional component where the inner product is negative definite.

In a Pontryagin space $(\Pi_\kappa, [\cdot, \cdot])$, symmetric and self-adjoint operators can be defined involving the indefinite inner product $[\cdot, \cdot]$ just as was done in the Hilbert space setting. The extension theory of symmetric operators works in much the same way as discussed above and in terms of parametrization of generalized resolvents, a similar formula to Krein's (1.9) holds.

A difference in the formula in contrast to the previous section arises from the indefinite scalar product. The indefiniteness is reflected in the fact that $Q(z)$ becomes a generalized Nevanlinna function (relation). If the Pontryagin space Π_κ has κ negative squares then the Q-function for the extension problem will belong to the class $\mathcal{N}_\kappa$. For further details, cf. [4; 18] and the references therein.

It should be noted that such extension problems as discussed in the above two sections can also be formulated in the language of boundary triplets. We will not require this theory in the following but point to [17] as well as to the references therein.

1.6. Perturbations of self-adjoint operators as extensions of symmetric operators
We start with a "non-example": Let us consider a densely defined self-adjoint operator $A = A^*$ in a Hilbert space $\mathcal{H}$ and let us perturb this operator with a rank-one operator, i.e., for real α and $\varphi \in \mathcal{H}$ one can consider the sum

$$A_\alpha := A + \alpha \langle \varphi, \cdot \rangle \varphi.$$

This sum is well-defined on dom A_α = dom A and again $A_\alpha = A_\alpha^*$. If we now define the operator $S := A|_{\varphi^\perp}$ then it turns out this is a symmetric operator but it is of course no longer densely defined. Nevertheless, it seems natural to think of A_α as a self-adjoint extension of S. One can calculate the resolvent of A_α and express it in terms of $A_0 = A$ to get

$$(A_\alpha - z)^{-1} = (A_0 - z)^{-1} - \frac{\langle (A_0 - \overline{z})^{-1}\varphi, \cdot \rangle}{\langle \varphi, (A_0 - z)^{-1}\varphi \rangle + \frac{1}{\alpha}} (A_0 - z)^{-1}\varphi,$$

with the Nevanlinna function $\langle (A_0 - z)^{-1}\varphi, \varphi \rangle$ in the denominator. Even though the theory we have seen so far was not applicable directly, this should still remind us somewhat of Krein's formula (2.5).

Before we go on, we need the following concept, cf. for example the general outline given in [32].

Definition 1.21. Let $A = A^*$ be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Define for $n \in \mathbb{Z}$ a mapping $\| \cdot \|_n := \|(|A| + 1)^{n/2} \cdot \|_{\mathcal{H}}$. Then one defines the scale of Hilbert spaces $\mathcal{H}_n(A)$ generated by A as follows:

- For $n \geq 0$ set $\mathcal{H}_n(A) := \mathrm{dom}(|A|^{n/2})$. Then $\| \cdot \|_n$ is a norm on this set and $\mathcal{H}_n(A)$ is complete in this norm.

- For $-n < 0$ define $\mathcal{H}_{-n}(A)$ as the closure of $\mathcal{H}$ in the norm $\| \cdot \|_{-n}$ or, alternatively, as the dual space of $\mathcal{H}_n(A)$, which is then again complete in the norm $\| \cdot \|_{-n}$.

Note that $|A|$ can be defined via the spectral theorem for (unbounded) self-adjoint operators. In the case of a semi-bounded operator, i.e., $A \geq c$ for some $c \in \mathbb{R}$, one can (potentially after a shift by a constant) take away the absolute value. In particular, this is true for a positive operator.

Remark 1.22. By the above procedure a scale of spaces is obtained such that $\mathcal{H}_m(A) \supset \mathcal{H}_n(A)$ for $n > m$ and the smaller space is densely contained in the larger space with respect the norm of the latter. The picture one should have in mind looks like

$$\cdots \supset \mathcal{H}_{-3} \supset \mathcal{H}_{-2} \supset \mathcal{H}_{-1} \supset \mathcal{H}_0 = \mathcal{H} \supset \mathcal{H}_1 \supset \mathcal{H}_2 \supset \mathcal{H}_3 \supset \ldots,$$

where for example $(\mathcal{H}_2(A), \| \cdot \|_2)$ is just the domain of A together with the graph norm. Furthermore, we also use $\langle f, g \rangle$ to denote the action of the functional $f \in \mathcal{H}_{-n}(A)$ on a function $g \in \mathcal{H}_n(A)$. If a self-adjoint operator has been fixed, we simply write $\mathcal{H}_n$ for the respective spaces. ◇

Example (Part IV)**.** If $\mathcal{H}$ and L_0 are chosen as before, then the scale of Hilbert spaces coincides with the Sobolev spaces $H^k = W^{k,2}$ and their respective dual spaces H^{-k}.

Singular Perturbations

In contrast to the "non-example" above, let us look at a situation where the extension theory of symmetric operators as outlined in the previous sections can be applied, namely in the case of a singular perturbation: That is, one considers φ outside (but "not too far" outside) of the original Hilbert space, namely, $\varphi \in \mathcal{H}_{-1} \setminus \mathcal{H}$ or $\varphi \in \mathcal{H}_{-2} \setminus \mathcal{H}_{-1}$, cf. [32] and also the references therein.

In this case the formal sum $A_\alpha := A + \alpha \langle \varphi, \cdot \rangle \varphi$ does not immediately make sense. The goal is nevertheless to understand it as an operator in the Hilbert space. This operator should be self-adjoint since the sum formally has this property. Moreover, when we vary α and compare different formal sums and their domains, the perturbation does not affect those elements u from $\operatorname{dom} A$ that satisfy $\langle \varphi, u \rangle = 0$. Hence, evaluation of the functional $\langle \varphi, \cdot \rangle$ takes the place of considering $\varphi^\perp$ above and thus we define a symmetric operator

$$S := A|_{\{u \in \operatorname{dom} A : \langle \varphi, u \rangle = 0\}}.$$

In this setting, S is now densely defined, closed and has deficiency indices $(1, 1)$. It is thus plausible to expect operators A_α to be found among the self-adjoint extensions of this symmetric operator.

