1-DIMENSIONAL SCHRÖDINGER OPERATORS WITH COMPLEX POTENTIALS

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Abstract. We discuss realizations of $L := -\partial_x^2 + V(x)$ as closed operators on $L^2]a, b[$, where V is complex, locally integrable and may have an arbitrary behavior at (finite or infinite) endpoints a and b. The main tool of our analysis are Green's operators, that is, various right inverses of L.

Contents

1. Introduction

The paper is devoted to operators of the form

$$L = -\partial_x^2 + V(x) \tag{1.1}$$

on $]a, b[$, where $a < b$, a can be $-\infty$ and b can be ∞. The potential V can be complex, have low regularity, and a rather arbitrary behavior at the boundary of the domain: we assume that $V \in L^1_{\rm loc}]a, b[$. We study realizations of L as closed operators on $L^2]a, b[$.

Operators of the form (1.1) are commonly called *1-dimensional Schrödinger operators* or, shorter, *1d Schrödinger operators.* They are special cases of *Sturm-Liouville operators*, that is operators of the form

$$-\frac{1}{w(x)}\partial_x p(x)\partial_x + \frac{q(x)}{w(x)}. \tag{1.2}$$

Note, however, that if $\frac{p(x)}{w(x)}$ is real, then under rather weak assumptions on w, p, q, a simple unitary transformation reduces (1.2) to (1.1). Therefore, it is not a serious restriction to consider 1d Schrödinger operators instead of Sturm-Liouville operators.

1d Schrödinger operators is a classic subject with a lot of literature. Most of the literature is devoted to real V, when L can be realized as self-adjoint operator. It is, however, quite striking that the usual theory well-known from the real (self-adjoint) case works almost equally well in the complex case. In particular, essentially the same theory for boundary conditions and the same formulas for *Green's operators* (right inverses of (1.1)) hold as in the real case. We will describe these topics in detail in this paper.

A large part of the literature on 1d Schrödinger operators assumes that potentials are L^1 near finite endpoints. Under this condition one can impose the so called *regular boundary conditions* (Dirichlet, Neumann or Robin). In this case, it is natural to use the so-called *Weyl-Titchmarsh function* and the formalism of the so-called *boundary triplets*, see e.g. [2] and references therein. We are interested in general boundary conditions, such as those considered in [4, 9, 10], where the above approach does not directly apply. See the discussion at the end of Subsect. 5.2.

One of the motivations of the present work is the study of exactly solvable Schrödinger operators, such as those given by the Bessel equation [4, 9], or the Whittaker equation [10]. Analysis of those operators indicates that non-real potentials are as good from the point of view of the exact solvability as real ones. It is also natural to organize exactly solvable Schrödinger operators in holomorphic families, whose elements are self-adjoint only in exceptional cases. Therefore, a theory for 1d Schrödinger operators with complex potentials and general boundary conditions provides a natural framework for the study of exactly solvable Hamiltonians.

As we mentioned above, we suppose that $V \in L^1_{\rm loc}]a,b[$. The theory is much easier if $V \in L^2_{\rm loc}]a,b[$, because one could then assume that the operator acts on $C^2_{\rm c}]a,b[$. Dealing with potentials in $L^1_{\rm loc}$ causes of a lot of trouble—this is however a rather natural assumption. We think that handling a more general case forces us to better understand the problem. Actually, one could consider even more singular potentials: it is easy to generalize our results to potentials V being Borel measures on $]a,b[$.

In the preliminary Sect. 2 we study the inhomogeneous problem given by the operator (1.1) by basic ODE methods. We introduce some distinguished Green's operators: The *two-sided Green's operators* are related to boundary conditions on both sides. The *forward* and *backward Green's operators* are related to the Cauchy problem at the endpoints of the interval. These operators belong to the most often used objects in mathematics. Usually they appear under the guise of *Green's functions*, which are the integral kernels of Green's operators.

Note that in the Hilbert space $L^2]a,b[$ we have a natural conjugation $f \mapsto \overline{f}$ and a bilinear form $\langle f|g\rangle := \int fg$. For an operator T it is natural to define its *transpose* $T^\# := \overline{T^*}$, where the bar denotes the complex conjugation. We say that T is *self-transposed* if $T^\# = T$ (in the literature the alternative name *J-self-adjoint* is also used). These concepts play an important role in the theory of differential operators on $L^2]a,b[$. Therefore, we devote Sect. 3 to a general theory of operators in a Hilbert space with a conjugation. We briefly recall the theory of restrictions/extensions of unbounded operators. The concept of self-transposed operators turns out to be a natural alternative to the concept of self-adjointness. It is well-known that self-adjoint operators are *well-posed* (possess non-empty resolvent set). Not every self-transposed operator is well-posed, however they often are.

The remaining sections are devoted to realizations of L given by (1.1) as closed operators on the Hilbert space $L^2]a,b[$. The most obvious realizations are the *minimal* one $L_{\min}$ and the *maximal* one $L_{\max}$. We prove that these operators are closed and densely defined. Under the assumption $V \in L^1_{\rm loc}]a,b[$ the proof is quite long and technical but, in our opinion, instructive. If we assumed $V \in L^2_{\rm loc}]a,b[$, the proof would be easy.

At this point it is helpful to recall basic theory of 1d Schrödinger operators for real potentials. One is usually interested in self-adjoint extensions of the Hermitian operator $L_{\min}$. They are are situated "half-way" between $L_{\min}$ and $L_{\max}$. More precisely, we have 3 possibilities:

(1) $L_{\min} = L_{\max}$: then $L_{\min}$ is already self-adjoint.
(2) The codimension of $\mathcal{D}(L_{\min})$ in $\mathcal{D}(L_{\max})$ is 2: if $L_\bullet$ is a self-adjoint extension of $L_{\min}$, the inclusions $\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_\bullet) \subset \mathcal{D}(L_{\max})$ are of codimension 1.
(3) The codimension of $\mathcal{D}(L_{\min})$ in $\mathcal{D}(L_{\max})$ is 4: if $L_\bullet$ is a self-adjoint extension of $L_{\min}$, the inclusions $\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_\bullet) \subset \mathcal{D}(L_{\max})$ are of codimension 2.

Note that in the literature it is common to use the theory of *deficiency indices*. The cases (1), (2), resp. (3) correspond to $L_{\min}$ having the deficiency indices $(0,0)$, $(1,1)$ and $(2,2)$. However, the deficiency indices do not have a straightforward generalization to the complex case.

Let us go back to complex potentials. Note that the Hermitian conjugate of an operator T, denoted T^*, turns out to be less useful than its transpose $T^\#$. In particular, the role of self-adjoint operators is taken up by self-transposed operators.

By choosing a subspace of $\mathcal{D}(L_{\max})$ closed in the graph topology and restricting $L_{\max}$ to this subspace we can define a closed operator. Such operators will be called *closed realizations of* L. We will show that in the complex case closed realizations of L possess a theory quite analogous to that of the real case.

We are mostly interested in realizations of L whose domain contains $\mathcal{D}(L_{\min})$, that is, operators $L_\bullet$ satisfying $L_{\min} \subset L_\bullet \subset L_{\max}$. Such realizations are defined by specifying boundary conditions. Similarly as in the real case, boundary conditions are given by functionals on $\mathcal{D}(L_{\max})$ that vanish on $\mathcal{D}(L_{\min})$. For each of endpoints, a and b, there is a space of functionals describing boundary conditions. We call the dimension of this space the *boundary index at* a, resp. b, and denote it $\nu_a(L)$, resp. $\nu_b(L)$. They can take the values 0 or 2 only. Therefore, we have the following classification of operators L:

$$\begin{aligned}&(1)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) = 0, \text{ or } L_{\min} = L_{\max},\\ &(2)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) = 2,\\ &(3)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) = 4.\end{aligned} \tag{1.3}$$

Let $\lambda \in \mathbb{C}$. It is natural to consider the space of solutions of $(L - \lambda)u = 0$ that are square integrable near a, resp. b. We denote these spaces by $\mathcal{U}_a(\lambda)$, resp. $\mathcal{U}_a(\lambda)$. We will prove that

$$\nu_a(L) = 0 \iff \dim \mathcal{U}_a(\lambda) \le 1\ \forall \lambda \in \mathbb{C} \iff \dim \mathcal{U}_a(\lambda) \le 1 \text{ for some } \lambda \in \mathbb{C}, \tag{1.4}$$

$$\nu_a(L) = 2 \iff \dim \mathcal{U}_a(\lambda) = 2\ \forall \lambda \in \mathbb{C} \iff \dim \mathcal{U}_a(\lambda) = 2 \text{ for some } \lambda \in \mathbb{C}. \tag{1.5}$$

The most useful realizations of L are well-posed. Not all L possess such realizations. One can classify such L's as follows. If L possesses a well-posed realization $L_\bullet$, then one of the following conditions holds:

$$\begin{aligned}&(1)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = 0, \text{ or } L_\bullet = L_{\max}\\ &(2)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = 1,\\ &(3)\ \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = 2.\end{aligned} \tag{1.6}$$

There is a strict correspondence between (1), (2) and (3) of (1.3) and (1), (2) and (3) of (1.6). In cases (1) and (2) from Table (1.6) we describe all realizations with nonempty resolvent set and their resolvents. We prove that if $L_\bullet$ is such a realization, then we can find $u \in \mathcal{U}_a(\lambda)$ and $v \in \mathcal{U}_b(\lambda)$ with the Wronskian equal to 1, so that the integral kernel of $(L_\bullet - \lambda)^{-1}$ can then be easily expressed in terms of u and v.

The case (3) is much richer. We describe all realizations of L that have *separated boundary conditions* (given by independent boundary conditions at a and b). If in addition they are self-transposed, then essentially the same formula as in (1) and (2) gives $(L_\bullet - \lambda)^{-1}$. There are however two other separated realizations of L, which are denoted L_a and L_b, with boundary conditions only at a, resp. b. They are not self-transposed, in fact, they satisfy $L_a^\# = L_b$. Their resolvents are given by what we call *forward* and *backward Green's operators*, which incidentally are cousins of the *retarded* and *advanced Green's functions*, well-known from the theory of the wave equation.

In the last section we discuss potentials with a negative imaginary part. We show that under some weak conditions they define dissipative 1d Schrödinger operators. We also describe Weyl's limit point–limit cricle method for such potentials. For real potentials, this method allows us to determine the dimension of $\mathcal{U}_a(\lambda)$ for $\mathrm{Im}(\lambda) > 0$: if a is limit point, then $\dim \mathcal{U}_a(\lambda) = 1$; if a is limit circle then $\dim \mathcal{U}_a(\lambda) = 2$. The picture is more complicated if the potential is complex: there are examples where the endpoint a is limit point and $\mathcal{U}_a(\lambda)$ is two-dimensional.

1d Schrödinger operators is one of the most classic topics in mathematics. Already in the first half of 19 century Sturm and Liouville considered second order differential operators on a finite interval with various boundary consitions. The theory was extended to a half-line and a line in a celebrated work by Weyl.

2nd order ODE's and 1d Schrödinger operators are considered in many textbooks, including Atkinson [1], Coddington-Levinson [5], Dunford-Schwartz [12, 13], Naimark [20], Pryce [21], de Alfaro-Regge [7], Reed-Simon [23], Stone [25], Titchmarsh [27], Teschl [26], Gitman-Tyutin-Voronov [17]. However, in the literature complex potentials are rarely studied in detail, and if so, then one does not pay attention to nontrivial boundary conditions. The monograph by Edmunds-Evans [14] is often considered as one of the most up-to-date source for results on this subject. Many results presented in our article have their counterpart in the literature, especially in [14]. Let us try to make a more detailed comparison of our paper with the literature

Most of the material of Sect. 2 is standard. However, we have not seen a separate discussion of semi-regular boundary condition, as described in Prop. 2.5 (2) and (3). The definitions of the canonical bisolution $G_\leftrightarrow$, various Green's operators $G_{u,v}$ $G_\leftarrow$, $G_\rightarrow$ and relations between them (2.21)–(2.23) are implicit in many works on the subject, however they are rarely separately emphasized.

The material of our Sect. 3 on Hilbert spaces with conjugation is to a large extent contained in Chap. 3 Sects 3 and 5 of [14]. It is based on previous results of Vishik [28], Galindo [16] and Knowles [19]. However, our presentation seems to be somewhat different. It shows in particular that the existence of a self-transposed extension follows almost trivially from a basic theory of symplectic spaces described in Appendix A. Another special feature of our Sect. 3 is a discussion of properties of right inverses of an unbounded operator.

The deepest result described in our paper is probably Theorem 6.15 about the characterization of boundary conditions by square integrable solutions. This result is actually not contained in [14]. It is based on Everitt and Zettl [15, Theorem 9.1], and uses [1, Theorem 9.11.2] of Atkinson and [22, Theorem 5.4] of Race.

The study of Green's operators contained in Sect. 7 is probably to a some extent new.

A separate subject that we discuss are potentials with negative imaginary part studied by means of the so-called Weyl limit circle/limit point method. Here the main reference is Sims [24], see also [3, 14].

The present manuscript grew out of the Appendix of [4] devoted to 1d Schrödinger operators with the potential $\frac{1}{x^2}$. [4] and its follow-up papers [9, 10] illustrated that 1d Schrödinger operators with complex potentials and unusual boundary conditions appear naturally in various situations. Motivated by these applications, we decided to write an exposition of basic general theory of 1d Schrödinger operators.

We decided to make our exposition as complete and self-contained as possible, explaining things that are perhaps obvious to experts, but often difficult to many readers. We use freely the modern operator theory—this is not the case of a large part of literature, which often sticks to old-fashioned approaches. We also use the terminology and notation which, we believe, is as natural as possible in the context we consider. For instance, we prefer the name "self-transposed" to "J-self-adjoint" found in a large part of the literature. We believe that our treatment of the subject is quite different from the one found in the literature. One of the main tools that we have found useful, rarely appearing in the literature, are right inverses, which in the context of 1d Schrödinger operators we call by the traditional name of *Green's operators*.

2. Basic ODE theory

2.1. **Notations.** Recall that $a < b$, a can be $-\infty$ and b can be ∞. The notation $[a, b]$ stands for the interval including the enpoints a and b, while $]a, b[$ for the interval without endpoints. $[a, b[$ and $]a, b]$ have the obvious meaning.

In some cases one could use the notation involving either $[a, b]$ or $]a, b[$ without a change of the meaning. For instance, $L^p\big([a, b]\big) = L^p\big(]a, b[\big)$. For esthetic reasons, we try to use a uniform notation—we usually write $L^p]a, b[$, dropping the round bracket for brevity.

In other cases, the choice of either $[a, b]$ or $]a, b[$ influences the meaning of a symbol. For instance, $C[a, b] \subsetneq C]a, b[$. For example, $f \in C[-\infty, b]$ implies that $\lim\limits_{x\to-\infty} f(x) =: f(-\infty)$ exists.

$f \in L^p_{\rm loc}]a, b[$ iff for any $a < a_1 < b_1 < b$, we have $f\Big|_{]a_1,b_1[} \in L^p]a_1, b_1[$. $f \in L^p_{\rm loc}[a, b[$ if in addition $f \in L^1[a, a_1[$ and similarly for $L^p_{\rm loc}]a, b]$.

$f \in L^p_{\rm c}]a, b[$ iff $f \in L^p]a, b[$ and supp$f$ is a compact subset of $]a, b[$. The analogous meaning has the subscript c in different situations.

$\oplus$ will mean the topological direct sum of two spaces.

2.2. **Absolutely continuous functions.** We will denote f' or ∂f the derivative of a distribution f. We will denote by $AC]a, b[$ the space of *absolutely continuous functions* on $]a, b[$, that is, distributions on $]a, b[$ whose derivative is in $L^1_{\rm loc}]a, b[$. This definition is equivalent to the more common definition: for every $\epsilon > 0$ there exists $\delta > 0$ such that for any family of non-intersecting intervals $[x_i, x_i']$ in $a, b[$ satisfying $\sum_{i=1}^n |x_i' - x_i| < \delta$ we have $\sum_{i=1}^n |f(x_i') - f(x_i)| < \epsilon$.

We have $AC]a, b[\subset C]a, b[$. If $f, g \in AC]a, b[$, then $fg \in AC]a, b[$ and the Leibniz rule holds:

$$(fg)' = f'g + fg'. \tag{2.1}$$

$AC^n]a,b[$ will denote the space of distributions whose nth derivative is in $AC]a,b[$.

Lemma 2.1. *Let $f_n \in AC]a,b[$ be a sequence such that for any $a < a_1 < b_1 < b$, $f_n \to f$ uniformly on $[a_1,b_1]$ and $f_n' \to g$ in $L^1[a_1,b_1]$. Then $f \in AC]a,b[$ and $g = f'$.*

We will denote by $AC[a,b]$ the space of functions on $[a,b]$ whose (distributional) derivative is in $L^1]a,b[$. Clearly, $AC[a,b] \subset C[a,b]$. If $f \in AC[a,b]$, then

$$\int_a^b f'(x)\mathrm{d}x = f(b) - f(a). \tag{2.2}$$

Note that a can be $-\infty$ and b can be ∞.

Obviously, if $f \in AC]a,b[$ and $a < a_1 < b_1 < b$ then $f\Big|_{[a_1,b_1]}$ belongs to $AC[a_1,b_1]$.

2.3. **Choice of functional-analytic setting.** Throughout the section, we assume that $V \in L^1_{\mathrm{loc}}]a,b[$ and we consider the differential expression

$$L := -\partial^2 + V. \tag{2.3}$$

Sometimes we restrict our operator to a smaller interval, say $]c,d[$, where $a \le c < d \le b$. Then (2.3) restricted to $]c,d[$ is denoted $L^{c,d}$.

Eventually, we would like to study operators in $L^2]a,b[$ associated to L, which in many respects seems the most natural setting for one dimensional Schrödinger operators. This introductory section, however, is devoted mostly to the *equation* $Lf = g$. We postpone considerations related to *operator realizations of* L to the later sections.

Suppose that we choose $L^1_{\mathrm{loc}}]a,b[$ as the target space for (2.3), which seems to be a rather general function space. Note that if $f \in L^\infty_{\mathrm{loc}}]a,b[$, the product fV is well defined and belongs to $L^1_{\mathrm{loc}}]a,b[$. Moreover, this is the best we can do if V is an arbitrary locally integrable function, i.e. we cannot replace L^∞_{loc} by a larger space. Then, if we consider L^∞_{loc} as the initial space for (2.3) and we require that the target space for (2.3) is $L^1_{\mathrm{loc}}]a,b[$, we are forced to work with functions $f \in L^\infty_{\mathrm{loc}}]a,b[$ such that $Lf \in L^1_{\mathrm{loc}}]a,b[$. But then $f'' \in L^1_{\mathrm{loc}}]a,b[$, and hence $f \in AC^1]a,b[$.

Therefore it is natural to consider (2.3) as an an operator $L : AC^1]a,b[\to L^1_{\mathrm{loc}}]a,b[$, which we will do throughout this paper. Restrictions of L to subspaces of $AC^1]a,b[$ which are sent into $L^2]a,b[$ by L are the objects of main interest in our study.

We equip $L^1_{\mathrm{loc}}]a,b[$ with the topology of local uniform convergene, i.e. a sequence $\{f_n\}$ converges to f if and only if $\lim\limits_{n\to\infty} \|f_n - f\|_{L^1(J)} = 0$ for any compact $J \subset]a,b[$. Clearly this is a complete space. It is convenient to think of L as an operator in $L^1_{\mathrm{loc}}]a,b[$ with domain $AC^1]a,b[$. Then L is densely defined and later on we will prove that it is is closed (see Corollary 2.17).

2.4. **The Cauchy problem.** For $g \in L^1_{\mathrm{loc}}]a,b[$ we consider the problem

$$Lf = g. \tag{2.4}$$

Proposition 2.2. *Let $a < d < b$. Then for any p_0, p_1 there exists a unique $f \in AC^1]a,b[$ satisfying (2.4) and*

$$f(d) = p_0, \quad f'(d) = p_1. \tag{2.5}$$

Proof. Define the operators Q_d and T_d by their integral kernels

$$Q_d(x,y) := \begin{cases} (y-x)V(y), & x < y < d, \\ (x-y)V(y), & x > y > d, \\ 0 & \text{otherwise}; \end{cases} \tag{2.6}$$

$$T_d(x,y) := \begin{cases} (y-x), & x < y < d, \\ (x-y), & x > y > d, \\ 0 & \text{otherwise}. \end{cases} \tag{2.7}$$

The Cauchy problem can be rewritten as $F(f) = f$ where F is a map on $C]a,b[$ given by

$$F(f)(x) := p_0 + p_1(x-d) + Q_d f(x) + T_d g(x). \tag{2.8}$$

If $a \le a_1 < d < b_1 \le b$ and we view Q_d as an operator on $C[a_1, b_1]$ with the supremum norm, then

$$\|Q_d\| \le \max\Big\{ \int_{a_1}^{d} |V(y)(y-a_1)|\mathrm{d}y,\ \int_{d}^{b_1} |V(y)(y-b_1)|\mathrm{d}y \Big\}. \tag{2.9}$$

If the interval $[a_1, b_1]$ is finite, the operator T_d is bounded from $L^1]a_1, b_1[$ into $C[a_1, b_1]$.

Thus, by choosing a sufficiently small interval $[a_1, b_1]$ containing d, we can make F well defined and contractive on $C[a_1, b_1]$. (F is contractive iff $\|Q_d\| < 1$). By Banach's Fixed Point Theorem (or the convergence of an appropriate Neumann series) there exists $f \in C[a_1, b_1]$ such that $f = F(f)$. Then note that we have

$$f'(x) = F(f)'(x) = p_1 + \int_d^x V(y)f(y)\mathrm{d}y + \int_d^x g(y)\mathrm{d}y$$

hence $f' \in AC[a_1, b_1]$ and $f \in AC^1[a_1, b_1]$.

Thus for every $d \in]a, b[$ we can find an open interval containing d on which there exists a unique solution to the Cauchy problem. We can cover $]a, b[$ with intervals $]a_j, b_j[$ containing d_j with the analogous property. This allows us to extend the solution with initial conditions at any $d \in]a, b[$ to the whole $]a, b[$. □

2.5. **Regular and semiregular endpoints.** One dimensional Schrödinger operators possess the simplest theory when $-\infty < a < b < \infty$ and $V \in L^1]a, b[$. Then we say that L *is a regular operator*. Most of the classical Sturm-Liouville theory is devoted to such operators. More generally, the following standard terminology will be convenient.

Definition 2.3. *The endpoint a is called* regular*, or L is called* regular at a*, if a is finite and $V \in L^1_{\mathrm{loc}}[a, b[$ (i.e. V is integrable around a). Similarly for b. Hence L is* regular *if both endpoints are regular.*

1d Schrödinger operators satisfying the following conditions are also relatively well behaved:

Definition 2.4. *The endpoint a is called* semiregular *if a is finite and $(x-a)V \in L^1_{\mathrm{loc}}[a, b[$ (i.e. $(x-a)V$ is integrable around a). Similarly for b.*

Proposition 2.5. *Let $g \in L^1_{\mathrm{loc}}[a, b[$.*

1. *Let a be a regular endpoint. Let p_0, p_1 be given. Then there exists a unique $f \in AC^1[a, b[$ satisfying $Lf = g$ and $f(a) = p_0, f'(a) = p_1$.*
2. *Let a be a semiregular endpoint. Then all solutions f have a limit at a.*
3. *Let a be a semiregular endpoint. Let p_1 be given. Then there exists a unique $f \in AC^1[a, b[$ satisfying $Lf = g$ and $f(a) = 0, f'(a) = p_1$.*

Proof. (1) is proven as Prop. 2.2, choosing $d = a$; the operators (2.6) and (2.7) are now

$$Q_a(x, y) := \begin{cases} (x-y)V(y), & x > y > a, \\ 0 & \text{otherwise}; \end{cases} \tag{2.10}$$

$$T_a(x, y) := \begin{cases} (x-y), & x > y > a, \\ 0 & \text{otherwise}. \end{cases} \tag{2.11}$$

To prove (2) we choose d inside $]a, b[$ such that $\int_a^d V(y)|y-a|\mathrm{d}y < 1$. This guarantees that the operator Q_d is contractive on $C[a, d]$.

To prove (3) we modify the proof of Prop. 2.2. We chose $d = a$ and use the Banach space $|x-a|^{-1}C]a, b_1[:= \{f \in C]a, b_1[\mid \|f\| := \sup \frac{|f(x)|}{|x-a|} < \infty\}$, where $a < b_1 < b$ is finite and will be chosen later. The Cauchy problem can be rewritten as $F(f) = f$ where F is given by $|x-a|^{-1}C]a, b_1[$ given by

$$F(f)(x) := p_1(x-a) + Q_a f(x) + T_a g(x). \tag{2.12}$$

Q_a is an operator on $|x-a|^{-1}C[a,b_1]$ with the norm

$$\|Q_a\| \leq \int_a^{b_1} |V(y)(y-a)|\mathrm{d}y. \tag{2.13}$$

The operator T_a is bounded from $L^1]a,b_1[$ into $|x-a|^{-1}C[a,b_1]$. Therefore, F is a well-defined map on $|x-a|^{-1}C[a,b_1]$. Then we argue similarly as in the proof of Prop. 2.2. For b_1 close enough to a the map F is contractive and we can apply Banach's Fixed Point Theorem. From

$$f'(x) = F(f)'(x) = p_1 + \int_a^x |y-a|V(y)|y-a|^{-1}f(y)\mathrm{d}y + \int_a^x g(y)\mathrm{d}y$$

we see that $f'(a) = p_1$. □

An example of a potential with a finite point which is not semiregular is $V(x) = \frac{c}{x^2}$ on $]0,\infty[$. For its theory see [4, 9].

2.6. **Wronskian.**

Definition 2.6. *The* Wronskian *of two differentiable functions u, v is*

$$W(u,v;x) = W_x(u,v) = u(x)v'(x) - u'(x)v(x). \tag{2.14}$$

Proposition 2.7. *Let $u, v \in AC^1]a,b[$. Then the* Lagrange identity *holds:*

$$\partial_x W(u,v;x) = -(Lu)(x)v(x) + u(x)(Lv)(x). \tag{2.15}$$

Consequently, if $Lu = Lv = 0$, then $W(u,v)$ is a constant function.

Proof. Since $u, u', v, v' \in AC]a,b[$, the Wronskian can be differentiated and a simple computation yields (2.15). □

Definition 2.8. *The set of solutions in $AC^1]a,b[$ of the homogeneous equation $Lf = 0$ will be denoted $\mathcal{N}(L)$.*

$\mathcal{N}(L)$ is a two dimensional complex space and the map $W : \mathcal{N}(L) \times \mathcal{N}(L) \to \mathbb{C}$ is bilinear and antisymmetric. $u, v \in \mathcal{N}(L)$ are linearly independent if and only if $W(u,v) \neq 0$. If $u_2 = \alpha u_1 + \beta v_1, v_2 = \gamma u_1 + \delta v_1$ then

$$W(u_2,v_2) = W(\alpha u_1, \delta v_1) + W(\beta v_1, \gamma u_1) = (\alpha\delta - \beta\gamma)W(u_1,v_1).$$

hence if $W(u_1,v_1) = 1$ then $W(u_2,v_2) = 1$ if and only if $\alpha\delta - \beta\gamma = 1$, and in this case a simple computation gives

$$u_2(x)v_2(y) - u_2(y)v_2(x) = u_1(x)v_1(y) - u_1(y)v_1(x), \quad x,y \in]a,b[. \tag{2.16}$$

Thus the function

$$G_\leftrightarrow(x,y) := u(x)v(y) - u(y)v(x) \tag{2.17}$$

is independent of the choice of the solutions u, v of the homogeneous equation $Lf = 0$ if they satisfy $W(u,v) = 1$. (2.17) can be interpreted as the integral kernel of an operator $G_\leftrightarrow : L^1_\mathrm{c}]a,b[\to AC^1]a,b[$, and will be called the *canonical bisolution of* L. It satisfies

$$LG_\leftrightarrow = 0, \quad G_\leftrightarrow L = 0, \quad G_\leftrightarrow(x,y) = -G_\leftrightarrow(y,x). \tag{2.18}$$

2.7. **Green's operators.**

The expression "Green's function" is commonly used to denote the integral kernel of a right inverse of a differential operator, usually of a second order. We will use the expression "Green's operator" for a right inverse of L.

Definition 2.9. *An operator $G_\bullet : L^1_\mathrm{c}]a,b[\to AC^1]a,b[$ is called a* Green's operator of L *if*

$$LG_\bullet g = g, \quad g \in L^1_\mathrm{c}]a,b[. \tag{2.19}$$

Note that we do not require that $G_\bullet L = \mathbb{1}$. Note also that $G_\leftrightarrow$ is not Green's operator—it is a bisolution. However, it is so closely related to various Green's operators that its symbol contains the same letter G.

There are many Green's operators. If $G_\bullet$ is a Green's operator, u, v are two solutions of the homogeneous equation, and $\phi, \psi \in L^\infty_{\mathrm{loc}}]a, b[$ are arbitrary, then

$$G_\bullet + |u\rangle\langle\phi| + |v\rangle\langle\psi|$$

is also a Green's operator. Recall that if E, F are vector spaces, g belongs to the dual of E, and $f \in F$, then $|f\rangle\langle g|$ is the linear map $E \to F$ defined by $e \mapsto g(e)f$.

Let us define some distinguished Green's operators. Let u, v be two solutions of the homogeneous equation such that $W(v, u) = 1$. We easily check that the operators $G_{u,v}$, G_a and G_b defined below are Green's operators in the sense of Def. 2.9:

Definition 2.10. Green's operator associated to u at a and v at b, *denoted* $G_{u,v}$, *is defined by its integral kernel*

$$G_{u,v}(x, y) := \begin{cases} u(x)v(y), & x < y, \\ v(x)u(y), & x > y. \end{cases}$$

Operators of the form $G_{u,v}$ will be sometimes called *two-sided Green's operators.*

Definition 2.11. Forward Green's operator $G_\rightarrow$ *has the integral kernel*

$$G_\rightarrow(x, y) := \begin{cases} 0, & x < y, \\ v(x)u(y) - u(x)v(y), & x > y. \end{cases} \tag{2.20}$$

Definition 2.12. Backward Green's operator $G_\leftarrow$ *has the integral kernel*

$$G_\leftarrow(x, y) := \begin{cases} u(x)v(y) - v(x)u(y), & x < y, \\ 0, & x > y. \end{cases}$$

By the comment after (2.16), the operators $G_\rightarrow$ and $G_\leftarrow$ are independent of the choice of u, v. For $a < b_1 < b$, $G_\rightarrow$ maps $L^1_{\mathrm{c}}]b_1, b[$ into functions that are zero on $]a, b_1]$. Similarly, for $a < a_1 < b$, $G_\rightarrow$ maps $L^1_{\mathrm{c}}]a, a_1[$ into functions that are zero on $[a_1, b[$.

Note also some formulas for differences of two kinds of Green's operators:

$$G_{u,v} - G_\rightarrow = |u\rangle\langle v|, \tag{2.21}$$

$$G_{u,v} - G_\leftarrow = |v\rangle\langle u|, \tag{2.22}$$

$$G_\rightarrow - G_\leftarrow = |v\rangle\langle u| - |u\rangle\langle v| = G_\leftrightarrow, \tag{2.23}$$

$$G_{u,v} - G_{u_1,v_1} = |u\rangle\langle v| - |u_1\rangle\langle v_1|, \tag{2.24}$$

The following definition introduces another class of Green's operators in the sense of Def. 2.9, which are generalizations of forward and backward Green's operators.

Definition 2.13. Green's operator associated to $d \in]a, b[$ *is defined by the integral kernel*

$$G_d(x, y) := \begin{cases} u(x)v(y) - v(x)u(y), & x < y < d, \\ v(x)u(y) - u(x)v(y), & x > y > d, \\ 0, & \textit{otherwise}. \end{cases}$$

As in the case of $G_\rightarrow$ and $G_\leftarrow$, these operators are independent of the choice of u, v. Note that if $a < a_1 < d < b_1 < b$, then G_d maps $L^1_{\mathrm{c}}]a, a_1[$ on functions that are zero on $[a_1, b[$, and $L^1_{\mathrm{c}}]b_1, b[$ on functions that are zero on $]a, b_1]$.

The proof of Prop. 2.2 suggests how to construct G_d without knowing v, u using the operators Q_d and T_d defined there. We have, at least formally,

$$G_d = (\mathbb{1} - Q_d)^{-1} T_d. \tag{2.25}$$

If we choose $a \leq a_1 < d < b_1 \leq b$ with a finite $[a, b]$ and

$$\max\left\{\int_{a_1}^{d} |V(x)(x-a_1)|\mathrm{d}x, \int_{d}^{b_1} |V(x)(x-b_1)|\mathrm{d}x\right\} < 1, \tag{2.26}$$

then (2.25) is given by a convergent Neumann series in the sense of an operator from $L^1]a_1, b_1[$ to $C[a_1, b_1]$.

Remark 2.14. *The 1-dimensional Schrödinger equation can be interpreted as the Klein Gordon equation on a 1+0 dimensional spacetime (no spacial dimensions, only time). The operators $G_\leftrightarrow$, $G_\rightarrow$ and $G_\leftarrow$ have important generalizations to globally hyperbolic spacetimes of any dimension— they are then usually called the Pauli-Jordan, retarded, resp. advanced propagator, see e.g. [11].*

2.8. **Some estimates.** The following elementary estimates will be useful later on.

Lemma 2.15. *Let J be an open interval of length $\nu < \infty$ and $f \in L^1(J)$ with $f'' \in L^1(J)$. Then f and f' are continuous functions on the closure of J and if a is an end point of J then*

$$|f(a)| + \nu|f'(a)| \leq C \int_J \left(\nu|f''(x)| + \nu^{-1}|f(x)|\right) \mathrm{d}x, \tag{2.27}$$

where C is a real number independent of f and J.

Proof. By a scaling argument we may assume $\nu = 1$. It suffices to assume that f is a distribution on $\mathbb{R}$ such that $f'' = 0$ outside J. Let $\theta : \mathbb{R} \to \mathbb{R}$ be of class C^∞ outside of 0 and such that $\theta(x) = 0$ if $x \leq 0$, $\theta(x) = x$ if $0 < x < 1/2$, $\theta(x) = 0$ if $x \geq 1$. Define η by $\theta'' = \delta - \eta$ where δ is the Dirac measure at the origin. Clearly η is of class C^∞ with support in $[1/2, 1]$. For any distribution f we have

$$f = \delta * f = \theta'' * f + \eta * f = \theta * f'' + \eta * f \quad \text{hence also} \quad f' = \theta' * f'' + \eta' * f.$$

This clearly implies (2.27) for $\nu = 1$ and a the right endpoint of J. □

Lemma 2.16. *Assume that $\ell := \sup_J \int_J |V(x)|\mathrm{d}x < \infty$ where J runs over all the intervals $J \subset]a, b[$ of length ≤ 1. Then there are numbers $C, \nu_0 > 0$ such that*

$$\|f\|_{L^\infty(J)} + \nu\|f'\|_{L^\infty(J)} \leq C\nu\|Lf\|_{L^1(J)} + C\nu^{-1}\|f\|_{L^1(J)} \tag{2.28}$$

for all $f \in L^\infty_{\mathrm{loc}}]a, b[$, all $\nu \leq \nu_0$, and all intervals $J \subset]a, b[$ of length ν.

Proof. Note that for a continuous f we have $f'' \in L^1_{\mathrm{loc}}$ if and only $Lf \in L^1_{\mathrm{loc}}$ and then f' is absolutely continuous. We take $\nu_0 \leq 1$ and strictly less than half the length of $]a, b[$. If $\nu \leq \nu_0$, then (2.27) gives for x such that $]x, x + \nu[\subset]a, b[$:

$$\begin{aligned}
|f(x)| + \nu|f'(x)| &\leq C \int_x^{x+\nu} \left(\nu|Lf| + \nu|Vf| + \nu^{-1}|f(y)|\right) \mathrm{d}y \\
&\leq C\|\nu|Lf| + \nu^{-1}|f|\|_{L^1(x,x+\nu)} + C\ell\nu\|f\|_{L^\infty(x,x+\nu)} \\
&\leq C\nu\|Lf\|_{L^1(J)} + C\nu^{-1}\|f\|_{L^1(J)} + C\ell\nu\|f\|_{L^\infty(J)}.
\end{aligned}$$

If $x \in]a, b[$ and $]x, x + \nu[\not\subset]a, b[$ then $]x - \nu, x[\subset]a, b[$ and we have an estimate as above with $]x, x + \nu[$ replaced by $]x - \nu, x[$. Hence

$$\|f\|_{L^\infty(J)} + \nu\|f'\|_{L^\infty(J)} \leq C\nu\|Lf\|_{L^1(J)} + C\nu^{-1}\|f\|_{L^1(J)} + C\ell\nu\|f\|_{L^\infty(J)}.$$

If ν_0 is such that $C\ell\nu_0 < 1$ we get the required estimate. □

Recall (see Subsect. 2.3) that $L^1_{\mathrm{loc}}]a, b[$ is equipped with the topology of local uniform convergence and that we think of L as an operator in $L^1_{\mathrm{loc}}]a, b[$ with domain $AC^1]a, b[$. The next result says that this operator is closed.

Corollary 2.17. *Let $\{f_n\}$ be a sequence in $AC^1]a, b[$ such that the sequences $\{f_n\}$ and $\{Lf_n\}$ are Cauchy in $L^1_{\mathrm{loc}}]a, b[$. Then the limits $f := \lim_{n\to\infty} f_n$ and $g := \lim_{n\to\infty} Lf_n$ exist in $L^1_{\mathrm{loc}}]a, b[$ and we have $f \in AC^1]a, b[$ and $Lf = g$.*

Proof. The estimate (2.28) implies that on every compact interval J we have uniform convergence of f_n to f (and also of f_n' to f'). Therefore, $Vf_n\big|_J \to Vf\big|_J$ in $L^1(J)$ for any such J. Hence, $-f_n'' = Lf_n - Vf_n$ converges in $L^1(J)$ to $g - Vf$. Therefore, by Lemma 2.1, $-f'' = g - Vf$. We know that $g - Vf \in L^1_{\rm loc}]a,b[$, hence $f \in AC^1]a,b[$. $\square$

3. Hilbert spaces with conjugation

3.1. **Bilinear scalar product.** Let $\mathcal{H}$ be a Hilbert space equipped with a *scalar product* $(\cdot|\cdot)$. One says that J is a *conjugation* if it is an antilinear operator on $\mathcal{H}$ satisfying $J^2 = \mathbb{1}$ and $(Jf|Jg) = \overline{(f|g)}$. In a Hilbert space with a conjugation J an important role is played by the *natural bilinear form*

$$\langle f|g\rangle := (Jf|g). \tag{3.1}$$

In our paper we usually consider the Hilbert space $\mathcal{H} = L^2]a,b[$, which has the obvious conjugation $f \mapsto \overline{f}$. Its scalar product and its bilinear form are as follows

$$(f|g) := \int_a^b \overline{f(x)}g(x)\mathrm{d}x, \tag{3.2}$$

$$\langle f|g\rangle := \int_a^b f(x)g(x)\mathrm{d}x = (\overline{f}|g). \tag{3.3}$$

Thus we use round brackets for the sesquilinear scalar product and angular brackets for the bilinear form. Note that in some sense the latter plays a more important role in our paper (and in similar problems) than the former. See e.g. [8, 10], where the same notation is used.