The obvious choice for a certain self-adjoint extension to compare other extensions with is $A_0 = A$. If $\varphi_z := (A_0 - z)^{-1} \varphi$ then the defect spaces of S are $\mathfrak{N}_z := \operatorname{span}\{\varphi_z\}$. A gamma field γ_z in this setting is easily obtained from the bijection $\gamma_{z_0} : \omega \mapsto \omega \varphi_{z_0}$ between $\mathbb{C}$ and $\mathfrak{N}_{z_0}$, where some $z_0 \in \mathbb{C}^+$ has been fixed. The Q-function appears from

$$\frac{q(z) - \overline{q(z_0)}}{z - \overline{z_0}} = \langle \varphi_{z_0}, \varphi_z \rangle$$

and we then get all generalized resolvents of S inside the Hilbert space $\mathcal{H}$ from Krein's formula, which appears as

$$(A_\tau - z)^{-1} = (A - z)^{-1} - \frac{\langle \varphi_{\overline{z}}, \cdot \rangle}{q(z) - \frac{1}{t}} \varphi_z$$

where $t \in \mathbb{R} \cup \{\infty\}$. Hence, via these resolvents the family (A_α) is defined in terms of the family (A_t). It turns out that given $\varphi \in \mathcal{H}_{-1}$ allows for one particular t-value to be associated with one particular α-value. This is essentially due to the fact that it is possible to decompose

$$(z - \overline{z_0}) \langle \varphi_{z_0}, \varphi_z \rangle = -\langle \varphi, (A - z_0)^{-1} \varphi \rangle + \langle \varphi, (A - z)^{-1} \varphi \rangle$$

where both summands are then well-defined. However, for more singular perturbation elements $\varphi \in \mathcal{H}_{-2} \setminus \mathcal{H}_{-1}$ connecting one α-value to one t-value requires additional assumptions.

1.7. Supersingular Perturbations In the case where $\varphi \in \mathcal{H}_{-n-2} \backslash \mathcal{H}_{-2}$ for $n \geq 1$, so-called supersingular perturbations, the above construction does not work.

- On the one hand, restricting $S := A|_{\{u \in \mathrm{dom}\, A : \langle \varphi, u \rangle = 0\}}$ does not give a symmetry with defect indices $(1, 1)$. Instead, this operator is essentially self-adjoint, i.e., its closure is a self-adjoint operator, namely A, and this is the only self-adjoint extension to work with in $\mathcal{H}$. This of course contrasts negatively with the expectation that (A_α) would still be an infinite family of self-adjoint operators.

- On the other hand, one could consider A in a smaller space $\mathcal{H}_n$, where its domain is then $\mathcal{H}_{n+2}$. Restricting A to obtain an operator S as above leads to S being symmetric with deficiency indices $(1, 1)$. Then, the machinery of Krein's formula can be applied and a family of self-adjoint operators in $\mathcal{H}_n$ is parametrised in terms of their resolvents. However, this approach has several disadvantages. For one, the rank-one operator in Krein's formula, that is

$$\frac{\langle \psi_{\bar{z}}, \cdot \rangle}{\tilde{q}(z) + \frac{1}{t}} \psi_z,$$

  involves the defect elements ψ_z, calculated in $\mathcal{H}_n$, that have no direct connection to the perturbation element $\varphi \in \mathcal{H}_{-n-2}$ as in the previous singular perturbation case.

There exist several operator models dealing with supersingular perturbations. On the one hand, is is possible to consider the perturbation problem in a Pontryagin space setting as was done in [10], for an application see for example also [11]. On the other hand, a different model due to Kurasov could give an interpretation of the perturbations in a Hilbert space, cf. the series of papers [21; 22; 24; 25] and in particular [23]. However, this latter model requires the operator A to be semi-bounded. A comparison of the two approaches, Pontryagin space and Hilbert space models, is presented in [9].

From our viewpoint the Hilbert space model is of particular interest. It is used in Papers I and II to analyse certain Sturm-Liouville differential expressions. Furthermore, in Paper III the requirement for A to be semi-bounded is investigated. We will thus give a short overview of this model here.

In the case of semibounded operators, one can consider $\mathbb{H} := \mathcal{H}_n \oplus \mathbb{C}^n$ and equip it with a Hilbert space structure. The smaller space $\mathcal{H}_n \subsetneq \mathcal{H}$ allows one to define a symmetric operator with deficiency indices $(1,1)$. The role of the extension $\mathbb{C}^n$ is to involve n elements of the form $(A - \mu_j)^{-1}\varphi$, which are

exactly the kind of elements that appear in Krein's formula in the case of singular perturbations. Hence, in order for Krein's formula to involve $(A-z)^{-1}\varphi$ one accordingly needs to add such elements to the space. Furthermore, this also connects the defect element in $\mathbb{H}$ and the perturbation element φ.

The Hilbert space structure on the component $\mathbb{C}^n$ is achieved by choosing $\mu_1,\ldots,\mu_n$ from the resolvent set of A, real and mutually different, a choice which clearly cannot be guaranteed for any (non-semibounded) self-adjoint operator. Note furthermore that there exists an embedding $\iota_{\mathbb{H}} : \mathbb{H} \to \mathcal{H}_{-n}$. Given $\mathbb{H}$ one can build two operators in this space, a maximal operator $A_{\max}$ and its adjoint $A_{\min} := A_{\max}^*$ in $\mathbb{H}$. The maximal operator arises when considering the restriction of A in $\mathcal{H}_n$ to the set $\{u \in \mathcal{H}_{n+2} : \langle \varphi, u \rangle = 0\}$, then taking the triplet adjoint $A^\dagger$ with respect to $\mathcal{H}_n \subset \mathcal{H} \subset \mathcal{H}_{-n}$ and then finally restricting $A^\dagger$ to $\mathbb{H}$. It then turns out that $A_{\min}$ is a symmetric operator with deficiency indices $(1,1)$. From this point on forwards it is a question of applying extension theory and using the resulting family of self-adjoint operators (A_t) to define (A_α). Finally, Krein's formula can then be restricted to $\mathcal{H}_n$, i.e., the first component, and embedded into the space of functionals $\mathcal{H}_{-n}$, giving rise to the formula

$$\iota_{\mathbb{H}}(A_t - z)^{-1}\Big|_{\mathcal{H}_n} = (A-z)^{-1} - \frac{\langle (A-\overline{z})^{-1}\varphi, \cdot \rangle}{b(z)(Q(z)+1/t)}(A-z)^{-1}\varphi, \qquad (1.11)$$

where $Q(z)$ is the Q-function from the extension in $\mathbb{H}$ and $b(z) = (z-\mu_1)\cdots(z-\mu_n)$ is a polynomial. Hence, one sees that building a Hilbert space model that closely mirrors Krein's formula from the singular perturbation case comes at the price of a generalized Nevanlinna function $b(z)Q(z)$ appearing in the denominator.

Remark 1.23. It should be noted that there are two formulations of the Hilbert space model. Informally speaking, the so-called "cascade" model (used in Papers I and II) involves a certain number of progressively less singular elements to build a Hilbert space, whereas the so-called "peak" model (appearing in Paper III) uses "equally singular" elements in such a construction. The above description of the model is based on the "peak" model. The formulations are, however, equivalent by way of the resolvent identity (1.3).

2 Sturm-Liouville Problems

The following section has been adapted from [30] and was shortened a little in the process. More information on some of the often well-known results can be found for example in [1; 34], see also the treatise [35]. Let us now start with a quite general definition to set the foundation.

Definition 2.1. Let (a, b) be a bounded or unbounded interval. Furthermore, let p, q, r be measurable complex-valued functions on (a, b). Suppose that r and p vanish at most on a set of measure zero and that r is nonnegative. Then

$$\tau := \frac{1}{r} \left(-\frac{d}{dx} \left(p \frac{d}{dx} \right) + q \right)$$

is called a Sturm-Liouville differential expression (with coefficients p, q, r).