If $\mathcal{G} \subset L^2]a,b[$, we will write

$$\mathcal{G}^\perp := \{f \in L^2]a,b[\mid (f|g) = 0,\ g \in \mathcal{G}\}, \tag{3.4}$$

$$\mathcal{G}^{\rm perp} := \{f \in L^2]a,b[\mid \langle f|g\rangle = 0,\ g \in \mathcal{G}\} = \overline{\mathcal{G}^\perp}. \tag{3.5}$$

3.2. **Transposition of operators.** If T is an operator, then $\mathcal{D}(T)$, $\mathcal{N}(T)$ and $\mathcal{R}(T)$ will denote the domain, the nullspace (kernel) and the range of T. $\overline{T}$ denotes the *complex conjugation of* T. This means,

$$\mathcal{D}(\overline{T}) := \{\overline{f} \mid f \in \mathcal{D}(T)\}, \quad \overline{T}f := \overline{T\overline{f}}, \quad f \in \mathcal{D}(\overline{T}). \tag{3.6}$$

Suppose that T is densely defined. We say that $u \in \mathcal{D}(T^\#)$ if

$$\langle u|Tv\rangle = \langle w|v\rangle, \quad u \in \mathcal{D}(T), \tag{3.7}$$

for some $w \in \mathcal{H}$. Then we set $T^\# u := w$. The operator $T^\#$ is called the *transpose of* T. Clearly, if T^* denotes the usual *Hermitian adjoint* of T, then $T^\# = \overline{T^*} = \overline{T}^*$.

If T is a bounded linear operator with

$$\big(Tf\big)(x) := \int_a^b T(x,y)f(y)\mathrm{d}y,$$

then

$$\big(T^*f\big)(x) = \int_a^b \overline{T(y,x)}f(y)\mathrm{d}y, \tag{3.8}$$

$$\big(T^\# f\big)(x) = \int_a^b T(y,x)f(y)\mathrm{d}y, \tag{3.9}$$

$$\big(\overline{T}f\big)(x) = \int_a^b \overline{T(x,y)}f(y)\mathrm{d}y. \tag{3.10}$$

An operator T is *self-adjoint* if $T = T^*$. We will say that it is *self-transposed* if $T^\# = T$. It is useful to note that a holomorphic function of a self-transposed operator is self-transposed.

Remark 3.1. It would be natural to call an operator satisfying $T \subset T^{\#}$ *symmetric.* The natural name for an operator satisfying $T \subset T^*$ would then be *Hermitian.* Unfortunately and confusingly, in a large part of mathematical literature the word *symmetric* is reserved for an operator satisfying the latter condition.

Many properties of the transposition have their exact analogs for the Hermitian conjugation and are proven similarly. Below we describe some of them.

Proposition 3.2. *Let T be a densely defined operator.*

(1) $T^{\#}$ is closed.
(2) If T is closed, then $T = T^{\#\#}$.
(3) Let $T \subset S$. Then $S^{\#} \subset T^{\#}$ and

$$\dim \mathcal{D}(S)/\mathcal{D}(T) = \dim \mathcal{D}(T^{\#})/\mathcal{D}(S^{\#}). \tag{3.11}$$

Lemma 3.3. *Let S, T be linear operators on a Hilbert space $\mathcal{H}$ such that:*
(1) *$\langle Sf|g\rangle = \langle f|Tg\rangle$ for all $f \in \mathcal{D}(S)$ and $g \in \mathcal{D}(T)$,*
(2) *T is surjective,*
(3) *$\mathcal{R}(S)^{\mathrm{perp}} \subset \mathcal{N}(T)$.*
Then S is densely defined.

Proof. We must show:
$$\langle f|h\rangle = 0, \ \forall f \in \mathcal{D}(S) \Rightarrow h = 0.$$
Since T is surjective, there is $g \in \mathcal{D}(T)$ such that $h = Tg$ and then we get $0 = \langle f|h\rangle = \langle f|Tg\rangle = \langle Sf|g\rangle$ by (1) for all $f \in \mathcal{D}(S)$. Thus $g \in \mathcal{R}(S)^{\mathrm{perp}}$ and (3) gives $Tg = 0$ hence $h = 0$. □

Here is a version of the closed range theorem [29, Sect. VII.5], which we will use in §3.4.

Theorem 3.4. *If T is a closed densely defined operator in $\mathcal{H}$, then the following assertions are equivalent:*
(1) *$\mathcal{R}(T)$ is closed,* (2) *$\mathcal{R}(T^{\#})$ is closed,*
(3) *$\mathcal{R}(T) = \mathcal{N}(T^{\#})^{\mathrm{perp}}$,* (4) *$\mathcal{R}(T^{\#}) = \mathcal{N}(T)^{\mathrm{perp}}$.*

Remark 3.5. In a large part of literature [14, 19] a different terminology and notation is used. If T is an operator, then JT^*J is called the *J-adjoint of T*; an operator T satisfying $T = JT^*J$ is called *J-self-adjoint*, etc. In the context of our paper $Jf = \overline{f}$. Moreover, $(Jf|g)$ and JT^*J are denoted $\langle f|g\rangle$, resp. $T^{\#}$. Our notation and terminology stresses the naturalness of the bilinear product $\langle\cdot|\cdot\rangle$ and of the transposition $T \mapsto T^{\#}$. Therefore, we prefer them instead of the notation and terminology of e.g. [14, 19], which puts J in many places.

3.3. **Spectrum.** Let T be a closed operator. We say that G is an *inverse* of T if G is bounded, $GT = \mathbb{1}$ on $\mathcal{D}(T)$, and $TG = \mathbb{1}$ on $\mathcal{H}$. An inverse of T, if it exists, is unique. If T possesses an inverse, we say that it is *invertible.*

We will denote by $\mathrm{rs}(T)$ the *resolvent set*, that is the set of $\lambda \in \mathbb{C}$ such that $T - \lambda$ is invertible. The spectrum of T is $\mathrm{sp}(T) := \mathbb{C}\backslash\mathrm{rs}(T)$.

Let T be densely defined. Then T is invertible iff $T^{\#}$ is, $T^{-1\#} = T^{\#-1}$ and $\mathrm{sp}(T) = \mathrm{sp}(T^{\#})$.

We say that a closed operator T is *Fredholm* if $\dim \mathcal{N}(T) < \infty$ and $\dim \mathcal{H}/\mathcal{R}(T) < \infty$. If T is a Fredholm operator, we define its *index*

$$\mathrm{ind}(T) = \dim \mathcal{N}(T) - \dim \mathcal{H}/\mathcal{R}(T). \tag{3.12}$$

If a closed operator T is densely defined, then we have an equivalent, more symmetric definition: T is Fredholm if $\mathcal{R}(T)$ is closed (equivalently, $\mathcal{R}(T^{\#})$ is closed), $\dim \mathcal{N}(T) < \infty$ and $\dim \mathcal{N}(T^{\#}) < \infty$. Besides,

$$\mathrm{ind}(T) = \dim \mathcal{N}(T) - \dim \mathcal{N}(T^{\#}). \tag{3.13}$$

One can introduce various varieties of the *essential resolvent set* and *essential spectrum*, [14]. One of them is

$$\mathrm{rs}_{\mathrm{F0}}(T) := \{\lambda \in \mathbb{C} \mid T - \lambda \quad \text{is Fredholm of index } 0\}, \quad \mathrm{sp}_{\mathrm{F0}}(T) := \mathbb{C}\backslash\mathrm{rs}_{\mathrm{F0}}(T). \tag{3.14}$$

Clearly, $\mathrm{rs}(T) \subset \mathrm{rs}_{\mathrm{F0}}(T)$.

3.4. **Restrictions of closed operators.** In this subsection we fix a closed operator on a Hilbert space $\mathcal{H}$. For consistency with the rest of the paper, this operator will be denoted by $L_{\max}$. Note that $\mathcal{D}(L_{\max})$ can be treated as a Hilbert space with the scalar product

$$(f|g)_L := (f|g) + (L_{\max}f|L_{\max}g). \tag{3.15}$$

We will investigate closed operators $L_\bullet$ contained in $L_{\max}$. Obviously, $L_\bullet \subset L_{\max}$ if and only if $L_\bullet - \lambda \subset L_{\max} - \lambda$, where λ is a complex number. Therefore, many of the statements in this and next subsections have obvious generalizations, where $L_{\max}$ is replaced with $L_{\max} - \lambda$. For simplicity of presentation, we keep $\lambda = 0$.

Proposition 3.6.

(1) We have a 1-1 correspondence between closed subspaces $\mathcal{L}_\bullet$ of $\mathcal{D}(L_{\max})$ and closed operators $L_\bullet \subset L_{\max}$ given by $\mathcal{L}_\bullet = \mathcal{D}(L_\bullet)$.

(2) If $L_{\max}$ is Fredholm and $L_\bullet \subset L_{\max}$ is closed, then $L_\bullet$ is Fredholm if and only if $\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) < \infty$, and then

$$\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = \mathrm{ind}(L_{\max}) - \mathrm{ind}(L_\bullet) \tag{3.16}$$

(3) If $\mathcal{R}(L_{\max}) = \mathcal{H}$, and $L_\bullet \subset L_{\max}$, then $\mathrm{ind}(L_\bullet) = 0$ iff

$$\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = \dim \mathcal{N}(L_{\max}). \tag{3.17}$$

Proof. (1) is obvious.

Since $L_\bullet$ is a restriction of $L_{\max}$, we have $\mathcal{N}(L_\bullet) \subset \mathcal{N}(L_{\max})$ and, $\mathcal{N}(L_\bullet)$ being a finite dimensional subspace of the Banach space $\mathcal{D}(L_\bullet)$, there is a closed subspace of $\mathcal{D}_\bullet$ of $\mathcal{D}(L_\bullet)$ such that $\mathcal{D}(L_\bullet) = \mathcal{N}(L_\bullet) \oplus \mathcal{D}_\bullet$. We have $\mathcal{D}_\bullet + \mathcal{N}(L_{\max}) \subset \mathcal{D}(L_{\max})$ with $\mathcal{D}_\bullet \cap \mathcal{N}(L_{\max}) = 0$ hence, since $\mathcal{N}(L_{\max})$ is finite dimensional, there is a closed subspace $\mathcal{D}_{\max}$ of $\mathcal{D}(L_{\max})$ which contains $\mathcal{D}_\bullet$ and such that $\mathcal{D}(L_{\max}) = \mathcal{N}(L_{\max}) \oplus \mathcal{D}_{\max}$. Then we clearly get

$$\begin{aligned}\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) &= \dim \mathcal{N}(L_{\max})/\mathcal{N}(L_\bullet) + \dim \mathcal{D}_{\max}/\mathcal{D}_\bullet \\ &= \dim \mathcal{N}(L_{\max}) - \dim \mathcal{N}(L_\bullet) + \dim \mathcal{D}_{\max}/\mathcal{D}_\bullet.\end{aligned}$$

The map $L_{\max} : \mathcal{D}_{\max} \to \mathcal{R}(L_{\max})$ is bijective and its restriction to $\mathcal{D}_\bullet$ has $\mathcal{R}(L_\bullet)$ as image hence by the closed map theorem it is a homeomorphism, so

$$\dim \mathcal{D}_{\max}/\mathcal{D}_\bullet = \dim \mathcal{R}(L_{\max})/\mathcal{R}(L_\bullet) = \dim \mathcal{H}/\mathcal{R}(L_\bullet) - \dim \mathcal{H}/\mathcal{R}(L_{\max}).$$

The last two relations imply (3.16).

Finally, (3) is an immediate consequence of (2). □

The following concept is useful in the study of invertible operators contained in $L_{\max}$:

Definition 3.7. *We say that $G_\bullet$ is a* right inverse *of $L_{\max}$ if it is a bounded operator on $\mathcal{H}$ such that $\mathcal{R}(G_\bullet) \subset \mathcal{D}(L_{\max})$ and*

$$L_{\max}G_\bullet = 1\!\!1. \tag{3.18}$$

Note that $L_{\max}$ can have many right inverses or none.

Proposition 3.8. *The following conditions are equivalent:*
(1) *$L_{\max}$ has right inverses,*
(2) *$\mathcal{R}(L_{\max}) = \mathcal{H}$,*
If in addition $L_{\max}$ is densely defined, then (1) and (2) are equivalent to
(3) *$L^{\#}_{\max} : \mathcal{D}(L^{\#}_{\max}) \to \mathcal{H}$ is injective and $\mathcal{R}(L^{\#}_{\max})$ is closed.*
(4) *$\mathcal{N}(L^{\#}_{\max}) = \{0\}$ and $\mathcal{R}(L^{\#}_{\max}) = \mathcal{N}(L_{\max})^{\mathrm{perp}}$.*
Under these conditions we have a bijective correspondence between
(a) *right inverses $G_\bullet$ of $L_{\max}$;*
(b) *invertible operators $L_\bullet$ contained in $L_{\max}$;*
(c) *closed subspaces $\mathcal{L}_\bullet$ of $\mathcal{D}(L_{\max})$ such that $\mathcal{D}(L_{\max}) = \mathcal{L}_\bullet \oplus \mathcal{N}(L_{\max})$.*
This correspondence is given by $G_\bullet = L_\bullet^{-1}$ and $\mathcal{D}(L_\bullet) = \mathcal{L}_\bullet$.

Proof. If $G_\bullet$ is a right inverse for $L_{\max}$ then $L_{\max}$ is surjective due to (3.18). Reciprocally, assume $L_{\max}$ is surjective. Let $\mathcal{L}_\bullet$ be the orthogonal complement of the closed subspace $\mathcal{N}(L_{\max})$ in the Hilbert space $\mathcal{D}(L_{\max})$. Then $\mathcal{D}(L_{\max}) = \mathcal{L}_\bullet \oplus \mathcal{N}(L_{\max})$. Now $L_\bullet = L_{\max}\big|_{\mathcal{L}_\bullet}$ is a bijective map $\mathcal{L}_\bullet \to \mathcal{H}$ and $G_\bullet := L_\bullet^{-1}$ is a right inverse of $L_{\max}$. This proves (1) ⇔ (2). The equivalence with (3) and (4) follows by the closed range theorem (see Theorem 3.4). □

Proposition 3.9. *Let $G_\bullet$ be a right inverse of $L_{\max}$. Then*

(1) $\mathcal{N}(G_\bullet) = \{0\}$.
(2) $G_\bullet$ is bounded from $\mathcal{H}$ to $\mathcal{D}(L_{\max})$.
(3) $P_\bullet := G_\bullet L_{\max}$ is a bounded projection in the space $\mathcal{D}(L_{\max})$ such that

$$\mathcal{R}(P_\bullet) = \mathcal{R}(G_\bullet), \quad \mathcal{N}(P_\bullet) = \mathcal{N}(L_{\max}).$$

(4) $\mathcal{R}(G_\bullet)$ is closed in $\mathcal{D}(L_{\max})$.
(5) $\mathcal{D}(L_{\max}) = \mathcal{R}(G_\bullet) \oplus \mathcal{N}(L_{\max})$.

Proof. (1) is obvious and

$$\|G_\bullet f\|_L^2 = \|L_{\max} G_\bullet f\|^2 + \|G_\bullet f\|^2 \le \big(1 + \|G_\bullet\|^2\big)\|f\|^2 \tag{3.19}$$

implies (2). Since $L_{\max} : \mathcal{D}(L_{\max}) \to \mathcal{H}$ is bounded, $P_\bullet$ is bounded on $\mathcal{D}(L_{\max})$. Then

$$P_\bullet^2 = G_\bullet (L_{\max} G_\bullet) L_{\max} = G_\bullet L_{\max} = P_\bullet$$

hence $P_\bullet$ is a projection.

It is obvious that $\mathcal{R}(P_\bullet) \subset \mathcal{R}(G_\bullet)$. If $g \in \mathcal{H}$, then

$$G_\bullet g = G_\bullet L_{\max} G_\bullet g = P_\bullet G_\bullet g.$$

Hence $\mathcal{R}(G_\bullet) \subset \mathcal{R}(P_\bullet)$. This shows that $\mathcal{R}(G_\bullet) = \mathcal{R}(P_\bullet)$.

It is obvious that $\mathcal{N}(L_{\max}) \subset \mathcal{N}(P_\bullet)$. If $0 = P_\bullet f$, then

$$0 = L_{\max} P_\bullet f = (L_{\max} G_\bullet) L_{\max} f = L_{\max} f.$$

Hence $\mathcal{N}(P_\bullet) \subset L_{\max}$. This shows that $\mathcal{N}(P_\bullet) = \mathcal{N}(L_{\max})$.

Thus we have shown (3), which implies immediately (4) and (5). □

Proposition 3.10. *Let $L_\bullet$ be a closed operator such that $L_\bullet \subset L_{\max}$ and $L_\bullet$ is invertible. Then*

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_\bullet) \oplus \mathcal{N}(L_{\max}). \tag{3.20}$$

Proof. $G_\bullet := L_\bullet^{-1}$ is a right inverse of $L_{\max}$. Now (3.20) is the same as Prop. 3.9.(5). □

Proposition 3.11. *Let $G_\bullet$ be a right inverse of $L_{\max}$. If $K : \mathcal{H} \to \mathcal{N}(L_{\max})$ is a linear continuous map, then $G_\bullet + K$ is also a right inverse of $L_{\max}$. Conversely, all right inverses of $L_{\max}$ are of this form.*

In particular, suppose that $\mathcal{N}(L_{\max})$ is n-dimensional and spanned by $u_1, \dots, u_n$. Then if G_1, G_2 are two right inverses of $L_{\max}$, there exist $\phi_1, \dots \phi_n \in \mathcal{H}$ such that

$$G_1 - G_2 = \sum_{j=1}^n |u_j\rangle\langle\phi_j|. \tag{3.21}$$

Proposition 3.12. *Suppose that $G_\bullet$ is a bounded operator on $\mathcal{H}$ and $\mathcal{D} \subset \mathcal{H}$ a dense subspace such that $G_\bullet \mathcal{D} \subset \mathcal{D}(L_{\max})$ and*

$$L_{\max} G_\bullet g = g, \quad g \in \mathcal{D}. \tag{3.22}$$

Then $G_\bullet$ is a right inverse of $L_{\max}$.