Definition 2.2. Let τ be a Sturm-Liouville differential expression. An operator

$$L : \begin{cases} L^2(a, b) \supseteq \operatorname{dom}(L) & \to & L^2(a, b) \\ f & \mapsto & \tau f \end{cases}$$

is called a realization of τ in the Hilbert space $L^2(a, b)$. It is called a symmetric or self-adjoint realization if L has the respective property, i.e., if $L \subseteq L^*$ or $L = L^*$.

Remark 2.3. Note that under certain conditions the equation

$$-(p(x)u'(x))' + q(x)u(x) = \lambda r(x)u(x),$$

together with some boundary conditions, can be transformed, by way of the Liouville transform, to the so-called Liouville normal form

$$-y''(x) + \tilde{q}(x)y(x) = \lambda y(x),$$

where λ is a complex parameter. ◇

Definition 2.1 is quite broad and for the purposes of this work more extensive than necessary. In the following, our main point of interest lies with the coefficient q. In the light of Remark 2.3, it will suffice to concentrate on the case where $p, r \equiv 1$. Furthermore, we want to investigate these differential expressions in the setting of self-adjoint operators acting in a Hilbert space. Thus, we want the image of q to be real, which will make the differential expression formally self-adjoint.

Hence, from now on we will only use the following

Definition 2.4. Let (a, b) be a bounded or unbounded interval. Furthermore, let q be a locally integrable real-valued function. Then by a Sturm-Liouville differential expression we will always mean an expression of the form

$$\tau := -\frac{d^2}{dx^2} + q(x). \tag{2.1}$$

The coefficient q is called the potential of τ. Furthermore, a realization of τ inside the Hilbert space $L^2(a, b)$ is also called a Schrödinger operator.

We also need the following endpoint classification.

Definition 2.5. If the left endpoint a is finite and if for some, and hence for any, $c \in (a, b)$ we have

$$\int_a^c |q(x)| dx < \infty$$

then a is a regular endpoint; otherwise it is called singular. Similarly, we define regularity/singularity of the endpoint b. If a and b are both regular endpoints, then the expression τ is called regular. Otherwise, τ is called singular.

There is an additional finer categorization of endpoints due to Weyl.

Definition 2.6. Consider the equation $\tau u = \lambda u$ for $\lambda \in \mathbb{C}$.

1. If for all $\lambda \in \mathbb{C}$ all its solutions are square integrable near the endpoint a then τ is said to be in the limit circle case at a.

2. If for all $\lambda \in \mathbb{C}$ there is at least one solution that is not square integrable at the endpoint a then τ is said to be in the limit point case.

Similarly, we define limit circle and limit point case at b.

It is clear from the definition that limit circle and limit point case exclude each other. Moreover, we have

Theorem 2.7 (Weyl's alternative)**.** *Let τ be a Sturm-Liouville differential expression. If there exists some $\lambda_0 \in \mathbb{C}$ such that all solutions of $\tau u = \lambda_0 u$ are square integrable at an endpoint, then the same is true for any $\lambda \in \mathbb{C}$. Consequently, τ is at any endpoint either in the limit circle or the limit point case.*

We point out that the limit point case does not say that no solution is square integrable at the respective endpoint. Instead, the following is true: a basis of the two-dimensional solution space of $\tau u = \lambda u$ can be chosen such that one vector is still square integrable at the endpoint whereas the other one cannot fulfill this requirement.
We note that a regular endpoint is automatically in the limit circle case. Hence, it is the singular endpoints that receive an additional distinction through this terminology.
In the following we will only deal with problems on the half-line, i.e., when the interval is given by $(0, \infty)$. Thus, the right endpoint is always singular and we assume it to be in the limit point case.
The potential q now determines what difficulties one faces when analysing a Sturm-Liouville problem. Historically, the analysis started with "nice" potentials that let τ be regular at the left endpoint — think of a test function

$q \in C_0^\infty(0,\infty)$ as an example. In the next section we will review the classical case of a differential expression τ with only one singular endpoint.

However, for a potential that fails to be integrable at the origin we end up with two singular endpoints. Depending on whether 0 will fall into the limit circle or limit point case we will need to adapt the classical approaches to some extent. In this situation one could consider the so-called Bessel potential $q(x) = \frac{q_0 + q_1 x}{x^2}$ as an example and continue from this starting point. This more general setup will be the topic of the later sections in the introduction.

2.1. The Classical Case In this section we assume that $q \in L^1_{loc}[0,\infty)$. In particular, this means that it is integrable at the left endpoint. Hence, the differential expression (2.1) has one regular and one singular endpoint. Furthermore, we assume the singular endpoint to be in the limit point case.

Titchmarsh-Weyl m-function

First, one can look at the problem from the viewpoint of ordinary differential equations. Thus, we take the equation

$$-u''(x) + q(x)u(x) = \lambda u(x) \qquad \lambda \in \mathbb{C}\setminus\mathbb{R} \tag{2.2}$$

together with the two sets of initial conditions

$$
\begin{array}{ccc}
u_1(0,\lambda) = 0 & & u_2(0,\lambda) = 1 \\
& \text{and} & \\
u_1'(0,\lambda) = 1 & & u_2'(0,\lambda) = 0
\end{array}
\tag{2.3}
$$

corresponding to a Dirichlet and a Neumann condition. From the standard theory we can thus find two solutions u_1 and u_2 to the respective second order initial value problems. By the chosen initial conditions it is apparent that they are linearly independent and, thus, they will span the space of solutions. Any two linearly independent solutions are called a fundamental system for the equation. In our case this fundamental system is already uniquely determined and its Wronskian is normalized due to the given boundary conditions, i.e.,

$$W_x(u_2, u_1) := W(u_2, u_1)(x) \equiv W(u_2, u_1)(0) = u_2(0)u_1'(0) - u_2'(0)u_1(0) = 1$$

Note also that since both solutions are continuous up to the left endpoint, they are clearly square integrable there. This reflects again the fact that the left endpoint is in the limit circle case.

On the other hand, the right endpoint should by assumption fall into the limit point case. This means that there exists a — unique up to a complex

factor — solution ψ to the above problem that will be square integrable near infinity. But as we already have chosen a basis for our solution space, it must be possible to express ψ in this basis, i.e.,

$$\psi(x,\lambda) = u_2(x,\lambda) + m(\lambda)u_1(x,\lambda) \qquad \lambda \in \mathbb{C}\backslash\mathbb{R}$$

for any fixed λ and it is now uniquely determined by this linear combination. This solution ψ is called the Weyl solution.