Proof. Let $f \in \mathcal{H}$ and $(f_n) \subset \mathcal{D}$ such that $f_n \underset{n\to\infty}{\to} f$. Then $G_\bullet f_n \underset{n\to\infty}{\to} G_\bullet f$ and $L_{\max} G_\bullet f_n = f_n \underset{n\to\infty}{\to} f$. By the closedness of $L_{\max}$, $G_\bullet f \in \mathcal{D}(L_{\max})$ and $L_{\max} G_\bullet f = f$. □

3.5. **Nested pairs of operators.** In this subsection we assume that $L_{\min}$ and $L_{\max}$ are two densely defined closed operators. We assume that they form a *nested pair*,

$$L_{\min} \subset L_{\max}. \tag{3.23}$$

Note that along with (3.23) we have a second nested pair

$$L_{\max}^{\#} \subset L_{\min}^{\#}. \tag{3.24}$$

In this subsection we do not assume that $L_{\min}^{\#} = L_{\max}$, so that the two nested pairs can be different.

Remark 3.13. *The notion of a nested pair is closely related to the notion of* conjugate pair*, often introduced in the literature, e.g. in [14]. Two operators A, B form a conjugate pair if $A \subset B^*$, and hence $B \subset A^*$. The pair of operators $L_{\min}$, $L_{\max}^*$ is an example of a conjugate pair.*

Proposition 3.14.

(1) *We have a direct decomposition*

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) \oplus \mathcal{N}(L_{\min}^* L_{\max} + 1), \tag{3.25}$$

where

$$\mathcal{N}(L_{\min}^* L_{\max} + 1) = \{u \in \mathcal{D}(L_{\max}) \mid L_{\max}u \in \mathcal{D}(L_{\min}^*) \text{ and } L_{\min}^* L_{\max}u + u = 0\}.$$

(2) *If in addition $\mathcal{R}(L_{\min}^{\#}) = \mathcal{H}$, then*

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) \oplus \mathcal{N}(L_{\min}^* L_{\max}). \tag{3.26}$$

where $\mathcal{N}(L_{\min}^* L_{\max}) = \{u \in \mathcal{D}(L_{\max}) \mid L_{\max}u \in \mathcal{D}(L_{\min}^*)$ and $L_{\min}^* L_{\max}u = 0\}$.

Proof. (1) We will show that

$$\mathcal{N}(L_{\min}^* L_{\max} + 1) = \mathcal{D}(L_{\min})^{\perp_L}, \tag{3.27}$$

where the superscript $\perp_L$ denotes the orthogonal complement with respect to the scalar product (3.15). In fact, $u \in \mathcal{D}(L_{\min})$ and $v \in \mathcal{D}(L_{\min})^{\perp_L}$ if and only if

$$0 = (v|u) + (L_{\max}v|L_{\max}u) = (v|u) + (L_{\max}v|L_{\min}u). \tag{3.28}$$

This means $L_{\max}v \in \mathcal{D}(L_{\min}^*)$ and

$$0 = (L_{\min}^* L_{\max}v + v|u). \tag{3.29}$$

Since $\mathcal{D}(L_{\min})$ is dense, we obtain

$$0 = v + L_{\min}^* L_{\max}v. \tag{3.30}$$

(2) $\mathcal{R}(L_{\min}^{\#}) = \mathcal{H}$ implies that $\mathcal{R}(L_{\min})$ is closed. Therefore,

$$\mathcal{H} = \mathcal{R}(L_{\min}) \oplus \mathcal{N}(L_{\min}^*). \tag{3.31}$$

Let $u \in \mathcal{D}(L_{\max})$. By (3.31), there exist $v \in \mathcal{D}(L_{\min})$ and $w \in \mathcal{N}(L_{\min}^*)$ such that

$$L_{\max}u = L_{\min}v + w. \tag{3.32}$$

Hence $L_{\max}(u - v) = w$. Therefore, $u - v \in \mathcal{N}(L_{\min}^* L_{\max})$. Thus we have proven that

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) + \mathcal{N}(L_{\min}^* L_{\max}). \tag{3.33}$$

Suppose now that $u \in \mathcal{D}(L_{\min}) \cap \mathcal{N}(L_{\min}^* L_{\max})$. Thus

$$0 = L_{\min}^* L_{\max}u = L_{\min}^* L_{\min}u. \tag{3.34}$$

This implies $L_{\min}u = 0$. But $\mathcal{R}(L_{\min}^{\#}) = \mathcal{H}$ implies $\mathcal{N}(L_{\min}) = \{0\}$. Hence $u = 0$. □

Our main goal in this and the next subsection is to study closed operators $L_\bullet$ satisfying $L_{\min} \subset L_\bullet \subset L_{\max}$. Such operators are the subject of the following proposition.

Proposition 3.15. *Let $L_\bullet$ be a closed operator such that $L_\bullet \subset L_{\max}$. Then $L_{\min} \subset L_\bullet$ if and only if $L_\bullet^{\#} \subset L_{\min}^{\#}$.*

Let us reformulate Proposition 3.15 for invertible $L_\bullet$, using right inverses as the basic concept:

Proposition 3.16. *Let $G_\bullet$ be a right inverse of $L_{\max}$ and $L_\bullet^{-1} = G_\bullet$. Then $L_{\min} \subset L_\bullet$ if and only if $G_\bullet^\#$ is a right inverse of $L_{\min}^\#$.*

The following proposition should be compared with Prop. 3.11.

Proposition 3.17. *Suppose that G_1 is a right inverse of $L_{\max}$ and $G_1^\#$ is a right inverse of $L_{\min}^\#$. Then G_2 is also a right inverse of $L_{\max}$ and $G_2^\#$ is a right inverse of $L_{\min}^\#$ if and only if*

$$G_1 - G_2 = K, \tag{3.35}$$

where K is a bounded operator in $\mathcal{H}$ with $\mathcal{R}(K) \subset \mathcal{N}(L_{\max})$ and $\mathcal{R}(K^\#) \subset \mathcal{N}(L_{\min}^\#)$.

In particular, let $\mathcal{N}(L_{\max})$ and $\mathcal{N}(L_{\min}^\#)$ be finite dimensional. Chose a basis $(u_1, \dots u_n)$ of $\mathcal{N}(L_{\max})$ and a basis $(w_1, \dots w_m)$ of $\mathcal{N}(L_{\min}^\#)$. Then

$$G_1 - G_2 = \sum_{i,j} \alpha_{ij} |u_i\rangle\langle w_j| \quad \textit{for some matrix} \quad [\alpha_{ij}].$$

3.6. **Nested pairs consisting of an operator and its transpose.** In this subsection we assume that the pair of densely defined closed operators $L_{\min}$, $L_{\max}$ satisfies

$$L_{\min}^\# = L_{\max}, \quad L_{\min} \subset L_{\max}, \tag{3.36}$$

Note that this is a special case of conditions of the previous subsection—now the two nested pairs (3.23) and (3.24) coincide with one another.

We will use the terminology related to symplectic vector spaces introduced in Appendix A.

Lemma 3.18. *Let $u, v \in \mathcal{D}(L_{\max})$. Consider*

$$\langle L_{\max} u | v\rangle - \langle u | L_{\max} v\rangle. \tag{3.37}$$

Then (3.37) is zero if $u \in \mathcal{D}(L_{\min})$ or $v \in \mathcal{D}(L_{\min})$. If we fix u and (3.37) is zero for all $v \in \mathcal{D}(L_{\max})$, then $u \in \mathcal{D}(L_{\min})$. Besides,

$$|\langle L_{\max} u | v\rangle - \langle u | L_{\max} v\rangle| \le \|u\|_L \|v\|_L. \tag{3.38}$$

If $\phi, \psi \in \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$ are represented by $u, v \in \mathcal{D}(L_{\max})$, we set

$$[\![\phi|\psi]\!] := \langle L_{\max} u | v\rangle - \langle u | L_{\max} v\rangle. \tag{3.39}$$

By Lemma 3.18, $[\![\cdot | \cdot]\!]$ is a well defined continuous symplectic form on $\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$.

To every closed operator $L_\bullet$ such that $L_{\min} \subset L_\bullet \subset L_{\max}$ we associate a closed subspace $\mathcal{W}_\bullet$ of $\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$ by

$$\mathcal{W}_\bullet := \mathcal{D}(L_\bullet)/\mathcal{D}(L_{\min}).$$

Proposition 3.19.

(1) The above correspondence is bijective.

(2) If $L_\bullet$ is mapped to $\mathcal{W}_\bullet$, then $L_\bullet^\#$ is mapped to $W_\bullet^{\mathrm{s}\perp}$ (the symplectic orthogonal complement of $\mathcal{W}_\bullet$).

(3) Self-transposed operators are mapped to Lagrangian subspaces.

The following result is quite striking and shows that in a certain respect the concept of self-transposedness is superior to the concept of self-adjointness. It is due to Galindo [16], with a simplified proof given by Knowles [19], see also [14]. It is a generalization of a well-known property of real Hermitian operators: they have a self-adjoint extension which commutes with the usual conjugation.

Theorem 3.20. *There exists a self-transposed operator $L_\bullet$ such that $L_{\min} \subset L_\bullet \subset L_{\max}$. Moreover, $\dim \mathcal{D}(L_{\max}^\#)/\mathcal{D}(L_{\min})$ is even or infinite and*

$$\dim \mathcal{D}(L_\bullet)/\mathcal{D}(L_{\min}) = \dim \mathcal{D}(L_{\max}^\#)/\mathcal{D}(L_\bullet) = \frac{1}{2} \dim \mathcal{D}(L_{\max}^\#)/\mathcal{D}(L_{\min}). \tag{3.40}$$

Proof. By Prop. A.1, there exists a Lagrangian subspace $\mathcal{W}_\bullet$ contained in the symplectic space $\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$. By Prop. A.2 it is closed. The corresponding operator $L_\bullet$ is self-transposed (Prop. 3.19). □

Proposition 3.21. *Suppose that $L_{\min} \subset L_\bullet \subset L_{\max}$ and*

$$\dim \mathcal{D}(L_\bullet)/\mathcal{D}(L_{\min}) = \dim \mathcal{D}(L_{\max}^{\#})/\mathcal{D}(L_\bullet) = \frac{1}{2}\dim \mathcal{D}(L_{\max}^{\#})/\mathcal{D}(L_{\min}) = 1. \tag{3.41}$$

Then $L_\bullet$ is self-transposed.

Proof. All 1-dimensional subspaces in a 2-dimensional symplectic space are Lagrangian. □

Here is a version of Prop. 3.14 adapted to the present context:

Proposition 3.22.

(1) *We have a direct decomposition*

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) \oplus \mathcal{N}(\overline{L}_{\max} L_{\max} + 1). \tag{3.42}$$

(2) *If in addition $\mathcal{R}(L_{\max}) = \mathcal{H}$, then*

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) \oplus \mathcal{N}(\overline{L}_{\max} L_{\max}). \tag{3.43}$$

Here is a consequence of Prop. 3.16

Proposition 3.23. *Suppose that $L_\bullet$ is invertible and $L_{\min} \subset L_\bullet \subset L_{\max}$. Then there exists a self-transposed invertible L_1 such that $L_{\min} \subset L_1 \subset L_{\max}$.*

Proof. $G_\bullet := L_\bullet^{-1}$ is a right inverse of $L_{\max}$. By Prop. 3.16, $G_\bullet^{\#}$ is also a right inverse of $L_{\max}$. Therefore, also $G_1 := (G_\bullet + G_\bullet^{\#})/2$ is a right inverse, which in addition is self-transposed. Now L_1 such that $L_1^{-1} = G_1$ has the required properties. □

Here is a version of Prop. 3.17 adapted to the present context:

Proposition 3.24. *Suppose that G_1 is a right inverse of $L_{\max}$ and $G_1^{\#}$ is a right inverse of $L_{\max}$. Then G_2 is also a right inverse of $L_{\max}$ and $G_2^{\#}$ is a right inverse of $L_{\max}$ if and only if*

$$G_1 - G_2 = K, \tag{3.44}$$

where K and $K^{\#}$ are bounded from $\mathcal{H}$ to $\mathcal{N}(L_{\max})$.

In particular, let $\mathcal{N}(L_{\max})$ be finite dimensional. Chose a basis $(u_1, \dots u_n)$ of $\mathcal{N}(L_{\max})$. Then

$$G_1 - G_2 = \sum_{i,j} \alpha_{ij} |u_i\rangle\langle u_j| \quad \textit{for some matrix} \quad [\alpha_{ij}].$$

Theorem 3.25. *Suppose that $L_{\min} \subset L_\bullet \subset L_{\max}$.*

(1) *If $L_\bullet$ is Fredholm of index 0, then*

$$\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet) = \mathcal{D}(L_\bullet)/\mathcal{D}(L_{\min}) = \frac{1}{2}\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}). \tag{3.45}$$

(2) *If $\dim \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) < \infty$ and (3.45) holds, then $L_\bullet$ is Fredholm of index 0.*

Remark 3.26. *Thm. 3.25 implies that if $L_{\min} \subset L_\bullet \subset L_{\max}$ and $\mathrm{rs}_{\mathrm{F0}}(L_\bullet) \neq \emptyset$, then $L_\bullet$ has to satisfy (3.45) (see (3.14) for the definition of $\mathrm{rs}_{\mathrm{F0}}$). Thus the most "useful" operators (which usually means well-posed ones) are "in the middle" between the minimal and maximal operator.*

4. Basic L^2 theory of 1d Schrödinger operators

4.1. The maximal and minimal operator.

As before, we assume that $V \in L^1_{\rm loc}]a,b[$. Recall that L is the differential expression

$$L := -\partial^2 + V. \tag{4.1}$$

In this section we present basic realizations of L as closed operators on $L^2]a,b[$.

Definition 4.1. *The* maximal operator $L_{\max}$ *is defined by*

$$\mathcal{D}(L_{\max}) := \big\{ f \in L^2]a,b[\cap AC^1]a,b[\mid Lf \in L^2]a,b[\big\}, \tag{4.2}$$
$$L_{\max} f := Lf, \quad f \in \mathcal{D}(L_{\max}). \tag{4.3}$$

We equip $\mathcal{D}(L_{\max})$ with the graph norm

$$\|f\|_L^2 := \|f\|^2 + \|Lf\|^2.$$

Remark 4.2. *Note that $L^2]a,b[\subset L^1_{\rm loc}]a,b[$. Therefore, as explained in Subsect. 2.3, $f \in L^\infty_{\rm loc}]a,b[$ and $Lf \in L^2]a,b[$ implies $f \in AC^1]a,b[$. Therefore, in (4.2) we can replace $AC^1]a,b[$ with $L^\infty_{\rm loc}]a,b[$ (or $C]a,b[$, or $C^1]a,b[$).*

Recall that $AC^1_{\rm c}]a,b[$ are once absolutely differentiable functions of compact support.

Definition 4.3. *We set*

$$\mathcal{D}(L_{\rm c}) := AC^1_{\rm c}]a,b[\cap \mathcal{D}(L_{\max}).$$

Let $L_{\rm c}$ be the restriction of $L_{\max}$ to $\mathcal{D}(L_{\rm c})$. Finally, $L_{\min}$ is defined as the closure of $L_{\rm c}$.

The next theorem is the main result of this subsection:

Theorem 4.4. *The operators $L_{\min}, L_{\max}$ have the following properties.*

(1) The operators $L_{\max}$ and $L_{\min}$ are closed, densely defined and $L_{\min} \subset L_{\max}$.

(2) $L_{\max}^{\#} = L_{\min}$ and $L_{\min}^{\#} = L_{\max}$.

(3) Suppose that $f_1, f_2 \in \mathcal{D}(L_{\max})$. Then there exist

$$W(f_1, f_2; a) := \lim_{d \searrow a} W(f_1, f_2; d), \tag{4.4}$$
$$W(f_1, f_2; b) := \lim_{d \nearrow b} W(f_1, f_2; d), \tag{4.5}$$

and the so-called Green's identity *(the integrated form of the Lagrange identity) holds:*

$$\langle L_{\max} f_1 | f_2 \rangle - \langle f_1 | L_{\max} f_2 \rangle = W(f_1, f_2; b) - W(f_1, f_2; a). \tag{4.6}$$

(4) We set $W_d(f_1, f_2) = W(f_1, f_2; d)$ for any $d \in [a,b]$ and $f_1, f_2 \in \mathcal{D}(L_{\max})$. Then for any $d \in [a,b]$ the map $W_d : \mathcal{D}(L_{\max}) \times \mathcal{D}(L_{\max}) \to \mathbb{C}$ is a continuous bilinear antisymmetric form, in particular

$$|W_d(f_1, f_2)| \leq C_d \|f_1\|_L \|f_2\|_L. \tag{4.7}$$

(5) $\mathcal{D}(L_{\min})$ coincides with

$$\big\{ f \in \mathcal{D}(L_{\max}) \ \mid \ W(f, g; a) = 0 \text{ and } W(f, g; b) = 0 \text{ for all } g \in \mathcal{D}(L_{\max}) \big\}. \tag{4.8}$$

(6) $\overline{L}_{\min} = \overline{L_{\min}} = L^*_{\max}$ and $\overline{L}_{\max} = \overline{L_{\max}} = L^*_{\min}$.

One of the things we will need to prove is the density of $\mathcal{D}(L_{\rm c})$ in $L^2]a,b[$. This is easy if $V \in L^2_{\rm loc}]a,b[$ (see Prop. 4.12), but with our assumptions on the potential the proof is not so trivial, because the idea of approximating an $f \in L^2(I)$ with smooth functions does not work: $\mathcal{D}(L_{\max})$ may not contain any "nice" function, as the example described below shows.

Example 4.5. Let $V(x) = \sum_\sigma c_\sigma |{\rm x} - \sigma|^{-1/2}$ where σ runs over the set of rational numbers and $c_\sigma \in \mathbb{R}$ satisfy $c_\sigma > 0$ and $\sum_\sigma c_\sigma < \infty$. Then $V \in L^1_{\rm loc}(\mathbb{R})$ but V is not square integrable on any nonempty open set. Hence there is no C^2 nonzero function in the domain of L in $L^2(\mathbb{R})$.

Before proving Thm 4.4, we first state an immediate consequence of Lemma 2.16:

Lemma 4.6. (1) *Let J be a finite interval whose closure is contained in $]a,b[$. Then*

$$\left\|f\big|_J\right\| \leq C_J \|f\|_L, \tag{4.9}$$

$$\left\|f'\big|_J\right\| \leq C_J \|f\|_L. \tag{4.10}$$

(2) *Let $\chi \in C^\infty]a,b[$ with $\chi' \in C_{\rm c}^\infty]a,b[$. Then*

$$\|\chi f\|_L \leq C_\chi \|f\|_L. \tag{4.11}$$

As in the previous section, we fix $u,v \in AC^1]a,b[$ that span $\mathcal{N}(L)$ and satisfy $W(v,u)=1$.

Our proof of Thm 4.4 uses ideas from [25, Theorem 10.11] and [20, Sect. 17.4] and is based on an abstract result described in Lemma 3.3. The following lemma about the regular case (cf. Definition 2.3) contains the key arguments of the proof of (1) and (2) of Thm 4.4:

Lemma 4.7. *If $V \in L^1]a,b[$ and $a,b \in \mathbb{R}$, then*

(1) $\mathcal{N}(L_{\max}) = \mathcal{N}(L)$.
(2) $\mathcal{R}(L_{\max}) = L^2]a,b[$.
(3) $\langle L_{\rm c} f|g\rangle = \langle f|L_{\max} g\rangle$, $f \in \mathcal{D}(L_{\rm c})$, $g \in \mathcal{D}(L_{\max})$.
(4) $\mathcal{R}(L_{\rm c}) = L_{\rm c}^2]a,b[\cap \mathcal{N}(L)^{\rm perp}$.
(5) $\mathcal{R}(L_{\rm c})^{\rm perp} = \mathcal{N}(L)$.
(6) $\mathcal{D}(L_{\rm c})$ is dense in $L^2]a,b[$.

Proof. Clearly, $\mathcal{N}(L) = \operatorname{Span}(u,v) \subset AC^1[a,b] \subset L^2]a,b[$. Therefore, $\mathcal{N}(L) \subset \mathcal{D}(L_{\max})$. This proves (1).

Recall that in (2.20) we defined the forward Green's operator $G_\to$. Under the assumptions of the present lemma, it maps $L^2]a,b[$ into $AC^1[a,b]$. Therefore, for any $g \in L^2]a,b[$, $\alpha,\beta \in \mathbb{C}$,

$$f = \alpha u + \beta v + G_\to g$$

belongs to $AC^1[a,b]$ and verifies $Lf = g$. Therefore, $f \in \mathcal{D}(L_{\max})$. Hence $L_{\max}$ is surjective. This proves (2).

To obtain (3) we integrate twice by parts. This is allowed by (2.1) and (2.2), since $f,g \in AC^1[a,b]$.

It is obvious that $\mathcal{R}(L_{\rm c}) \subset L_{\rm c}^2]a,b[$. $\mathcal{R}(L_{\rm c}) \subset \mathcal{N}(L_{\max})^{\rm perp}$ follows from (3).

Let us prove the converse inclusions. Let $g \in L_{\rm c}^2]a,b[\cap \mathcal{N}(L)^{\rm perp}$. Set $f := G_\to g$. Clearly, $Lf = g$. Using $\int_a^b gu = \int_a^b gv = 0$ we see that f has compact support. Hence $f \in \mathcal{D}(L_{\rm c})$. This proves (4).

$L_{\rm c}^2]a,b[$ is dense in $L^2]a,b[$ and $\mathcal{N}(L)^{\rm perp}$ has a finite codimension. Therefore, by Lemma 4.8, given below, $L_{\rm c}^2]a,b[\cap \mathcal{N}(L)^{\rm perp}$ is dense in $\mathcal{N}(L)$. This implies (5).

By applying Lemma 3.3 with $T := L_{\max}$ and $S := L_{\rm c}$, we obtain (6). □

Lemma 4.8. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{K}$ a closed subspace of finite codimension. If $\mathcal{Z}$ is a dense subspace of $\mathcal{H}$, then $\mathcal{Z} \cap \mathcal{K}$ is dense in $\mathcal{K}$.*

Proof. The lemma is obvious if the codimension is 1. Then we apply induction. □

Proof of Thm 4.4. It follows from Lemma 4.7 (6) that $\mathcal{D}(L_{\rm c})$ is dense in $L^2]a,b[$. We have

$$L_{\rm c}^\# \supset L_{\max} \tag{4.12}$$

by integration by parts, as in the proof of (3), Lemma 4.7.

Suppose that $h,k \in L^2]a,b[$ such that

$$\langle L_{\rm c} f|h\rangle = \langle f|k\rangle, \quad f \in \mathcal{D}(L_{\rm c}). \tag{4.13}$$

In other words, $h \in \mathcal{D}(L_{\rm c}^\#)$ and $L_{\rm c}^\# h = k$. Choose $d \in]a,b[$. We set $h_d := G_d k$, where G_d is defined in Def. 2.13. Clearly, $Lh_d = k$. For $f \in \mathcal{D}(L_{\rm c})$, set $g := L_{\rm c} f$. We can assume that $\operatorname{supp} f \subset [a_1,b_1]$ for $a < a_1 < b_1 < b$. Now

$$\langle g|h_d\rangle = \langle L_{\rm c} f|h_d\rangle = \langle f|Lh_d\rangle = \langle f|k\rangle = \langle L_{\rm c} f|h\rangle = \langle g|h\rangle.$$

By Lemma 4.7 (4) applied to $[a_1.b_1]$,

$$h = h_d + \alpha u + \beta v \tag{4.14}$$

on $[a_1, b_1]$. But since a_1, b_1 were arbitrary under the condition $a < a_1 < b_1 < b$, (4.14) holds on $]a, b[$. Hence $Lh = k$. Therefore, $h \in \mathcal{D}(L_{\max})$ and $L_{\max}h = k$. This proves that

$$L_{\mathrm{c}}^{\#} \subset L_{\max}. \tag{4.15}$$

From (4.12) and (4.15) we see that $L_{\mathrm{c}}^{\#} = L_{\max}$. In particular, $L_{\max}$ is closed and L_{c} is closable. We have

$$L_{\min} = L_{\mathrm{c}}^{\#\#} = L_{\max}^{\#}. \tag{4.16}$$

This ends the proof of (1) and (2).

For $f, g \in \mathcal{D}(L_{\max})$ and $a < a_1 < b_1 < b$ we have

$$\begin{aligned}\int_{a_1}^{b_1} (Lf(x)g(x) - f(x)Lg(x))\mathrm{d}x &= \int_{a_1}^{b_1} (f(x)g'(x) - f'(x)g(x))'\mathrm{d}x \\ &= W(f, g; a_1) - W(f, g; b_1).\end{aligned} \tag{4.17}$$

The lhs of (4.17) clearly converges as $a_1 \searrow a$. Therefore, the limit (4.4) exists. Similarly, by taking $b_1 \nearrow b$ we show that the limit (4.5) exists. Taking both limits we obtain (4.6). This proves (3).

If $d \in]a, b[$, then (4.7) is an immediate consequence of (4.9) and (4.10). We can rewrite (4.17) as

$$W(f, g; a) = -\int_a^d \big((Lf)(x)g(x) - f(x)Lg(x)\big)\mathrm{d}x + W(f, g; d). \tag{4.18}$$

Now both terms on the right of (4.18) can be estimated by $C\|f\|_L\|g\|_L$. This shows (4.7) for $d = a$. The proof for $d = b$ is analogous.

Let L_w be L restricted to (4.8). By (4.7), (4.8) is a closed subspace of $\mathcal{D}(L_{\max})$. Hence, L_w is closed. Obviously, $L_{\mathrm{c}} \subset L_w$. By (4.6), $L_w \subset L_{\max}^{\#}$. By (2), we know that $L_{\max}^{\#} = L_{\min}$. But $L_{\min}$ is the closure of L_{c}. Hence $L_w = L_{\min}$. This proves (5). □

Remark 4.9. Here is an alternative, more direct proof of the closedness of $L_{\max}$. Let $f_n \in \mathcal{D}(L_{\max})$ be a Cauchy sequence wrt the graph norm. This means that f_n and Lf_n are Cauchy sequences wrt $L^2]a, b[$. Let $f := \lim_{n\to\infty} f_n$, $g := \lim_{n\to\infty} Lf_n$. Let J be an arbitrary sufficiently small closed interval in $]a, b[$. We have

$$\|f_n - f_m\|_{L^1(J)} \le \sqrt{|J|}\|f_n - f_m\|_{L^2(J)}, \tag{4.19}$$

$$\|Lf_n - Lf_m\|_{L^1(J)} \le \sqrt{|J|}\|Lf_n - Lf_m\|_{L^2(J)}. \tag{4.20}$$

Hence f_n satisfies the conditions of Cor. 2.17. Hence $f \in AC^1]a, b[$ and $g = Lf$. Hence $f \in \mathcal{D}(L_{\max})$ and it is the limit of f_n in the sense of the graph norm. Therefore, $\mathcal{D}(L_{\max})$ is complete. Hence $L_{\max}$ and $L_{\min}$ are closed.

4.2. **Smooth functions in the domain of $L_{\max}$.** We point out a certain pathology of the operators $L_{\max}$ and $L_{\min}$ if V is only locally integrable.

Lemma 4.10. *(1) The imaginary part of V is locally square integrable if and only if $\mathcal{D}(L_{\mathrm{c}})$ is stable under conjugation and in this case $\mathcal{D}(L_{\min})$ and $\mathcal{D}(L_{\max})$ are also stable under conjugation.*

(2) If the imaginary part of V is not square integrable on any open set, then for $f \in \mathcal{D}(L_{\max})$ we have $\overline{f} \in \mathcal{D}(L_{\max})$ only if $f = 0$. In other words, $\mathcal{D}(L_{\max}) \cap \mathcal{D}(\overline{L}_{\max}) = \{0\}$. Hence $\mathcal{D}(L_{\max})$ does not contain any nonzero real function.

Proof. (1): Write $Lf = -f'' + V_1 f + iV_2 f$ if $V = V_1 + iV_2$ with V_1, V_2 real. Then if $V_2 \in L^2_{\mathrm{loc}}]a, b[$ and $f \in AC^1_{\mathrm{c}}]a, b[$ we have $V_2 f \in L^2]a, b[$ so $-f'' + Vf \in L^2]a, b[$ if and only if $-f'' + V_1 f \in L^2]a, b[$ hence $-\overline{f}'' + V_1\overline{f} \in L^2]a, b[$ so we get $-\overline{f}'' + V\overline{f} \in L^2]a, b[$, thus $\mathcal{D}(L_{\mathrm{c}})$ is stable under conjugation.

The corresponding assertion concerning $\mathcal{D}(L_{\min})$ follows by taking the completion, and that concerning $\mathcal{D}(L_{\max})$ follows by taking the transposition.

Reciprocally, assume that $\mathcal{D}(L_{\mathrm{c}})$ is stable under conjugation and let $x_0 \in]a,b[$. Then there is $f \in \mathcal{D}(L_{\mathrm{c}})$ such that $f(x_0) \neq 0$ and we may assume that its real part $g = (f+\overline{f})/2$ does not vanish on a neighbourhood of x_0. Then $g \in \mathcal{D}(L_{\mathrm{c}})$ hence $-g'' + V_1 g + iV_2 g \in L^2]a,b[$ and so must be the imaginary part of this function hence V_2 is square integrable on a neighbourhood of x_0.

(2): Assume now that V_2 is not square integrable on any open set. If $f \in AC^1$ is real then $-f'' + Vf \in L^2$ if and only if $-f'' + V_1 f \in L^2$ and $V_2 f \in L^2$ and if $f \neq 0$ then the second condition implies $f = 0$. Finally, if $f \in \mathcal{D}(L_{\max})$ and $\overline{f} \in \mathcal{D}(L_{\max})$ then the functions $f + \overline{f}$ and $f - \overline{f}$ will be zero by (1). □

Remark 4.11. Clearly, $L_{\min}^* = \overline{L}_{\max}$. Thus, by Prop. 4.10 (2), if the imaginary part of V is not square integrable on any open set then $\mathcal{D}(L_{\min}) \cap \mathcal{D}(L_{\min}^*) = \{0\}$. On the other hand, if the imaginary part of V is locally square integrable, then $\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_{\min}^*)$.

If $V \in L^2_{\mathrm{loc}}$, many things simplify:

Proposition 4.12. *If $V \in L^2_{\mathrm{loc}}]a,b[$ then $C_{\mathrm{c}}^\infty]a,b[$ is a dense subspace of $\mathcal{D}(L_{\min})$.*

Proof. Clearly $C_{\mathrm{c}}^\infty]a,b[\subset \mathcal{D}(L_{\mathrm{c}})$. Let $f \in C_{\mathrm{c}}]a,b[$. Then $Lf \in L^2]a,b[$ if and only if $f'' \in L^2]a,b[$. Fix some $\theta \in C_{\mathrm{c}}^\infty(\mathbb{R})$ with $\int \theta = 1$ and let $\theta_n(x) := n\theta(nx)$ with $n \geq 1$. Then for n large $f_n := \theta_n * f \in C_{\mathrm{c}}^\infty]a,b[$ and has support in a fixed small neighbourhood of $\mathrm{supp} f$. Moreover, $f_n \to f$ in $C_{\mathrm{c}}^1]a,b[$, in particular $f_n \to f$ uniformly with supports in a fixed compact, which clearly implies $Vf_n \to Vf$ in $L^2]a,b[$. Moreover $f_n'' \to f''$ in $L^2]a,b[$. □

4.3. **Closed operators contained in $L_{\max}$.** If $\mathcal{D}(L_\bullet)$ is a subspace of $\mathcal{D}(L_{\max})$ closed in the $\|\cdot\|_L$ norm, then the operator

$$L_\bullet := L_{\max}\Big|_{\mathcal{D}(L_\bullet)} \tag{4.21}$$

is closed and contained in $L_{\max}$. We can call such an operator $L_\bullet$ a *closed realization of L*.

We will be mostly interested in operators $L_\bullet$ that satisfy

$$\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_\bullet) \subset \mathcal{D}(L_{\max}) \tag{4.22}$$

so that

$$L_{\min} \subset L_\bullet \subset L_{\max}. \tag{4.23}$$

They are automatically densely defined. Note that we can use the theory developed in Subsect. 3.5 and 3.6. In particular, as descibed in Prop. 3.15, one can easily check if a realization of L contains $L_{\min}$ with the help of the following criterion:

Proposition 4.13. *Suppose that $L_\bullet$ is a closed densely defined operator contained in $L_{\max}$. Then $L_\bullet^\#$ is contained in $L_{\max}$ if and only if $L_{\min} \subset L_\bullet$. In particular, if $L_\bullet^\# = L_\bullet$, then $L_{\min} \subset L_\bullet$.*

The most obvious examples of such operators are given by one-sided boundary conditions:

Definition 4.14. *Set*

$$\mathcal{D}(L_a) := \{f \in \mathcal{D}(L_{\max}) \mid W(f,g;a) = 0 \text{ for all } g \in \mathcal{D}(L_{\max})\}, \tag{4.24}$$

$$\mathcal{D}(L_b) := \{f \in \mathcal{D}(L_{\max}) \mid W(f,g;b) = 0 \text{ for all } g \in \mathcal{D}(L_{\max})\}. \tag{4.25}$$

Let L_a, resp. L_b be $L_{\max}$ restricted to $\mathcal{D}(L_a)$, resp. $\mathcal{D}(L_b)$.

Proposition 4.15. *L_a and L_b are closed and densely defined operators satisfying*

$$L_a^\# = L_b, \quad L_b^\# = L_a, \tag{4.26}$$

$$L_{\min} \subset L_a \subset L_{\max}, \quad L_{\min} \subset L_b \subset L_{\max}. \tag{4.27}$$

5. Boundary conditions

5.1. **Regular endpoints.** Recall that the endpoint a is regular if it is finite and V is integrable close to a.

Proposition 5.1. *If L is regular at a then any function $f \in \mathcal{D}(L_{\max})$ extends to a function of class C^1 on the left closed interval $[a, b[$, hence $f(a)$ and $f'(a)$ are well defined, and for $f, g \in \mathcal{D}(L_{\max})$ we have $W_a(f, g) = f(a)g'(a) - f'(a)g(a)$. Similarly if L is regular at b. Thus if L is regular then $\mathcal{D}(L_{\max}) \subset C^1[a, b]$ and Green's identity (4.6) has the classical form*

$$\langle L_{\max} f_1 | f_2 \rangle - \langle f_1 | L_{\max} f_2 \rangle = \big(f_1(b)f_2'(b) - f_1'(b)f_2(b)\big) - \big(f_1(a)f_2'(a) - f_1'(a)f_2(a)\big).$$

Thus if L is a regular operator then we have four continuous linear functionals on $f \in \mathcal{D}(L_{\max})$

$$f \mapsto f(a), \quad f \mapsto f'(a), \tag{5.1}$$

$$f \mapsto f(b), \quad f \mapsto f'(b), \tag{5.2}$$

which give a convenient description of closed operators $L_\bullet$ such that $L_{\min} \subset L_\bullet \subset L_{\max}$. In particular, $\mathcal{D}(L_{\min})$ is the intersection of the kernels of (5.1) and (5.2), $\mathcal{D}(L_a)$ is the intersection of the kernels of (5.1) and $\mathcal{D}(L_b)$ is the intersection of the kernels of (5.2).

5.2. **Boundary functionals.** It is possible to extend the strategy described above to the case of an arbitrary L by using an abstract version of the notion of boundary value of a function. We shall do it in this section.

The abstract theory of boundary value functionals goes back to J. W. Calkin's thesis [6] who used it for the classification of self-adjoint extensions of Hermitian operators. The theory was adapted to Hermitian differential operators of any order by Naimark [20] and to operators with complex coefficients of class C^∞ by Dunford and Schwarz in [12, ch. XIII]. In this section we shall use this technique in the case of second order operators with potentials which are only locally integrable: this loss of regularity is a problem for some arguments in [12].

Recall that $\mathcal{D}(L_{\max})$ is equipped with the Hilbert space structure associated to the norm $\|f\|_L = \sqrt{\|f\|^2 + \|Lf\|^2}$. Following [12, §XXX.2], we introduce the following notions.

Definition 5.2. *A* boundary functional for L *is any linear continuous form on $\mathcal{D}(L_{\max})$ which vanishes on $\mathcal{D}(L_{\min})$. A* boundary functional at a *is a boundary functional ϕ such that $\phi(f) = 0$ for all $f \in \mathcal{D}(L_{\max})$ with $f(x) = 0$ near a;* boundary functionals at b *are defined similarly. $\mathcal{B}(L)$ is the set of boundary functionals for L and $\mathcal{B}_a(L), \mathcal{B}_b(L)$ the subsets of boundary functionals at a and b.*

$\mathcal{B}(L)$ is a closed linear subspace of the topological dual $\mathcal{D}(L_{\max})'$ of $\mathcal{D}(L_{\max})$ and $\mathcal{B}_a(L), \mathcal{B}_b(L)$ are closed linear subspaces of $\mathcal{B}(L)$. By using a partition of unity on $]a, b[$ it is easy to prove that

$$\mathcal{B}(L) = \mathcal{B}_a(L) \oplus \mathcal{B}_b(L), \tag{5.3}$$

a topological direct sum.

Definition 5.3. *We define*

$$\begin{aligned} \textit{the } \text{boundary index for } L \text{ at } a, &\quad \nu_a(L) := \dim \mathcal{B}_a(L), \\ \textit{the } \text{boundary index for } L \text{ at } b, &\quad \nu_b(L) := \dim \mathcal{B}_b(L), \\ \textit{and the } \text{total boundary index for } L, &\quad \nu(L) := \dim \mathcal{B}(L) = \nu_a(L) + \nu_b(L). \end{aligned}$$

By definition, the subspace $\mathcal{B}(L) \subset \mathcal{D}(L_{\max})'$ is the polar set of the closed subspace $\mathcal{D}(L_{\min})$ of $\mathcal{D}(L_{\max})$. Hence it is canonically identified with the dual space of $\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$:

$$\mathcal{B}(L) = \big(\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})\big)'. \tag{5.4}$$

Clearly one may also define $\mathcal{B}_a(L)$ as the set of continuous linear forms on $\mathcal{D}(L_{\max})$ which vanish on the closed subspace $\mathcal{D}(L_a)$, and similarly for $\mathcal{B}_b(L)$. Thus

$$\mathcal{B}_a(L) = \big(\mathcal{D}(L_{\max})/\mathcal{D}(L_a)\big)'. \tag{5.5}$$

Definition 5.4. *For each $f \in \mathcal{D}(L_{\max})$ and $x \in [a,b]$, we introduce the functional*

$$\vec{f}_x : \mathcal{D}(L_{\max}) \to \mathbb{C} \quad \text{defined by} \quad \vec{f}_x(g) = W_x(f,g). \tag{5.6}$$

By Theorem 4.4 it is a well defined linear continuous form on $\mathcal{D}(L_{\max})$.