We note that our Sturm-Liouville equation (2.2) depends analytically on the spectral parameter λ, as do the intial conditions (2.3). Hence, its solutions will display the same kind of dependence on λ. This implies that $m(\lambda)$ is in fact an analytic function on the upper and lower half plane, called the Titchmarsh-Weyl m-function. It is, furthermore, easy to see that $m(\lambda)$ is in fact a Nevanlinna function Hence, $m(\lambda)$ has an integral representation involving a measure μ, cf. (1.4), which will play a role below.

Finally, this function may have discontinuities on $\mathbb{R}$. We will at the end of the section see how the location and type of discontinuities is connected to the spectrum of a certain self-adjoint realization.

Example (Part V). As an illustration let us consider $q \equiv 0$, which will connect back to the Example Part I-IV we have seen so far. Equation (2.2) simplifies to $-u''(x) = \lambda u(x)$. The initial conditions (2.3) allow us to find the fundamental system

$$u_1(x,\lambda) = \frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}} \quad \text{and} \quad u_2(x,\lambda) = \cos(\sqrt{\lambda}x),$$

where $(-\infty, 0]$ is again the branch cut for the root. To obtain the Weyl solution, we must find $m(\lambda)$ such that for $\lambda \in \mathbb{C}\backslash\mathbb{R}$ the function

$$\psi(x,\lambda) = \cos(\sqrt{\lambda}x) + m(\lambda)\frac{\sin(\sqrt{\lambda}x)}{\sqrt{\lambda}}$$

is square integrable near infinity. We see that this is the case if we choose

$$m(\lambda) := -\sqrt{-\lambda} = \begin{cases} i\sqrt{\lambda} & \lambda \in \mathbb{C}^+ \\ -i\sqrt{\lambda} & \lambda \in \mathbb{C}^- \end{cases}$$

and, thus, the Weyl solution is

$$\psi(x,\lambda) = e^{-\sqrt{-\lambda}x} = \begin{cases} e^{i\sqrt{\lambda}x} & \lambda \in \mathbb{C}^+ \\ e^{-i\sqrt{\lambda}x} & \lambda \in \mathbb{C}^- \end{cases} .$$

In other words, we have recovered the Weyl solution as the defect element of the operator $L_{\min}$. Note that $m(\lambda)$ is clearly analytic on the upper and lower halfplane, it maps $\mathbb{C}^+$ into itself, and satisfies the symmetry condition since

$$m(\bar{\lambda}) = -\sqrt{-\bar{\lambda}} = \overline{-\sqrt{\lambda}} = \overline{m(\lambda)}.$$

Hence, it is indeed a Nevanlinna function. ◇

Spectral transform and measure

Given a Sturm-Liouville differential expression τ we have so far seen how the function $m(\lambda)$ and, via (1.4), the measure μ can be associated to it. In terms of operators, it is on the one hand possible to consider the so-called Dirichlet realization L_0 of τ in $L^2(0,\infty)$, see the section immediately below for a definition.

On the other hand, one can look at the new Hilbert space $L^2(\mathbb{R}, \mu)$ and try to recapture the operator L_0 in this space. It turns out that the multiplication operator in this new space and L_0 in the original Hilbert space are in fact unitarily equivalent by way of the transformation

$$U : \begin{cases} L^2(0,\infty) & \to & L^2(\mathbb{R}, \mu) \\ f & \mapsto & \int_0^\infty u_1(x,\lambda) f(x) dx \end{cases}$$

with inverse

$$(U^{-1}F)(x) = \int_{\mathbb{R}} u_1(x,\lambda) F(\lambda) d\mu(\lambda).$$

Note that $\int_0^\infty u_1(\lambda, x) f(x) dx$ is not obviously well-defined but should be understood as the limit $\lim_{N\to\infty} \int_0^N u_1(x,\lambda) f(x) dx$ in the space $L^2(\mathbb{R}, \mu)$. The definition of the inverse involves a similar limit in $L^2(0,\infty)$.

Hence, one can choose between working with a more difficult second derivative operator and the Lebesgue measure or with a simpler operator of multiplication by the independent variable at the cost of a more complicated measure μ.

Example (Part VI)**.** For the Titchmarsh-Weyl function $m(\lambda) = -\sqrt{-\lambda}$ one can employ the Stieltjes inversion formula (1.6) to find that the associated spectral measure is $d\mu = \pi^{-1} \chi_{[0,\infty)} \sqrt{t} \, dt$. The measure is concentrated along the set where $-\sqrt{-\lambda}$ "feels" the branch cut for the square root. ◇

Realizations via extension theory

It is also possible to analyze τ via its self-adjoint realizations in the Hilbert space $L^2(0,\infty)$. To this end we first look at the maximal operator $L_{\max}$ —

note the obviously parallel definitions of the operators in the Example Part I — defined on

$$\text{dom}(L_{\max}) := \left\{ f \in L^2(0,\infty) \mid f, f' \in AC_{loc}(0,\infty), \tau f \in L^2(0,\infty) \right\},$$

i.e., its domain are all functions such that an application of τ gives again an element of $L^2(0,\infty)$, and the minimal operator $L_{\min}$ with

$$\text{dom}(L_{\min}) := \left\{ f \in \text{dom}(L_{\max}) \mid f(0) = f'(0) = 0 \right\}.$$

Alternatively, the minimal operator appears after considering a realization of τ defined on $C_0^\infty(0,\infty)$, i.e., all smooth and compactly supported functions, and then taking the closure in $L^2(0,\infty)$.

Neither of these two operators is self-adjoint in the current situation of a τ with only one singular endpoint, but integration by parts shows that $L_{\min}$ is symmetric. Furthermore, its adjoint turns out to be $L_{\max}$ and its deficiency indices are $(1,1)$. Hence, we know again that there exists a whole family of self-adjoint extensions $(L_s)_{s\in\mathbb{R}\cup\{\infty\}}$ of $L_{\min}$. It turns out that the domains can be characterized as

$$\text{dom}(L_s) := \left\{ f \in \text{dom}(L_{\max}) \mid f(0) - s f'(0) = 0 \right\}.$$

Compare even this to the Example Part II.

One immediately notes that the choice $s = 0$ corresponds to the Dirichlet boundary condition $f(0) = 0$, which then lends its name to the so-called Dirichlet realization L_0 of τ. In the following, L_0 serves as the point of reference, that is to compare different self-adjoint extensions to this fixed one.

Remark 2.8. The choice $s = \infty$ gives the boundary condition $f'(0) = 0$, which is easily seen from the equivalent formulation $\frac{1}{s} f(0) - f'(0) = 0$. Hence, L_∞ is referred to as the Neumann realization of τ. ⬦

A direct calculation of the resolvent of L_s and comparing it to the one of L_0 reveals

$$(L_s - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle \psi(\cdot, \overline{\lambda}), \cdot \rangle}{m(\lambda) - \frac{1}{s}} \psi(\cdot, \lambda). \tag{2.4}$$

Example (Part VII). We use $\{u_1, u_2\}$, the already determined fundamental system for $-u'' = \lambda u$ as well as the respective m-function $m(\lambda) = -\sqrt{-\lambda}$. Furthermore, the Weyl solution was shown to be $\psi(x, \lambda) = exp(-\sqrt{-\lambda}x)$. Hence, the above formula for the resolvent of L_s is

$$(L_s - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle e^{-\sqrt{-\overline{\lambda}}\cdot}, \cdot \rangle}{-\sqrt{-\lambda} - \frac{1}{s}} e^{-\sqrt{-\lambda}\cdot}.$$

This should of course already remind us of (1.10) in Example Part III. ⬦

Realizations via perturbation theory

Consider finally also the formal perturbations of the self-adjoint Dirichlet realization L_0

$$L_0 + t\langle \varphi, \cdot \rangle \varphi \qquad t \in \mathbb{R} \cup \{\infty\}.$$

To analyze τ it turns out that the perturbation element φ should be defined with the help of the Weyl solution $\psi(\cdot, \lambda)$. In fact, φ should be given by

$$\varphi := (L_0 - \lambda)\psi(\cdot, \lambda)$$

but this definition is not immediately meaningful. Even though the Weyl solution is square integrable it is not guaranteed to be in the domain of L_0. At the very least the perturbation element φ can then however be found in $\mathcal{H}_{-1}(L_0)$ or $\mathcal{H}_{-2}(L_0)$. Thus, the framework of singular perturbations is available.

Through integration by parts one finds

$$\langle \varphi, f \rangle = \langle (L_0 - \lambda)\psi(\cdot, \lambda), f \rangle = \langle \psi(\cdot, \lambda), (L_0 - \overline{\lambda})f \rangle = f'(0)\overline{\psi(0, \lambda)}$$

and thus that the condition $\langle \varphi, f \rangle = 0$ is nothing but $f'(0) = 0$. Hence, following the approach leading to Krein's formula means that the symmetry $S := L_0|_{\{f \in \text{dom}(L_0): f'(0) = 0\}}$ is nothing but the operator $L_{\min}$ from the previous section.

The defect space $\mathfrak{N}_\lambda$ is spanned by the Weyl solution $\psi(\cdot, \lambda)$ and after picking a Gamma-field and a Q-function, Krein's formula takes the form

$$(L_t - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle (L_0 - \overline{\lambda})^{-1}\varphi, \cdot \rangle}{Q(\lambda) + \frac{1}{t}}(L_0 - \lambda)^{-1}\varphi. \qquad (2.5)$$

The singularities of the Q-function are again in a direct correspondence to the spectrum of the underlying symmetric operator $L_{\min}$.

Connections between the approaches

We can start by comparing formulae (2.4) and (2.5). Both describe the same family of self-adjoint extensions of $L_{\min}$. Furthermore, $(L_0 - \lambda)^{-1}\varphi = \psi(\cdot, \lambda)$ holds by definition. Thus, even the numerators in the respective fractions must be equal, which implies that

$$Q(\lambda) - m(\lambda) \equiv \text{const.}$$

Secondly, we saw that L_0 in $L^2(0, \infty)$ was unitarily equivalent to the multiplication operator $Af(t) := tf(t)$ in $L^2(\mathbb{R}, \mu)$. Since unitary equivalence

preserves the spectrum, $\sigma(A) = \sigma(L_0)$ holds. The spectrum of a multiplication operator is, however, determined by the support of the measure in the underlying Hilbert space. On the other hand, μ is also connected to the Titchmarsh-Weyl m-function via (1.4). Hence, singularities of μ translate to those of $m(\lambda)$.

Finally, this now implies that

$$\sigma(L_0) = \{\text{singularities of } m\} = \{\text{singularities of } Q\}$$

and

$$\sigma(L_s) = \left\{\text{singularities of } -\frac{1}{m - \frac{1}{s}}\right\} \qquad s \in (\mathbb{R}\backslash\{0\}) \cup \{\infty\}.$$

2.2. Generalisations to two singular endpoints In the previous section, the potential q was assumed to be locally integrable up to the left endpoint. We will now drop this requirement and from now on let

$$q \in L^1_{loc}(0,\infty)\backslash L^1_{loc}[0,\infty).$$

This means that we are now considering more singular potentials and differential expressions with two singular endpoints. However, as by Weyl's alternative, we can divide this more general setup into yet another two cases. One of them, namely when the left endpoint is in the limit circle case, is easier to handle, as we see in the following

Remark 2.9. The treatment of τ is quite similar to before even when the left endpoint is no longer regular but still in the limit circle case.

- There are still fundamental systems of the equation $\tau u = \lambda u$ such that both basic solutions are square integrable at zero. It requires some extra work to ensure analyticity in the spectral parameter. It is then possible to define ψ and m as before and even see that m is a Nevanlinna function.

- One can again use the Stieltjes inversion formula (1.6) to associate a measure μ to m. With some additional work it can be identified as the spectral measure of a self-adjoint realization of τ and there is again a unitary transformation of this realization to a multiplication operator in $L^2(\mathbb{R}, \mu)$.

- The operator $L_{\min}$ is still symmetric with deficiency index $(1,1)$. From standard extension theory we thus again get a family of self-adjoint extensions $(L_s)_{s \in \mathbb{R} \cup \{\infty\}}$ and also (2.4).

- The element $\varphi := (L_0 - \lambda)\psi(\cdot, \lambda)$ still can be found in either $\mathcal{H}_{-1}$ or $\mathcal{H}_{-2}$. Hence, Krein's formula (2.5) in the perturbation theory picture carries over without modifications.

We can thus draw the conclusion that the singular limit circle case at zero does not pose any greater conceptual difficulties than the regular case. ⋄

Assumption. From now on let the differential expression τ be in the limit point case at both endpoints.

It seems clear that generalizations of the classical approaches should in the end again be somehow comparable. Recall that in the above this boiled down to the statement

$$m(\lambda) - Q(\lambda) \equiv const,$$

i.e., both the m-function that was found in a differential equation picture as well as the Q-function that stemmed from a perturbation problem and Krein's description of resolvents contained all important information about the underlying τ. Hence, a similar connection even in the more singular setting would be the outcome to expect.

However, the setup looks fundamentally different in this case:

- Finding a "good" fundamental system of $\tau u = \lambda u$ via properties at 0 is problematic, not to mention the question of analyticity in λ. There is then also no obvious way to read off the m-function nor a spectral measure.

- One could think of splitting the problem in two, by which we mean splitting the interval via $(0, \infty) = (0, c] \cup [c, \infty)$. However, this leads to two m-functions, one on each subinterval, which can then be combined to one 2×2-matrix valued Titchmarsh-Weyl-function and corresponding matrix-valued spectral measure. For many potentials, a scalar m-function and spectral measure should be enough, though.

- On the operator theoretic side, $L_{\min} = L_{\max} = L_{\min}^*$, i.e., there is only one self-adjoint operator.

- The Weyl-solution is no longer square integrable at zero and, thus, $\psi \notin L^2(0, \infty)$. Hence, in the perturbation image, we cannot easily make sense of φ.

It is thus necessary to use different techniques in the analysis of differential expressions τ.