Remember that if $x \in]a,b[$, then we can write

$$\vec{f}_x(g) = f(x)g'(x) - f'(x)g(x) = W_x(f,g) \quad \forall g \in C^1]a,b[. \tag{5.7}$$

If $x = a$, in general we cannot write (5.7) (unless a is regular). However we know that for all $x \in [a,b]$ (5.6) depends weakly continuously on x. Thus in general

$$\mathrm{w} - \lim_{x\to a} \vec{f}_x = \vec{f}_a. \tag{5.8}$$

It is easy to see that $\vec{f}_a \in \mathcal{B}_a$, cf. (4.24) for example. We shall prove below that any boundary value functional at the endpoint a is of this form.

Theorem 5.5. (i) *$f \mapsto \vec{f}_a$ is a linear surjective map $\mathcal{D}(L_{\max}) \to \mathcal{B}_a(L)$.*

(ii) *$W_a(f,g) = 0$ for all $f,g \in \mathcal{D}(L_{\max})$ if and only if $\mathcal{B}_a(L) = \{0\}$.*

(iii) *$W_a(f,g) \neq 0$ if and only if the functionals $\vec{f}_a, \vec{g}_a$ are linearly independent.*

(iv) *If $W_a(f,g) \neq 0$ then $\{\vec{f}_a, \vec{g}_a\}$ is a basis in $\mathcal{B}_a(L)$; then $\forall h \in \mathcal{D}(L_{\max})$ we have*

$$\vec{h}_a = cW_a(g,h)\vec{f}_a + cW_a(h,f)\vec{g}_a \quad \text{with } c = -1/W_a(f,g). \tag{5.9}$$

Proof. Let $\mathcal{W}_a$ be the set of linear forms of the form $\vec{f}_a$, this is a vector subspace of $\mathcal{B}_a(L)$ and we shall prove later that $\mathcal{W}_a = \mathcal{B}_a(L)$. For the moment, note that $\mathcal{W}_a$ separates the points of $\mathcal{Y}_a := \mathcal{D}(L_{\max})/\mathcal{D}(L_a)$, i.e. we have $W_a(f,g) = 0$ for all f if and only if $g \in \mathcal{D}(L_a)$, cf. (4.8) and (4.24). On the other hand, (5.5) implies that $\mathcal{B}_a(L) = \{0\}$ is equivalent to $\mathcal{D}(L_{\max}) = \mathcal{D}(L_a)$ which in turn is equivalent to $W_a(f,g) = 0$ for all $f,g \in \mathcal{D}(L_{\max})$ by (4.24). This proves (ii).

For the rest of the proof we need *Kodaira's identity* [21, pp. 151–152], namely: if f,g,h,k are C^1 functions on $]a,b[$ then

$$W(f,g)W(h,k) + W(g,h)W(f,k) + W(h,f)W(g,k) = 0, \tag{5.10}$$

with the usual definition $W(f,g) = fg' - f'g$. The relation obviously holds pointwise on $]a,b[$. If $f,g,h,k \in \mathcal{D}(L_{\max})$, then the relation extends to $[a,b]$, in particular

$$W_a(f,g)W_a(h,k) + W_a(g,h)W_a(f,k) + W_a(h,f)W_a(g,k) = 0, \tag{5.11}$$

and similarly at b. This implies (5.9) if $W_a(f,g) \neq 0$ from which it follows that $\{\vec{f}_a, \vec{g}_a\}$ is a basis in the vector space $\mathcal{W}_a$, in particular $\mathcal{W}_a$ has dimension 2. But $\mathcal{W}_a \subset \mathcal{Y}_a'$ separates the points of $\mathcal{Y}_a$ hence $\mathcal{W}_a = \mathcal{Y}_a' = \mathcal{B}_a(L)$ which proves the surjectivity of the map $f \mapsto \vec{f}(a)$. This proves (i) and (iv) completely and also one implication in (iii). It remains to prove that $\vec{f}_a, \vec{g}_a$ are linearly dependent if $W_a(f,g) = 0$.

We prove this but with a different notation which allows us to use what we have already shown. Let f such that $\vec{f}_a \neq 0$. Then $\vec{f}_a$ is part of a basis in $\mathcal{W}_a = \mathcal{B}_a(L)$, hence there is g such that $\{\vec{f}_a, \vec{g}_a\}$ is a basis in $\mathcal{B}_a(L)$. Then $W_a(f,g) \neq 0$ and we have (5.9). Thus if $W_a(h,f) = 0$ then $\vec{h}_a = cW_a(g,h)\vec{f}_a$, so $\vec{h}_a, \vec{f}_a$ are linearly dependent. □

The space $\mathcal{B}_a$ is naturally a symplectic space. In fact, if $\mathcal{B}_a$ is nontrivial, then we can find k,h with $W_a(k,h) \neq 0$. By the Kodaira identity,

$$\begin{aligned} W_a(f,g) &= \frac{-W_a(f,k)W_a(g,h) + W_a(f,h)W_a(g,k)}{W_a(h,k)} \\ &= \frac{-\vec{f}_a(k)\vec{g}_a(h) - \vec{f}_a(h)\vec{g}_a(k)}{W_a(h,k)}. \end{aligned} \tag{5.12}$$

Thus if we set for $\phi, \psi \in \mathcal{B}_a$ with $\vec{f}_a = \phi$, $\vec{g}_a = \psi$,

$$[\![\phi|\psi]\!]_a := W_a(f,g), \tag{5.13}$$

then $[\![\cdot|\cdot]\!]_a$ is a well defined symplectic form on $\mathcal{B}_a$. Moreover, $f\mapsto \vec{f}_a$ maps the form W_a onto $[\![\cdot|\cdot]\!]_a$. If $[\![\phi|\psi]\!]_a=1$, then by the Kodaira identity

$$W(h,k)=\phi(h)\psi(k)-\psi(h)\phi(k). \tag{5.14}$$

In the literature boundary functionals are usually described using the notion of *boundary triplet*. Let us make a comment on this concept. Suppose, for definiteness, that $\nu_a=\nu_b=2$. Choose bases

$$\phi_a,\psi_a,\ \text{of } \mathcal{B}_a \text{ and } \phi_b,\psi_b \text{ of } \mathcal{B}_b \tag{5.15}$$

such that $[\![\phi_a|\psi_a]\!]_a=[\![\phi_b|\psi_b]\!]_b=1$. We have the maps

$$\mathcal{D}(L_{\max})\ni f\mapsto \phi(f):=\big(\phi_a(f),\phi_b(f)\big)\in\mathbb{C}^2; \tag{5.16}$$

$$\mathcal{D}(L_{\max})\ni f\mapsto \psi(f):=\big(\psi_a(f),\psi_b(f)\big)\in\mathbb{C}^2. \tag{5.17}$$

Then we can rewrite Green's formula (4.6) as

$$\langle L_{\max}f|g\rangle-\langle f|L_{\max}g\rangle=\langle\psi(f)|\phi(g)\rangle-\langle\phi(f)|\psi(g)\rangle. \tag{5.18}$$

The triplet $(\mathbb{C}^2,\phi,\psi)$ is often called in the literature a *boundary triplet*, see e.g. [2] and references therein. It can be used to characterize operators in between $L_{\min}$ and $L_{\max}$.

Thus a boundary triplet is essentially a choice of a basis (5.15) in the space of boundary functionals. Such a choice is often natural: in particular this is the case of regular boundary conditions, see (5.1), (5.2). In our paper we consider rather general potentials for which there may be no natural choice for (5.15). Therefore, we do not use the boundary triplet formalism.

5.3. **Classification of endpoints and of realizations of L.** The next fact is a consequence of Theorem 5.5. One may think of the assertion "$\nu_a(L)$ can only take the values 0 or 2" as a version of Weyl's dichotomy, cf. §6.2.

Theorem 5.6. *$\nu_a(L)$ can be 0 or 2: we have $\nu_a(L)=0\Leftrightarrow W_a=0$ and $\nu_a(L)=2\Leftrightarrow W_a\neq 0$. Similarly for $\nu_b(L)$, hence $\nu(L)\in\{0,2,4\}$.*

Remark 5.7. According to the terminology in [12], we might say that L has *no boundary values at a* if $\nu_a(L)=0$ and that L has *two boundary values at a* if $\nu_a(L)=2$.

Example 5.8. If L is regular at the endpoint a then $\nu_a(L)=2$. It is clear that $f\mapsto f(a)$ and $f\mapsto f'(a)$ are linearly independent and Theorem 5.6 implies that they form a basis in $\mathcal{B}_a(L)$.

Example 5.9. If L is semiregular at a then we also have $\nu_a(L)=2$. Indeed, $\dim\mathcal{U}_a(\lambda)=2$ (Prop. 2.5) and this implies $\nu_a(L)=2$ by (the easy part of) Theorem 6.15. We also have the distinguished boundary functional $f\mapsto f(a)$, as shown in Prop. 2.5 (2). If u is the solution of $Lu=0$ satisfying $u(a)=0$, $u'(0)=1$, whose existence is guaranteed by Prop. 2.5 (3), then this functional coincides with $\vec{u}_a$. However, in general, we do not have another, linearly independent distinguished boundary functional.

As a consequence of Theorem 5.6 we get the following classification of 1d Schrödinger operators in terms of the boundary functionals.

(1) $\nu_a(L)=\nu_b(L)=0$. This is equivalent to $L_{\min}=L_a=L_b=L_{\max}$.
(2) $\nu_a(L)=0$, $\nu_b(L)=2$, Then $\mathcal{D}(L_{\min})$ is a subspace of codimension 2 in $\mathcal{D}(L_{\max})$. This is equivalent to $L_a=L_{\max}$, and to $L_{\min}=L_b$.
(3) $\nu_a(L)=2$, $\nu_b(L)=0$. Then $\mathcal{D}(L_{\min})$ is a subspace of codimension 2 in $\mathcal{D}(L_{\max})$. This is equivalent to $L_b=L_{\max}$, and to $L_{\min}=L_a$.
(4) $\nu_a(L)=\nu_b(L)=2$. Then $\mathcal{D}(L_{\min})$ is a subspace of codimension 4 in $\mathcal{D}(L_{\max})$.

In case (2) the operators $L_\bullet$ with $L_{\min}\subsetneq L_\bullet\subsetneq L_{\max}$ are defined by nonzero boundary value functionals ϕ at a: $\mathcal{D}(L_\bullet)=\{f\in\mathcal{D}(L_{\max})\mid\phi(f)=0\}$. Similarly in case (3).

Consider now the case (4). The domain of nontrivial realizations $L_\bullet$ could be then of codimension $1,2$, or 3 in $\mathcal{D}(L_{\max})$. We will see that realizations of codimension 2 are the most important.

Each realization of L extending $L_{\min}$ is defined by a subspace $\mathcal{C}_\bullet \subset \mathcal{B}_a \oplus \mathcal{B}_b$.

$$\mathcal{D}(L_\bullet) := \{f \in \mathcal{D}(L_{\max}) \mid \phi(f) = 0, \quad \phi \in \mathcal{C}_\bullet\} \tag{5.19}$$

The space $\mathcal{C}_\bullet$ is called the *space of boundary conditions for* $L_\bullet$. The dimension of $\mathcal{C}_\bullet$ coincides with the codimension of $\mathcal{D}(L_\bullet)$ in $\mathcal{D}(L_{\max})$.

Definition 5.10. *We say that the boundary conditions* $\mathcal{C}_\bullet$ *are* separated *if*

$$\mathcal{C}_\bullet = \mathcal{C}_\bullet \cap \mathcal{B}_a \oplus \mathcal{C}_\bullet \cap \mathcal{B}_b. \tag{5.20}$$

For instance, L_a and L_b are given by separated boundary conditions $\mathcal{B}_a$, resp. $\mathcal{B}_b$.

Definition 5.11. *Let* $\phi \in \mathcal{B}_a$ *and* $\psi \in \mathcal{B}_b$. *Then the realization of* L *with the boundary condition* $\mathbb{C}\phi \oplus \mathbb{C}\psi$ *will be denoted* $L_{\phi,\psi}$.

Clearly, $L_{\phi,\psi}$ has separated boundary conditions and depends only on the complex lines determined by ϕ and ψ. More explicitly,

$$\mathcal{D}(L_{\phi,\psi}) = \{f \in \mathcal{D}(L_{\max}) \mid \phi(f) = \psi(f) = 0\}.$$

Recall that if $\phi \neq 0$ then $\phi(f) = 0 \Leftrightarrow \exists c(f) \in \mathbb{C}$ such that $\vec{f_a} = c(f)\phi$. We abbreviate $L_\phi = L_{\phi,0}$ if $\psi = 0$ and define similarly L_ψ if $\phi = 0$. Thus L_ϕ involves no boundary condition at b:

$$\mathcal{D}(L_\phi) = \{f \in \mathcal{D}(L_{\max}) \mid \phi(f) = 0\} = \{f \in \mathcal{D}(L_{\max}) \mid \exists c(f) \text{ such that } \vec{f_a} = c(f)\phi\} \tag{5.21}$$

where the second equality holds if $\phi \neq 0$. Note that $L_{0,0} = L_{\max}$.

5.4. **Properties of boundary functionals.** The next proposition is a version of [12, XIII.2.27] in our context.

Proposition 5.12. *If* $\phi \in \mathcal{B}_a(L)$ *then there are continuous functions* $\alpha, \beta :]a, b[\to \mathbb{C}$ *such that*

$$\phi(f) = \lim_{x \to a} \big(\alpha(x)f(x) + \beta(x)f'(x)\big) \quad \forall f \in \mathcal{D}(L_{\max}).$$

Reciprocally, if α, β *are complex functions on* $]a, b[$ *and* $\lim_{x\to a} \big(\alpha(x)f(x) + \beta(x)f'(x)\big) =: \phi(f)$ *exists* $\forall f \in \mathcal{D}(L_{\max})$, *then* $\phi \in \mathcal{B}_a(L)$.

Proof. The first assertion follows from Theorem 5.5-(i) and relations (5.8), (5.7) while the second one is a consequence of Banach-Steinhaus theorem. □

Recall that for $d \in [a, b]$ the symbol $L^{a,d}$ denotes the operator $-\partial^2 + V$ on the interval $]a, d[$.

Lemma 5.13. *Let* $d \in]a, b[$. *Then*

$$\dim \mathcal{B}_a(L) = \dim \mathcal{B}_a(L^{a,d}). \tag{5.22}$$

Proof. Since d is a regular endpoint for L^d, the maximal operator $L^{a,d}_{\max}$ associated to $L^{a,d}$ has the property $\mathcal{D}(L^{a,d}_{\max}) \subset C^1]a, d]$. Thus the restriction map $R : f \mapsto f\big|_{]a,d[}$ is a surjective map $\mathcal{D}(L_{\max}) \to \mathcal{D}(L^{a,d}_{\max})$ such that $R\mathcal{D}(L_a) = \mathcal{D}(L^{a,d}_a)$. If ϕ is a boundary value functional at a for $L^{a,d}$ then clearly $\phi \circ R$ is a boundary value functional at a for $L^{a,d}$ and the map $\phi \mapsto \phi \circ R$ is a bijective map $\mathcal{B}_a(L) \to \mathcal{B}_a(L^{a,d})$. □

We note that the space $\mathcal{B}(L)$ and its subspaces $\mathcal{B}_a(L), \mathcal{B}_b(L)$ depend on L only through the domains $\mathcal{D}(L_{\max})$ and $\mathcal{D}(L_{\min})$. So in order to compute them one can sometimes change the potential and consider an operator $L^U := -\partial^2 + U$ instead of $L := -\partial^2 + V$. This is especially useful if U is real: for example, U could be the real part of V, if its imaginary part is bounded.

Proposition 5.14. *Let* $U :]a, b[\to \mathbb{C}$ *measurable such that* $\|(U - V)f\| \leq \alpha\|Lf\| + \beta\|f\|$ *for some real numbers* α, β *with* $\alpha < 1$ *and all* $f \in \mathcal{D}(L_{\max})$. *Then* $\mathcal{D}(L_{\max}) = \mathcal{D}(L^U_{\max})$ *and* $\mathcal{D}(L_{\min}) = \mathcal{D}(L^U_{\min})$. *Hence* $\mathcal{B}(L) = \mathcal{B}(L^U)$ *and*

$$\nu_a(L) = \nu_a(L^U), \quad \nu_b(L) = \nu_b(L^U). \tag{5.23}$$

Proof. We have

$$(1 - \alpha)\|Lf\| - \beta\|f\| \leq \|L^U f\| \leq (1 + \alpha)\|Lf\| + \beta\|f\|$$

so the norms $\|\cdot\|_L$ and $\|\cdot\|_{L^U}$ are equivalent. Then we use (5.4). □

5.5. **Infinite endpoints.** Suppose now that our interval is right-infinite. We will show that if the potential stays bounded in average at infinity, then all elements of the maximal domain converge to zero at ∞ together with their derivative, which obviously implies that their Wronskian converges to zero.

Proposition 5.15. *Suppose that $b = \infty$ and*

$$\limsup_{c\to\infty} \int_c^{c+1} |V(x)|\mathrm{d}x < \infty. \tag{5.24}$$

Then

$$f \in \mathcal{D}(L_{\max}) \quad \Rightarrow \quad \lim_{x\to\infty} f(x) = 0, \ \lim_{x\to\infty} f'(x) = 0. \tag{5.25}$$

Hence $\nu_b = 0$.

Of course, an analogous statement is true for $a = -\infty$ on left-infinite intervals.
Proof of Prop. 5.15. Let $\nu < \nu_0$ and let $J_n := [a + n\nu, a + (n+1)\nu]$. Then, using first (2.28) and then the Schwarz inequality, we obtain

$$\begin{aligned} \|f\|_{L^\infty(J_n)} + \nu\|f'\|_{L^\infty(J_n)} &\le C_1\|Lf\|_{L^1(J_n)} + C_2\|f\|_{L^1(J_n)} \\ &\le C_1\sqrt{\nu}\|Lf\|_{L^2(J_n)} + C_2\sqrt{\nu}\|f\|_{L^2(J_n)} \underset{n\to\infty}{\to} 0. \end{aligned}$$

This implies (5.25). □

6. Solutions square integrable near endpoints

6.1. **Spaces $\mathcal{U}_a(\lambda)$ and $\mathcal{U}_b(\lambda)$.** In this section we will show that one can compute the boundary indices with the help of eigenfunctions of the operator L which are square integrable around a given endpoint.

Definition 6.1. *If $\lambda \in \mathbb{C}$ then $\mathcal{U}_a(\lambda)$ is the set of $f \in AC^1]a, b[$ such that $(L - \lambda)f = 0$ and f is L^2 on $]a, d[$ for some, hence for all d such that $a < d < b$. Similarly we define $\mathcal{U}_b(\lambda)$.*

Proposition 6.2. *If a is a semiregular endpoint for L, then $\dim\mathcal{U}_a(\lambda) = 2$ for all $\lambda \in \mathbb{C}$. Besides, if a is regular, we can choose $u, v \in \mathcal{N}(L - \lambda)$ such that*

$$u(a) = 1, \quad u'(a) = 0, \tag{6.1}$$

$$v(a) = 0, \quad v'(a) = 1. \tag{6.2}$$

Similarly for b.