2.3. The hydrogen atom example As an example for this case one can consider the potential

$$q(x) = \frac{q_0 + q_1 x}{x^2} \qquad q_0 \geq \frac{3}{4},$$

where the requirement on q_0 ensures the limit point case at the origin.

Remark 2.10. Note that the potential comes from describing a hydrogen atom in three dimensions. After a separation into an angular and a radial part, the latter gives the above q. The calculation is carried out in, for example, [33], Sections 10.2-4. Cf. also [13], Section 39. ◇

We want to shortly describe three different approaches to the analysis of the respective differential expression τ.

ODE theory - Fulton [14]

In this example one can employ Frobenius theory to solve second order differential equations of the form

$$a(x) y''(x) + b(x) y'(x) + c(x) y(x) = \lambda y(x) \qquad x \in (0, \infty), \; \lambda \in \mathbb{C},$$

where the coefficient functions satisfy that $a(x), x b(x), x^2 c(x)$ all are analytic at 0. Clearly this is the case in our situation.

One can now make a generalized power series Ansatz. Eventually, one then arrives at a fundamental system of solutions

$$
\begin{aligned}
y_1(x, \lambda) &= x^{r_1} + \sum_{k=1}^{\infty} a_k(\lambda) x^{k + r_1} \\
y_2(x, \lambda) &= x^{r_2} + \sum_{k=1}^{\infty} b_k(\lambda) x^{k + r_2}
\end{aligned}
\tag{2.6}
$$

Here, r_1, r_2 are the roots of the so-called indicial equation, satisfying $r_1 \geq r_2$ and $r_1 + r_2 = 1$. Due to the limit point case at zero, $r_1 \geq 3/2$. It should be noted that the second solution y_2 might have additional logarithmic terms if $r_1 - r_2 \in \mathbb{N}$ but the argument runs generally the same course.

The important thing to take away here is that y_1 is square integrable at the origin ("regular" solution), whereas y_2 is not ("singular" solution).

However, it turns out that both solutions and their derivatives are entire in the spectral parameter λ and satisfy the symmetry condition $\overline{y_i(x, \lambda)} = y_i(x, \overline{\lambda})$. Furthermore, the fundamental system can be normalized, i.e., the Wronskian of the solutions is one.

In a further step one can define a coefficient $m(\lambda)$ by requiring that the linear combination

$$\psi(\cdot, \lambda) := y_2(\cdot, \lambda) + m(\lambda) y_1(\cdot, \lambda)$$

gives the Weyl solution, i.e., the solution that is square integrable at infinity. We note the following:

- $m(\lambda)$ is called a generalized Titchmarsh-Weyl coefficient. It is not a Nevanlinna function, but later turned out to be a generalized Nevanlinna function, i.e., belonging to $\mathcal{N}_\kappa$.

- Fulton could associate a scalar measure to the m-function, which then leads to a spectral transform.

- The outlined approach even works for other potentials, e.g., one can add an analytic perturbation to the potential in the hydrogen atom example and Frobenius theory is still available, cf. also [15].

Operator theory - Dijksma & Shondin [11]

For the slightly more specialized potential where $q_1 = 0$, i.e., the Bessel potential $q(x) = q_0/x^2$, the authors gave a model for perturbations of the form

$$L_0 + t\langle\varphi,\cdot\rangle\varphi$$

where φ is supersingular. This model made use of a Pontryagin space and in the description of the resolvents of the perturbed operator a Q-function appeared.

In this example it then holds that Fulton's m-function and the Q-function of Dijksma and Shondin coincide.

Operator theory - Kurasov & Luger [26] For the full example of arbitrary $q_1 \in \mathbb{R}$, Kurasov and Luger also used a model for the supersingular perturbation

$$L_0 + t\langle\varphi,\cdot\rangle\varphi,$$

this time, however, in a Hilbert space. The perturbation element is defined as $\varphi = (L_0 - \lambda)\psi(\cdot,\lambda)$, where ψ is again the Weyl solution of the problem $\tau u = \lambda u$.

A priori it is only known that φ is not inside the space $\mathcal{H}_{-2}(L_0)$. However, utilizing the fundamental system $\{y_1, y_2\}$ that appeared in Fulton's approach above, it is possible to analyze the asymptotic behaviour of the Weyl solution at the origin. Note that it is the behaviour of the "singular" solution y_2 at the origin that determines the asymptotic properties of ψ, i.e.,

$$\psi(x,\lambda) = o(x^{r_2}) \qquad x \searrow 0.$$

The key observation is now to notice that the coefficients of the lowest powers of x is independent of the spectral parameter λ in (2.6). Hence, if the difference $\psi(\cdot, \lambda) - \psi(\cdot, \mu)$ is considered, the singularity at the origin will become better, namely

$$\psi(x, \lambda) - \psi(x, \mu) = o(x^{r_2 + 2}) \qquad x \searrow 0.$$

It follows from the recursive calculation of the coefficients $a_k(\lambda)$ and $b_k(\lambda)$ in (2.6) that the coefficient of the lowest power in x in the above difference of Weyl solutions only depends on $\lambda - \mu$. Thus, by dividing out this factor, one can work with two such differences and regularize the solution even more at the origin, i.e.,

$$\left(\frac{\psi(x, \lambda) - \psi(x, \mu)}{\lambda - \mu} \right) - \left(\frac{\psi(x, \mu) - \psi(x, \nu)}{\mu - \nu} \right) = o(x^{r_2 + 4}) \qquad x \searrow 0.$$

This approach models applying the resolvent of L_0 for different points in the resolvent set. Doing this sufficiently often one arrives at an element from $L^2(0, \infty)$. Hence, the perturbation element belongs to some $\mathcal{H}_{-n}$ with $n \geq 3$. One can thus employ the theory of supersingular perturbations described in Section 1.7 and arrive at the Q-function of the problem. This Q-function $Q(\lambda)$ will itself be a usual Nevanlinna function since the extension problem is modeled in a Hilbert space. However, after embedding the model into the space $\mathcal{H}_{-n}$, cf. (1.11), one can compare the function $b(\lambda)Q(\lambda)$ with $m(\lambda)$. It then turns out that this product of a polynomial and a Q-function and Fulton's m-function only differ up to a polynomial of low degree. In fact, the degree of the polynomial depends on the strength of the singularity of the potential at the origin, which is regulated by the coefficient q_0.

In conclusion, an agreement between the different approaches is achieved for the Hydrogen atom example.

2.4. Strongly singular potentials Naturally, the question now arises how general the potentials can be. From the start we should already exclude potentials that lead to double spectrum, in which case e.g. a scalar m-function will not do. The following two paragraphs describe some results on the Titchmarsh-Weyl function side, which are an important starting point for Papers I and II.

Gesztesy & Zinchenko [16] In this work the authors introduce a class of functions often referred to as strongly singular potentials. The important assumption here is the existence of a certain "regular" solution of $\tau u = \lambda u$. In essence, it is required that there exists a solution $\phi(x, \lambda)$, analytic in an open neighbourhood $\mathcal{O}$ of $\mathbb{R}$ and square integrable at 0 for all $\lambda \in \mathcal{O}$.