Proof. We apply Prop. 2.5. □

6.2. **Two-dimensional $\mathcal{U}_a(\lambda)$.** The next proposition contains the main technical fact about the dimensions of the $\mathcal{U}_a(\lambda)$.

Proposition 6.3. *Assume that all the solutions of $Lf = 0$ are square integrable near a. If $f \in C^1]a, b[$ and $|Lf| \le B|f|$ for some $B > 0$, then f is square integrable near a. In particular, if $U \in L^\infty]a, b[$ then all the solutions of $(L + U)f = 0$ are square integrable near a.*

Proof. We may clearly assume that b is a regular endpoint and $f \in C^1]a, b]$. Let $G_\leftarrow$ be the backward Green's operator of L (Definition 2.12). If $Lf = g$, then $L(f - G_\leftarrow g) = 0$. Therefore

$$f(x) = \alpha u(x) + \beta v(x) + \int_x^b \big(u(x)v(y) - v(x)u(y)\big)g(y)\mathrm{d}y, \tag{6.3}$$

for some α, β. Set $A := \sqrt{|\alpha|^2 + |\beta|^2}$ and $\mu(x) := \sqrt{|u(x)|^2 + |v(x)|^2}$. Then

$$|f(x)| \le A\mu(x) + \mu(x)\int_x^b \mu(y)|g(y)|\mathrm{d}y \le \mu(x)\Big(A + B\int_x^b \mu(y)|f(y)|\mathrm{d}y\Big),$$

and the Gronwall Lemma applied to $|f|/\mu$ implies

$$|f(x)| \leq A\mu(x)\exp\Big(B\int_x^b \mu^2(y)\mathrm{d}y\Big). \tag{6.4}$$

Clearly the right hand side of (6.4) is square integrable. □

The above proposition has the following important consequence.

Proposition 6.4. *If* $\dim\mathcal{U}_a(\lambda) = 2$ *for some* $\lambda \in \mathbb{C}$ *then* $\dim\mathcal{U}_a(\lambda) = 2$ *for all* $\lambda \in \mathbb{C}$. *Besides, if this is the case, then* $\nu_a(L) = 2$.

6.3. **The kernel of $L_{\max}$.** Let us describe the relationship between the dimension of the kernel of $L_{\max} - \lambda$ and the dimensions of spaces $\mathcal{U}_a(\lambda)$ and $\mathcal{U}_b(\lambda)$.

The first proposition is a corrolary of Prop. 6.4:

Proposition 6.5. *The following statements are equivalent:*

(1) $\dim\mathcal{N}(L_{\max} - \lambda) = 2$ *for some* $\lambda \in \mathbb{C}$.
(2) $\dim\mathcal{N}(L_{\max} - \lambda) = 2$ *for all* $\lambda \in \mathbb{C}$.
(3) $\dim\mathcal{U}_a(\lambda_a) = \dim\mathcal{U}_b(\lambda_b) = 2$ *for some* $\lambda_a, \lambda_b \in \mathbb{C}$.
(4) $\dim\mathcal{U}_a(\lambda) = \dim\mathcal{U}_b(\lambda) = 2$ *for all* $\lambda \in \mathbb{C}$.

Besides, if this is the case, then $\nu_a(L) = \nu_b(L) = 2$.

The next two propositions are essentially obvious:

Proposition 6.6. *Let* $\lambda \in \mathbb{C}$. *We have* $\dim\mathcal{N}(L_{\max} - \lambda) = 1$ *if and only if one of the following statements is true:*

(1) $\dim\mathcal{U}_a(\lambda) = \dim\mathcal{U}_b(\lambda) = 1$ *and* $\mathcal{U}_a(\lambda) = \mathcal{U}_b(\lambda)$.
(2) $\dim\mathcal{U}_a(\lambda) = 2$ *and* $\dim\mathcal{U}_b(\lambda) = 1$.
(3) $\dim\mathcal{U}_a(\lambda) = 1$ *and* $\dim\mathcal{U}_b(\lambda) = 2$.

Proposition 6.7. *Let* $\lambda \in \mathbb{C}$ *and* $\mathcal{U}_a(\lambda) \neq \{0\}$, $\mathcal{U}_b(\lambda) \neq \{0\}$. *Then* $\dim\mathcal{N}(L_{\max} - \lambda) = 0$ *if and only if* $\dim\mathcal{U}_a(\lambda) = \dim\mathcal{U}_b(\lambda) = 1$ *and* $\mathcal{U}_a(\lambda) \neq \mathcal{U}_b(\lambda)$.

6.4. **First order ODE's.** We will need some properties of vector-valued ordinary differential equations. We will denote by $B(\mathbb{C}^n)$ the space of $n \times n$ matrices.

The following statement can be proven by the same methods as Prop. 2.2. Clearly, in the following proposition $\mathbb{C}^n$ can be easily replaced by an arbitrary Banach space.

Proposition 6.8. *Let* $u_0 \in \mathbb{C}^n$ *and the function* $[a, b[\ni x \mapsto A(x) \in B(\mathbb{C}^n)$ *be in* $L^1_{\mathrm{loc}}\big([a, b[, B(\mathbb{C}^n)\big)$. *Then there exists a unique solution in* $AC\big([a, b[, \mathbb{C}^n\big)$ *of the following Cauchy problem:*

$$\partial_x u(x) = A(x)u(x), \quad u(a) = u_0. \tag{6.5}$$

In particular, the dimension of the space of solutions of $\partial_x u(x) = A(x)u(x)$ *is* n.

If $A \in L^1\big(]a, b[, B(\mathbb{C}^n)\big)$ *then* $u \in AC\big([a, b], \mathbb{C}^n\big)$, *hence* u *is continuous up to* b.

The following theorem is much more interesting. It is borrowed from Atkinson [1, Th. 9.11.2]. Note that in this theorem the finite dimensionality of the space $\mathbb{C}^n$ seems essential.

Theorem 6.9. *Suppose that* A, B *are functions* $[a, b[\to B(\mathbb{C}^n)$ *belonging to* $L^1_{\mathrm{loc}}([a, b[, B(\mathbb{C}^n))$ *satisfying* $A(x) = A^*(x) \geq 0$, $B(x) = B^*(x)$. *Let* J *be an invertible matrix satisfying* $J^* = -J$ *and such that* $J^{-1}A(x)$ *is real. If for some* $\lambda \in \mathbb{C}$ *all solutions of*

$$J\partial_x\phi(x) = \lambda A(x)\phi(x) + B(x)\phi(x) \tag{6.6}$$

satisfy

$$\int_a^b \big(\phi(x)|A(x)\phi(x)\big)\mathrm{d}x < \infty \tag{6.7}$$

then for all $\lambda \in \mathbb{C}$ *all solutions of (6.6) satisfy (6.7).*

Proof. For $\lambda \in \mathbb{C}$, let $[a,b[\ni x \mapsto Y_\lambda(x) \in B(\mathbb{C}^n)$ be the solution of

$$J\partial_x Y_\lambda(x) = \lambda A(x)Y_\lambda(x) + B(x)Y_\lambda(x), \quad Y_\lambda(a) = 1\!\!1. \tag{6.8}$$

Then the theorem is equivalent to the following statement: if for some $\lambda \in \mathbb{C}$ we have

$$\int_a^b \operatorname{Tr} Y_\lambda^*(x)A(x)Y_\lambda(x)\mathrm{d}x < \infty, \tag{6.9}$$

then for all $\lambda \in \mathbb{C}$ we have (6.9). We are going to prove this in the following.

First note that

$$\overline{\operatorname{Tr} J^{-1}B(x)} = \operatorname{Tr}\,(J^{-1}B(x))^* = -\operatorname{Tr} B(x)J^{-1} = -\operatorname{Tr} J^{-1}B(x). \tag{6.10}$$

Therefore, $\operatorname{Tr} J^{-1}B(x) \in \mathrm{i}\mathbb{R}$. By the same argument $\operatorname{Tr} J^{-1}A(x) \in \mathrm{i}\mathbb{R}$. But $\operatorname{Tr} J^{-1}A(x)$ is real. Hence $\operatorname{Tr} J^{-1}A(x) = 0$, and so for arbitrary $\lambda \in \mathbb{C}$ we have $\operatorname{Tr}\big(\lambda A(x) + B(x)\big) \in \mathrm{i}\mathbb{R}$. Therefore,

$$\partial_x \det Y_\lambda(x) = \operatorname{Tr}\big(\lambda A(x) + B(x)\big)\det Y_\lambda(x) \tag{6.11}$$

implies

$$|\det Y_\lambda(x)| = |\det Y_\lambda(a)| = 1. \tag{6.12}$$

Therefore, $Y_\lambda(x)$ is invertible for all $x \in]a,b]$.

Now let $\mu \in \mathbb{C}$ and assume that (6.9) holds for $\lambda = \mu$. We have

$$\partial_x Y_\mu^*(x)JY_\mu(x) = (\mu - \overline{\mu})Y_\mu^*(x)A(x)Y_\mu(x), \quad Y_\mu^*(a)JY_\mu(a) = J. \tag{6.13}$$

Hence

$$Y_\mu^*(x)JY_\mu(x) = J + (\mu - \overline{\mu})\int_a^x Y_\mu^*(y)A(y)Y_\mu(y)\mathrm{d}y. \tag{6.14}$$

Using (6.9) we see that $Y_\mu^*(x)JY_\mu(x)$ is bounded uniformly in $x \in [a,b[$. By (6.12), its inverse is also bounded uniformly in $x \in [a,b[$. (Here we use the finiteness of the dimension of $\mathbb{C}^n$!)

Set $Z_\lambda(x) := Y_\mu^{-1}(x)Y_\lambda(x)$. We have

$$\partial_x Z_\lambda = (\lambda - \mu)Y_\mu^{-1}J^{-1}AY_\lambda = (\lambda - \mu)\big(Y_\mu^* JY_\mu\big)^{-1}Y_\mu^* AY_\mu Z_\lambda. \tag{6.15}$$

We have proven that $\big(Y_\mu^* JY_\mu\big)^{-1}$ is uniformly bounded. By (6.9) the norm of $Y_\mu^* AY_\mu$ is in $L^1]a,b[$. Hence by the second part of Prop. 6.8, $\|Z_\lambda\|$ is uniformly bounded on $[a,b[$. Now, by using

$$Y_\lambda^*(x)A(x)Y_\lambda(x) = Z_\lambda^*(x)Y_\mu^*(x)A(x)Y_\mu(x)Z_\lambda(x) \tag{6.16}$$

we see that (6.9) for $\lambda = \mu$ implies (6.9) for all λ. □

Remark 6.10. *Set*

$$J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad A := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad B(x) := \begin{pmatrix} -V(x) & 0 \\ 0 & 1 \end{pmatrix}. \tag{6.17}$$

Then $Lf = \lambda f$ can be rewritten as (6.6), that is,

$$J\partial_x\phi(x) = \lambda A(x)\phi(x) + B(x)\phi(x), \tag{6.18}$$

with $\phi = \begin{pmatrix} f \\ f' \end{pmatrix}$. Moreover

$$\int_a^b \big(\phi(x)|A(x)\phi(x)\big) = \int |f(x)|^2\mathrm{d}x, \tag{6.19}$$

hence the condition (6.7) means that $f \in L^2]a,b[$. Note also that the conditions of Thm 6.9 on J, A and B are satisfied. Thm 6.9 therefore implies that if all solutions of $Lf = \lambda f$ are square integrable for one λ, they are square integrable for all λ. We thus obtain an alternative proof of Prop. 6.4.

6.5. **Von Neumann decomposition.** Von Neumann's theory for the classification of self-adjoint extensions of a Hermitian operators is well known, cf. [25, 12]. In the present subsection we will investigate how to adapt it to the case of complex potentials.

First recall that $\mathcal{D}(L_{\max})$ has a Hilbert space structure inherited from its graph, which is a closed subspace of $L^2]a,b[\oplus L^2]a,b[$, namely

$$(f|g)_L := (Lf|Lg) + (f|g) = \langle \overline{Lf}|Lg\rangle + \langle \overline{f}|g\rangle. \tag{6.20}$$

Therefore, by the Riesz representation theorem $\mathcal{D}(\overline{L}_{\max})$ can be identified with the dual of $\mathcal{D}(L_{\max})$:

$$\mathcal{D}(\overline{L}_{\max}) \ni f \mapsto (\overline{f}|\cdot)_L \in \mathcal{D}(L_{\max})'. \tag{6.21}$$

Hence the space of boundary functionals $\mathcal{B}(L) \subset \mathcal{D}(L_{\max})'$ can be viewed as a subspace of $\mathcal{D}(\overline{L}_{\max})$.

The following lemma follows from Prop. 3.22 (1):

Lemma 6.11. *With the identification (6.21), there is a canonical linear isomorphism*

$$\mathcal{B}(L) \simeq \mathcal{N}(L_{\max}\overline{L}_{\max} + 1) = \{f \in \mathcal{D}(\overline{L}_{\max}) \mid \overline{L}f \in \mathcal{D}(L_{\max}) \text{ and } L\overline{L}f + f = 0\}. \tag{6.22}$$

Von Neumann's formalism is particularly efficient for real potentials and gives more precise results than in the complex case, so for completeness we begin with some comments on the real case. Then we explore what can be done for arbitrary complex potentials. The differences between the real and complex case are significative, the difficulties being related to the fact that in the complex case there is no simple relation between the (geometric) limit point/circle method and the dimension of the spaces $\mathcal{U}_a(\lambda)$, cf. Subsect. 8.5.

If V is real then $\overline{L} = L$, $L_{\min}$ is Hermitian, and $L_{\max} = L_{\min}^*$, hence

$$\mathcal{B}(L) \simeq \mathcal{N}(L_{\max}^2 + 1). \tag{6.23}$$

Then by using the relation $L^2 + 1 = (L - \mathrm{i})(L + \mathrm{i})$ it is easy to prove that

$$\mathcal{B}(L) \simeq \mathcal{N}(L_{\max} - \mathrm{i}) + \mathcal{N}(L_{\max} + \mathrm{i}). \tag{6.24}$$

The last sum is obviously algebraically direct but also orthogonal for the scalar product (6.20) hence we have an orthogonal direct sum decomposition

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_{\min}) \oplus \mathcal{B}(L) = \mathcal{D}(L_{\min}) \oplus \mathcal{N}(L_{\max} - \mathrm{i}) \oplus \mathcal{N}(L_{\max} + \mathrm{i}). \tag{6.25}$$

The map $f \mapsto \overline{f}$ is a real linear isomorphism of $\mathcal{N}(L_{\max} - \mathrm{i})$ onto $\mathcal{N}(L_{\max} + \mathrm{i})$ hence these spaces have equal dimension ≤ 2 and so $\dim \mathcal{B}(L) = 2 \dim \mathcal{N}(L_{\max} - \mathrm{i}) \in \{0, 2, 4\}$. Of course, we have already proved this in a much simpler way, but (6.25) also gives via a simple argument the following: if V is real then

(1) $\nu_a(L) = 0 \Leftrightarrow \dim \mathcal{U}_a(\lambda) = 1 \ \forall \lambda \in \mathbb{C} \setminus \mathbb{R}$;
(2) $\nu_a(L) = 2 \Leftrightarrow \dim \mathcal{U}_a(\lambda) = 2 \ \forall \lambda \in \mathbb{C}$.

The simplicity of the treatment in the real case is due to the possibility of working with (6.24), which involves only the second order operators $L_{\max} \pm \mathrm{i}$, instead of (6.23), which involves the operator $L_{\max}^2$ of order 4. We do not have such a simplification in the complex case where $L_{\max}\overline{L}_{\max} + 1$ is formally a fourth order differential operator with very singular coefficients, since V is only locally L^1.

Let us show how to generalize von Neumann's analysis to the complex case. We will follow [15, Theorem 9.1] which in turn is a consequence of [1, Theorem 9.11.2]. The nontrivial part of Theorem 6.15 is due to D. Race [22, Theorem 5.4].

We need to study the equation

$$(L\overline{L} + \lambda)f = 0. \tag{6.26}$$

More precisely, by a solution of (6.26) we will mean $f \in AC^1]a,b[$ such that $\overline{L}f \in AC^1]a,b[$ and $L(\overline{L}f) + \lambda f = 0$ holds.

Let us rewrite (6.26) as a 2nd order system of 2 equations. To this end, introduce

$$Q := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \mathcal{I} := \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad W := \begin{pmatrix} 0 & V \\ \overline{V} & -1 \end{pmatrix}, \tag{6.27}$$

$$\mathcal{L} := -Q\partial^2 + W = \begin{pmatrix} 0 & L \\ \overline{L} & -1 \end{pmatrix}. \tag{6.28}$$

Consider the equation

$$(\mathcal{L} + \lambda\mathcal{I})F = 0, \tag{6.29}$$

on $AC^1\big(]a,b[,\mathbb{C}^2\big)$. The equations (6.26) and (6.29) are equivalent in the following sense:

Lemma 6.12. *The map $f \mapsto F := \begin{pmatrix} f \\ \overline{L}f \end{pmatrix}$ is an isomorphism of the space of solutions of $(L\overline{L} + \lambda)f = 0$ onto the space of solutions of $(\mathcal{L} + \lambda\mathcal{I})F = 0$.*

Proof. It is immediate to see that if $(L\overline{L}f + \lambda)f = 0$, then $\begin{pmatrix} f \\ \overline{L}f \end{pmatrix} \in AC^1(]a,b[,\mathbb{C}^2)$ and $(\mathcal{L} + \lambda\mathcal{I}) \begin{pmatrix} f \\ \overline{L}f \end{pmatrix} = 0$.

Reciprocally, if $(\mathcal{L} + \lambda\mathcal{I}) \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = 0$, then $f_1, f_2 \in AC^1]a,b[$ and $\begin{pmatrix} \lambda f_1 + Lf_2 \\ \overline{L}f_1 - f_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$. Thus $f_2 = \overline{L}f_1$ and $(L\overline{L} + \lambda)f_1 = 0$. □

We still prefer to transform (6.29) to a 1st order system of 4 equations. To this end we introduce

$$J = \begin{pmatrix} 0 & -Q \\ Q & 0 \end{pmatrix}, \quad A = \begin{pmatrix} \mathcal{I} & 0 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} W & 0 \\ 0 & -Q \end{pmatrix}$$

Consider the equation

$$J\partial_x\phi = (\lambda A + B)\phi, \tag{6.30}$$

where $\phi \in AC\big(]a,b[,\mathbb{C}^4\big)$.