With this solution one can build a fundamental system, i.e., also find a "singular" solution $\theta(x, \lambda)$, analytic in λ in some neighbourhood $\mathcal{O}' \subseteq \mathcal{O}$ of the real line for every x, and such that the system is normalized via its Wronskian.

It now follows that there is again a generalized Titchmarsh-Weyl coefficient to uniquely express the Weyl solution ψ in this system. In general, this m-function is not a Nevanlinna function. However, one can still associate a scalar measure ρ to this m-function. This gives rise to a spectral transformation akin to the classical case.

Finally, it should be noted that it is not a-priori clear whether a given potential indeed allows us to find a "regular" solution as above. The authors give a list of sufficient conditions that ensure for this assumption to hold, cf. [16], Examples 3.10 and 3.13. While this list is not optimized in the sense of giving all potentials for which this approach works, it nevertheless includes those examples that play a role in the Papers I and II, namely

$$\frac{l(l+1)}{x^2} + \text{``less singular terms''} \qquad \text{and} \qquad \frac{1}{x^4}.$$

Kostenko, (Sakhnovich) & Teschl [19; 20]   Within this framework of strongly singular potentials, several improvements could be achieved.

For a start, Kostenko, Sakhnovich and Teschl in [19] gave two equivalent formulations of the regularity condition posed for the "regular" solution ϕ. First, one can ask for ϕ to be analytic for all $\lambda \in \mathbb{C}$ instead of just in an open neighbourhood $\mathcal{O}$ of $\mathbb{R}$ and for it to belong to L^2 at the left endpoint for all λ. Secondly, one can also state it as $L_0|_{(0,c]}$, for any $c \in (0, \infty)$, having discrete spectrum.

Furthermore, they manage to describe all possible Titchmarsh-Weyl coefficients, give integral representations, and obtain the spectral types from the boundary behaviour of the generalized Titchmarsh-Weyl function, amongst other results. As an application inverse problems are treated.

Later, Kostenko and Teschl in [20] consider the case of the perturbed spherical Schrödinger operator

$$\tau = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + q(x) \tag{2.7}$$

with $xq(x) \in L^1[0,1]$ (meaning that the determining singularity is in the x^{-2} term) and $l \geq 1/2$ (to ensure the limit point case at 0) in more detail. In particular, they study the behaviour of the m-function in dependence of the choice of the fundamental system $\{\phi, \theta\}$. It is shown that the fundamental system can always be taken in such a way as to make the m-function a

generalized Nevanlinna function, i.e., $m \in \mathcal{N}_\kappa$ with κ given in terms of the parameter l describing the strength of the potential at zero.

Hence, if one can treat such potentials in the supersingular perturbation picture, a comparison of the appearing Q-function to this $m(\lambda)$ is of interest.

2.5. Further results In all the above treatment the singularity of the potentials is firmly set at the left endpoint. This restriction of sorts has, however, also been lifted in the literature. To exemplify this point, we draw attention to the paper by Brown, Langer and Langer [5].

There, the authors consider a Bessel-type differential equation

$$-v''(x) + \frac{\alpha}{2}\left(\frac{\alpha}{2} + 1\right)\frac{v(x)}{(x-1)^2} = \lambda v(x) \qquad x \in [0, a].$$

If $a > 1$, the singularity will lie at the inner point $x = 1$ of the interval $[0, a]$. Rewriting the equation in the so-called impedence form

$$-\left(\frac{1}{|x-1|^\alpha} y'(x)\right)' = \lambda \frac{1}{|x-1|^\alpha} y(x) \qquad x \in [0, a] \tag{2.8}$$

one notices that the equation is regular for $\alpha \in (-1, 1)$ and the singularity at $x = 1$ is in the limit circle case from both sides. This corresponds roughly to the study of the classical case above.

However, for $\alpha \geq 1$ the above equations are in the limit point case at $x = 1$ from both sides. If the boundary conditions at the endpoints of the interval are fixed, there is only one self-adjoint realization inside $L^2(0, a)$. In fact, this operator is an orthogonal sum of the respective self-adjoint operators on the left and right side of the singularity, where also the Hilbert space is split accordingly as $L^2(0, 1) \oplus L^2(1, a)$.

In the paper, the singular measure μ_α with density $|x-1|^{-\alpha}$ on $[0, a]$ is used to build an — indeterminate with κ negative squares — inner product on $C^k[0, a]$ (for appropriate k and κ). This space plus the inner product can then be lifted to a Pontryagin space $\Pi_\kappa(\mu_\alpha)$. Amongst other results, the authors then describe all self-adjoint relations or operators in $\Pi_\kappa(\mu_\alpha)$ that can be associated to (2.8) via interface conditions while leaving the boundary conditions at $x = 0$ and $x = a$ fixed.

We finally also mention that there are yet other approaches to analyze singular potentials. In particular, by rewriting the differential equation in the problem to a system of first order equations one arrives at canonical systems, which are of the form

$$Y'(x) = \lambda J H(x) Y(x) \qquad x \in [0, L), \qquad \text{where } J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},$$

Y is vector valued and $H(x)$ is a real, locally integrable 2×2-matrix-valued function on $[0, L]$ (called the Hamiltonian of the system and playing roughly the role of the potential). See for example [28] and the references therein.

3 Summary of Papers

To conclude this introductory section, we will give a short presentation of the papers included in this thesis. The first two papers, Paper I and II, were already included in [30] and are concerned with slightly more concrete problems. The third paper is more theoretical in nature as it also investigates the theory that was used in the previous two papers. The fourth paper, finally, employs these findings in the case of a particular self-adjoint operator.

Paper I

We consider the differential expression

$$\tau := -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + q(x)$$

on the halfline $(0, \infty)$, where the singularity at the origin is stemming from the x^{-2}-term. We assume that $l \geq 1/2$ to get limit point case at the origin and we assume that the potential q is such that limit point case also holds at the right endpoint. Studying this expression in the framework of ODEs, as was done in [20], one arrives at the Titchmarsh-Weyl function $m(\lambda)$ which turns out to be a generalized Nevanlinna function.

Building on the treatment of the hydrogen example in [26] we ask the question if it is also possible to investigate this class of potentials by operator methods. Namely, is it possible to employ the Hilbert space model for supersingular perturbations? Will the appearing Q-function be close to the function $m(\lambda)$ that has already been described in the literature? In this case, is it even possible to get complete agreement, something that already happened for the hydrogen atom example in the Pontryagin space formulation of Dijksma and Shondin and the ODE analysis due to Fulton?

In the paper, we first select an appropriate fundamental system of the equation $\tau u = \lambda u$ via its properties at 0. As expected, one solution can be chosen as square integrable at the origin whereas the other solution cannot have this property. Nevertheless, they allow us to study the Weyl solution $\psi(\lambda, \cdot)$ and its dependence on the spectral parameter. We see that certain differences of the Weyl solution in different spectral points, e.g., $\psi(\mu_1, \cdot) - \psi(\mu_2, \cdot)$, have a less problematic singularity at the origin.

This allows us to find a — supersingular — perturbation element $\varphi \in \mathcal{H}_{-n-2}$, where $n := \lfloor l + \frac{1}{2} \rfloor$, to carry out the analysis of τ as an extension problem in a new Hilbert space $\mathbb{H}$.

It is possible to embed $\mathbb{H}$ in the space of functionals $\mathcal{H}_{-n}$. Studying an embedded version of Krein's formula in this setting we get a generalized Nevanlinna function $\tilde{Q}$ — this is the Q-function from the formulation in $\mathbb{H}$ multiplied with a polynomial of degree n stemming from the embedding — and find that

$$\tilde{Q}(\lambda) - m(\lambda)$$

is indeed a polynomial of degree at most n.

Additionally, we answer also the last question of when this difference can be zero: given the parameters of the Hilbert space model, thus $\tilde{Q}$ is chosen first, one can pick a fundamental system that gives an m-function that coincides with this $\tilde{Q}$.

Paper II

Continuing with the investigation in Paper I, the question one can immediately ask is how far the approach via supersingular perturbations can be pushed. In particular, we concentrate on the class of strongly singular potentials introduced in the paper [16], for which on the ODE side a "good" fundamental system exists so that a Titchmarsh-Weyl function could be defined. Especially for this class it would be interesting to know if the operator approach is as powerful as the ODE one. Hints that this might be possible could be found in the literature, cf. for example [28].

However, we find that the operator approach has certain limits. In particular, we study the expression

$$\tau = -\frac{d^2}{dx^2} + \frac{1}{x^4}$$

on the halfline. We find again a suitable fundamental system for $\tau u = \lambda u$. Studying the behaviour of these fundamental solutions at the origin, we find that the singular solution behaves as $\exp(1/x)$ there. The Weyl-solution ψ then shares this property. Even though taking the same kind of differences of several Weyl solutions as in Paper I works well formally, that is the dependence on the spectral parameter can be handled easily, it however does not smooth out the nonintegrable singularity at the origin.

Consequently, we find that we cannot localize ψ in one of the rigged spaces $\mathcal{H}_{-n}$ with a finite index n. Hence, the technique of supersingular perturbations cannot be employed here. We thus find a negative answer to our ques-

tion: The class of strongly singular potentials includes potentials where operator methods can fail while an analysis via Weyl-Titchmarsh m-functions is still possible.

Paper III

The differential expressions involving the negative second derivative operator have the property that they introduce nonnegative operators into the picture along the way. Consequently, the model developed by Kurasov could be employed as it requires that the self-adjoint operator that will be perturbed to be semi-bounded.

We thus ask if this is requirement can be lifted? In particular, we consider a self-adjoint operator $A = A^*$ with its spectrum potentially covering all of the real line. The aim is to find an interpretation for the formal perturbation

$$A + \alpha \langle \varphi, \cdot \rangle \varphi, \qquad \alpha \in \mathbb{R} \cup \{\infty\}$$

where the perturbation element $\varphi \in \mathcal{H}_{-n-2}(A) \backslash \mathcal{H}_{-2}(A)$ with $n \geq 1$, i.e., φ is supersingular. As a potential generalisation of Kurasov's model we want to preserve two of its key features:

(F1) The model space has a Hilbert space structure.

(F2) Embedding the model space into the space of functionals $\mathcal{H}_{-n}$ gives a nice version of Krein's formula, involving a generalized Nevanlinna function, that parametrises these perturbations.

It turns out that assuring both properties in a model relies heavily on the operator's spectrum to at least have a gap on the real line. In other words, if $\sigma(A) = \mathbb{R}$ no such model has been found.

In the case of a Hilbert space model to keep **(F1)**: We diagonalise the operator $A = A^+ \oplus (-A^-)$ so that $A^\pm$ are positive operators. In both associated subspaces of $\mathcal{H} = \mathcal{H}^+ \oplus \mathcal{H}^-$ we employ Kurasov's model for semibounded operators. This means that we can choose real numbers $\mu_1, \ldots, \mu_n < 0$ as regularisation points from which we can build positive definite inner products on $\mathcal{H}_n^+ \oplus \mathbb{C}^n$ and $\mathcal{H}_n^- \oplus \mathbb{C}^n$. It is then possible to obtain a Hilbert space model for A via gluing together the respective separate models. However, after the embedding of the model space into $\mathcal{H}_{-n}$ there appears a certain twist in Krein's formula, which is essentially due to the diagonalisation procedure. Thus, the second feature **(F2)** fails.

In the case where **(F2)** is preserved from the start, no such diagonalisation is carried out and the eventual embedded version of Krein's formula appears just as wanted. Instead, we have to find a suitable structure for a space of

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the form $\mathcal{H}_{2k} \oplus \mathbb{C}^{2k}$. We assume the index $n = 2k$ to be even so that we can use $v_1, \ldots, v_k \in \mathbb{C}^+$ and their conjugates as regularisation points. While $\mathcal{H}_{2k}$ is unproblematic in terms of finding a suitable positive definite inner product, this becomes more involved for the finite dimensional component $\mathbb{C}^{2k}$. It turns out that we will necessarily have to have k negative squares in the inner product there. Hence, the resulting model space will always be a Pontryagin space, which stems from choosing nonreal regularisation points.

Finally we also analyze the (embedded) Q-functions that appear in each construction. We find that they are always generalized Nevanlinna functions, which was in a sense to be expected from generalising Kurasov's model. Furthermore, given the perturbation element φ the functions arising in the Hilbert space and in the Pontryagin space model are equal modulo certain polynomials of low degree that are symmetric with respect to the real axis.

Paper IV

While the previous paper could shed some light onto how to define super-singular perturbations of general self-adjoint operators it necessarily lacks some more concrete results. Thus, we take the operator of multiplication by the independent variable, A, in the Hilbert space $L^2(\mathbb{R})$ as a model case for a self-adjoint operator whose spectrum covers all of the real line. A natural choice for supersingular perturbations is readily available in the form of the functions $|x|^{m/2}$ for $m \geq 1$.

We first build the Hilbert and Pontryagin space model in this particular situation and some of the formulas simplify. However, it also allows us to in fact calculate the Q-functions $Q^{\mathbb{H}}$ and $Q^{\mathbb{K}}$ that appear in the formulations of the model.

Studying the behaviour of these functions allows us then to describe some aspects of the spectra that appear for the families of self-adjoint operators we use to define the supersingular perturbations. In particular we see that in either formulation we always find a single operator from the respective families that has an embedded eigenvalue at the origin and calculate the respective eigenfunction. Finally, varying the parameters of the models, especially in the Pontryagin space case, can lead to operators exhibiting quite curious spectral properties, which can be used as illustrating examples.

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