Lemma 6.13. *The map $F \mapsto \phi := \begin{pmatrix} F \\ -F' \end{pmatrix}$ is an isomorphism of the space of solutions of $(\mathcal{L} + \lambda\mathcal{I})F = 0$ onto the space of solutions of $J\partial_x\phi = (\lambda A + B)\phi$.*

Proof. It is immediate to see that if $(\mathcal{L} + \lambda\mathcal{I})F = 0$, then

$$\begin{pmatrix} F \\ -F' \end{pmatrix} \in AC\big(]a,b[,\mathbb{C}^4\big) \quad \text{and} \quad (-J\partial_x + \lambda A + B)\begin{pmatrix} F \\ -F' \end{pmatrix} = 0.$$

Reciprocally, if $(-J\partial_x + \lambda A + B)\begin{pmatrix} F \\ G \end{pmatrix} = 0$, then

$$F, G \in AC\big(]a,b[,\mathbb{C}^2\big) \quad \text{and} \quad \begin{pmatrix} QG' + (W + \lambda\mathcal{I})F \\ -QF' + QG \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Therefore, $G = F'$, so that $F \in AC^1\big(]a,b[,\mathbb{C}^2\big)$, and $QF'' + (W + \lambda\mathcal{I})F = 0$. □

Lemma 6.14. *Suppose that L is regular at b. If all solutions of $(L\overline{L} + \lambda)f = 0$ are square integrable for some λ, then all solutions of $(L\overline{L} + \lambda)f = 0$ are square integrable for all λ.*

Moreover, if this is the case, then all solutions of $Lf = 0$ are square integrable.

Proof. By Lemmas 6.12 and 6.13, instead of $(L\overline{L} + \lambda)f = 0$ we can consider $J\partial_x\phi = (\lambda A + B)\phi$, and the square integrability of f is equivalent to the integrability of $\big(\phi(x)|A\phi(x)\big) = |\phi_1(x)|^2$, since $f = \phi_1$ under the identification. Note that J, A are constant 4×4 matrices with $J^* = -J$, $A^* = A$, $J^{-1}A$ is a real matrix, and $B(x)^* = B(x)$ belongs to $L^1_{\rm loc}]a,b]$. Thus the equation (6.30) satisfies the assumptions of Thm 6.9. The theorem says that if for some λ all solutions ϕ of (6.30) $\big(\phi(x)|A\phi(x)\big)$ is integrable, then this is so for any λ. This proves the first statement of the lemma.

Now suppose that all solutions of $(L\overline{L}+\lambda)f=0$ belong to $L^2]a,b[$ for all λ. In particular, all solutions of $L\overline{L}f=0$ are square integrable. Since $\overline{L}f=0 \Rightarrow L\overline{L}f=0$, any solution of $\overline{L}f=0$ is square integrable. Hence also any solution of $Lf=0$. □

Theorem 6.15. *The following assertions are equivalent and true:*

$$\nu_a(L)=0 \iff \dim\mathcal{U}_a(\lambda)\leq 1\ \forall\lambda\in\mathbb{C} \iff \dim\mathcal{U}_a(\lambda)\leq 1 \text{ for some } \lambda\in\mathbb{C}, \tag{6.31}$$

$$\nu_a(L)=2 \iff \dim\mathcal{U}_a(\lambda)=2\ \forall\lambda\in\mathbb{C} \iff \dim\mathcal{U}_a(\lambda)=2 \text{ for some } \lambda\in\mathbb{C}. \tag{6.32}$$

If V is a real function, then

$$\nu_a(L)=0 \iff \dim\mathcal{U}_a(\lambda)=1\ \forall\lambda\in\mathbb{C}\setminus\mathbb{R}. \tag{6.33}$$

Proof. The equivalences (6.31) follow from (6.32) by taking into account Theorem 5.6 and the fact that the dimension of $\mathcal{U}_a(\lambda)$ is ≤ 1 if it is not 2. Thus we only have to discuss (6.32). The second equivalence from (6.32) is a consequence of Proposition 6.4.

It is easy to see that $\nu_a(L)=2$ if $\dim\mathcal{U}_a(\lambda)=2$ for some complex λ. Indeed, let u,v be solutions of the equation $(L-\lambda)f=0$ such that $W(u,v)=1$. Then if all the solutions of $(L-\lambda)f=0$ are square integrable near a, we get $W_a(u,v)=1$, hence $W_a\neq 0$, so that $\nu_a(L)=2$.

In what follows we consider the nontrivial part of the theorem: we assume $\nu_a(L)=2$ and show that $\dim\mathcal{U}_a(0)=2$. Clearly we may assume that b is a regular end, if not we replace it by any number between a and b. Then $\nu(L)=2\Leftrightarrow\nu_a(L)=0$ and $\nu(L)=4\Leftrightarrow\nu_a(L)=2$ so we have to show that $\nu(L)=4\Rightarrow\dim\mathcal{N}(L_{\max})=2$. Since $\nu(L)=\dim\mathcal{B}(L)$ and $\mathcal{N}(L_{\max}\overline{L}_{\max}+1)\simeq\mathcal{B}(L)$ by (6.22), it suffices to prove

$$\dim\mathcal{N}(L_{\max}\overline{L}_{\max}+1)=4\Rightarrow\dim\mathcal{N}(L_{\max})=2. \tag{6.34}$$

By Prop. 6.8, the space of solutions of the 1st order system (6.30) is 4-dimensional. Therefore, Lemmas 6.12 and 6.13 imply that the space of solutions of $L\overline{L}f+\lambda f=0$ is 4-dimensional. Hence $\dim\mathcal{N}(L_{\max}\overline{L}_{\max}+1)=4$ implies that all solutions of $(L\overline{L}+1)f=0$ are square integrable. Now by Lemma 6.14 applied to $\lambda=1$, all solutions of $Lf=0$ are square integrable. □

7. Spectrum and Green's operators

7.1. **Integral kernel of Green's operators.** Recall that in Def. 3.7 we introduced the concept of a *right inverse of a closed operator*. In the context of 1d Schrödinger operators right inverses of $L_{\max}$ will be called L^2 *Green's operators*. Thus $G_\bullet$ is a L^2 Green's operator if it is bounded, $\mathcal{R}(G_\bullet)\subset\mathcal{D}(L_{\max})$ and $L_{\max}G_\bullet=\mathbb{1}$.

Let $G_\bullet$ be a Green's operator in the sense of Definition 2.9. Clearly, $L^2_{\mathrm{c}}]a,b[$ is contained in $L^1_{\mathrm{c}}]a,b[$. Besides, $L^2_{\mathrm{c}}]a,b[$ is dense in $L^2]a,b[$. Therefore, if the restriction of $G_\bullet$ to $L^2_{\mathrm{c}}]a,b[$ is bounded, then it has a unique extension to a bounded operator on $L^2]a,b[$. This extension, which by Prop. 3.12 is a L^2 Green's operator, will be denoted by the same symbol $G_\bullet$.

Note that the pair $L_{\max},L_{\min}$ satisfies $L_{\min}=L_{\max}^{\#}\subset L_{\max}$, which are precisely the properties discussed in Subsect 3.6. Recall from that subsection that L^2 Green's operators whose inverse contains $L_{\min}$ correspond to realizations of L that are between $L_{\min}$ and $L_{\max}$. The following proposition is devoted to properties of such Green's operators.

Recall that for any $x\in]a,b[$ we denote by $L^{a,x}$, resp. $L^{x,b}$ the restriction of L to $L^2]a,x[$, resp. $L^2]x,b[$. We also can define $L^{a,x}_{\max}$ and $L^{x,b}_{\max}$, etc. Note that x is a regular point of both $L^{a,x}$ and $L^{x,b}$ (V is integrable on a neighbourhood of x).

Proposition 7.1. *Suppose that $L_{\min}\subset L_\bullet\subset L_{\max}$, $L_\bullet$ is invertible and $G_\bullet:=L_\bullet^{-1}$. Then $G_\bullet$ is an integral operator whose integral kernel*

$$]a,b[\times]a,b[\ni(x,y)\mapsto G_\bullet(x,y)\in\mathbb{C}$$

is a function separately continuous in x and y which has the following properties:
(1) for each $a<x<b$ the function $G_\bullet(x,\cdot)$ restricted to $]a,x[$, resp. $]x,b[$ belongs to $\mathcal{D}(L^{a,x}_{\max})$,

resp. $\mathcal{D}(L_{\max}^{x,b})$ *and satisfies* $LG_\bullet(x,\cdot)=0$ *outside* x*. Besides,* $G_\bullet(x,\cdot)$ *and its derivative have limits at* x *from the left and the right satisfying*

$$\begin{aligned} G_\bullet(x,x-0)-G_\bullet(x,x+0)&=0,\\ \partial_2 G_\bullet(x,x-0)-\partial_2 G_\bullet(x,x+0)&=1; \end{aligned}$$

(2) for each $a<y<b$ *the function* $G_\bullet(\cdot,y)$ *restricted to* $]a,y[$*, resp.* $]y,b[$ *belongs to* $\mathcal{D}(L_{\max}^{a,y})$*, resp.* $\mathcal{D}(L_{\max}^{y,b})$ *and satisfies* $LG_\bullet(\cdot,y)=0$ *outside* y*. Besides,* $G_\bullet(\cdot,y)$ *and its derivative have limits at* y *from the left and the right satisfying*

$$\begin{aligned} G_\bullet(y-0,y)-G_\bullet(y+0,y)&=0,\\ \partial_1 G_\bullet(y-0,y)-\partial_1 G_\bullet(y+0,y)&=1; \end{aligned}$$

Proof. We shall use ideas from the proof of Lemma 4 p. 1315 in [12]. $G_\bullet$ is a continuous linear map $G_\bullet : L^2]a,b[\to\mathcal{D}(L_{\max})$ and for each $x\in]a,b[$ we have a continuous linear form $\varepsilon_x : f\mapsto f(x)$ on $\mathcal{D}(L_{\max})$, hence we get a continuous linear form $\varepsilon_x\circ G_\bullet : L^2]a,b[\to\mathbb{C}$. Thus for each $x\in]a,b[$ there exists a unique $\phi_x\in L^2]a,b[$ such that

$$(G_\bullet f)(x)=\int_a^b \phi_x(y)f(y)\mathrm{d}y,\quad \forall f\in L^2]a,b[\,.$$

We get a map $\phi :]a,b[\to L^2]a,b[$ which is continuous, and even locally Lipschitz, because if $J\subset]a,b[$ is compact and $x,y\in J$ then

$$\begin{aligned} \left|\int_a^b(\phi_x(z)-\phi_y(z))f(z)\mathrm{d}z\right| &= |(G_\bullet f)(x)-(G_\bullet f)(y)|\leq \|(G_\bullet f)'\|_{L^\infty(J)}|x-y|\\ &\leq C_1\|G_\bullet f\|_{\mathcal{D}(L_{\max})}|x-y|\leq C_2\|f\||x-y|, \end{aligned}$$

hence $\|\phi_x-\phi_y\|\leq C_2|x-y|$. By taking $f=L_\bullet g$, $g\in\mathcal{D}(L_\bullet)$, we get

$$g(x)=\int_a^b\phi_x(y)(L_\bullet g)(y)\mathrm{d}y. \tag{7.1}$$

Set $\phi_x^a:=\phi_x\big|_{]a,x[}$ and $\phi_x^b:=\phi_x\big|_{]x,b[}$. (7.1) can be rewritten as

$$g(x)=\int_a^x\phi_x^a(y)(L_\bullet g)(y)\mathrm{d}y+\int_x^b\phi_x^b(y)(L_\bullet g)(y)\mathrm{d}y. \tag{7.2}$$

Since $G_\bullet^\#$ is also an L^2 Green's operator, we have $L_{\min}\subset L_\bullet\subset L_{\max}$. Assuming that $g\in\mathcal{D}(L_{\min})$ and $g(y)=0$ in a neighborhood of x, we can rewrite (7.2) as

$$0=\int_a^x\phi_x^a(y)(L_{\min}^{a,x}g)(y)\mathrm{d}y+\int_x^b\phi_x^b(y)(L_{\min}^{a,x}g)(y)\mathrm{d}y. \tag{7.3}$$

Such functions g are dense in $\mathcal{D}(L_{\min}^{a,x})\oplus\mathcal{D}(L_{\min}^{x,b})$. Therefore, ϕ_x^a belongs to $\mathcal{D}(L_{\max}^{a,x})$ and ϕ_x^b belongs to $\mathcal{D}(L_{\max}^{x,b})$. Since x is a regular end of both intervals $]a,x[$ and $]x,b[$ the function ϕ_x and its derivative ϕ_x' extend to continuous functions on $]a,x]$ and $[x,b[$. However, these extensions are not necessarily continuous on $]a,b[$, i.e. we must distinguish the left and right limits at x, denoted $\phi_x(x\pm0)$ and $\phi_x'(x\pm0)$.

We now take $g\in\mathcal{D}(L_{\min})$ in (7.1). By taking into account (5) of Theorem 4.4 and what we proved above we have $W(\phi_x,g;a)=0$ and $W(\phi_x,g;b)=0$. Denote ϕ_x^a and ϕ_x^b the restrictions of ϕ_x to the intervals $]a,x[$ and $]x,b[$. Then by using Green's identity on $]a,x[$ and $]x,b[$ in (7.2) we get

$$g(x)=-W(\phi_x^a,g;x)+W(\phi_x^b,g;x).$$

We may compute the last two terms explicitly because x is a regular end of both intervals:

$$\begin{aligned} W(\phi_x^a,g;x)&=\phi_x(x-0)g'(x)-\phi_x'(x-0)g(x),\\ W(\phi_x^b,g;x)&=\phi_x(x+0)g'(x)-\phi_x'(x+0)g(x). \end{aligned}$$

Thus we get

$$g(x) = (\phi_x(x+0) - \phi_x(x-0))g'(x) + (\phi_x'(x-0) - \phi_x'(x+0))g(x).$$

The values $g(x)$ and $g'(x)$ may be specified in an arbitrary way under the condition $g \in \mathcal{D}(L_{\min})$ so we get $\phi_x(x+0) - \phi_x(x-0) = 0$ and $\phi_x'(x-0) - \phi_x'(x+0) = 1$. Thus ϕ_x must be a continuous function which is continuously differentiable outside x and its derivative has a jump $\phi_x'(x+0) - \phi_x'(x-0) = -1$ at x.

Thus $G_\bullet$ is an integral operator with kernel $G_\bullet(x,y) = \phi_x(y)$. But $G_\bullet^\#$ is also an L^2 Green's operator and clearly $G_\bullet^\#$ has kernel $G_\bullet^\#(x,y) = \phi_y(x)$. Repeating the above arguments applied to $G_\bullet^\#$ we obtain the remaining statements of the proposition. □

Let us describe a consequence of the above proposition; we use the notation of Definition 6.1.

Proposition 7.2. *If there exists a realization of L such that $\lambda \in \mathbb{C}$ is in its resolvent set, then* $\dim \mathcal{U}_a(\lambda) \geq 1$ *and* $\dim \mathcal{U}_b(\lambda) \geq 1$.

Proof. Suppose that L possesses a realization with $\lambda \in \mathbb{C}$ contained in its resolvent set. This means that $L - \lambda$ possesses an L^2 Green's operator $G_\bullet$. By Proposition 3.23 it can be chosen to satisfy $G_\bullet = G_\bullet^\#$. Then Proposition 7.1 implies that for any $x \in]a,b[$ the function $G_\bullet(x,\cdot) \in L^2]a,b[$ belongs to $L^2]a,b[$ and satisfies $LG_\bullet(x,\cdot) = 0$ on $]a,x[$ and $]x,b[$. We will prove that there is x such that $G_\bullet(x,\cdot)\big|_{]x,b[} \neq 0$, which implies $\dim \mathcal{U}_b(\lambda) \geq 1$. In order to prove that $\dim \mathcal{U}_a(\lambda) \geq 1$ it suffices to show that there is x such that $G_\bullet(x,\cdot)\big|_{]a,x[} \neq 0$ and the argument is similar.

If the required assertion is not true, then $G_\bullet(x,\cdot)\big|_{]x,b[} = 0$ for any x, in other terms $G_\bullet(x,y) = 0$ for all $a < x < y < b$. Since $G_\bullet$ is self-transposed, (3.9) gives $G_\bullet(x,y) = G_\bullet(y,x)$ $\forall x,y$. Hence we will also have $G_\bullet(x,y) = 0$ for $a < y < x < b$. But this means $G_\bullet = 0$, which is not true. □

7.2. **Forward and backward Green's operators.** Let us study the L^2 theory of the forward Green's operator $G_\rightarrow$. Recall that if u, v span $\mathcal{N}(L)$ with $W(v,u) = 1$, then $G_\rightarrow$ is given by

$$G_\rightarrow g(x) = v(x)\int_a^x u(y)g(y)\mathrm{d}y - u(x)\int_a^x v(y)g(y)\mathrm{d}y. \tag{7.4}$$

Note that elements of $\mathcal{N}(L)$ do not have to be square integrable. We have $\mathcal{N}(L_{\max}) = \mathcal{N}(L) \cap L^2]a,b[$. In the following proposition we consider the case $\mathcal{N}(L) = \mathcal{N}(L_{\max})$:

Proposition 7.3. *Assume* $\dim \mathcal{N}(L_{\max}) = 2$. *Then*

1. *$G_\rightarrow$ is Hilbert-Schmidt. In particular, it is an L^2 Green's operator of L.*
2. *Let L_a be the operator defined in Def. 4.14. Then L_a has an empty spectrum, $(L_a - \lambda)^{-1}$ is compact for avery $\lambda \in \mathbb{C}$, and we have $L_a^{-1} = G_\rightarrow$.*
3. *Every $f \in \mathcal{D}(L_{\max})$ has a unique decomposition as*
$$f = \alpha u + \beta v + f_a, \quad f_a \in G_\rightarrow L^2]a,b[= \mathcal{D}(L_a). \tag{7.5}$$
4. *$G_\leftarrow$ has analogous properties. In particular, we have*
$$G_\rightarrow^\# = G_\leftarrow, \quad L_b^{-1} = G_\leftarrow. \tag{7.6}$$

Proof. By hypothesis, $u, v \in L^2]a,b[$. The Hilbert-Schmidt norm of $G_\rightarrow$ is clearly bounded by $\sqrt{2}\|u\|_2\|v\|_2$. Then by Proposition 3.10 zero belongs to the resolvent set of L_a, $L_a^{-1} = G_a$, and

$$\mathcal{D}(L_{\max}) = \mathcal{D}(L_a) \oplus \mathcal{N}(L_{\max}), \tag{7.7}$$

which can be restated as the decomposition (7.5). If $\lambda \in \mathbb{C}$ and V is replaced by $V - \lambda$ then the new $G_\rightarrow$ will be the resolvent at λ of L_a, which proves the second assertion in (2). Finally, (7.6) is proved by a simple computation. □

Proposition 7.4. *$G_\rightarrow$ is bounded if and only if* $\dim \mathcal{N}(L_{\max}) = 2$ *(so that the assumptions of Prop. 7.3 are valid).*

Proof. Let $G_\to$ be bounded. Then so is $G_\to^\# = G_\leftarrow$. Let us recall the identity (2.23):

$$G_\to - G_\leftarrow = |v\rangle\langle u| - |u\rangle\langle v|. \tag{7.8}$$

But the boundedness of the rhs of (7.8) implies $v, u \in L^2]a,b[$. □

$G_\to$ is useful even if it not a bounded operator, especially if $\dim \mathcal{U}_a(0) = 2$:

Proposition 7.5. *Assume that* $\dim \mathcal{U}_a(0) = 2$*. Then* $G_\to$ *extends as a map from* $L^2]a,b[$ *to* $C^1]a,b[$ *satisfying the bounds*

$$|G_\to g(x)| \leq \Big(|u(x)|\|v\|_x + |v(x)|\|u\|_x\Big)\|g\|_x, \tag{7.9}$$

$$|\partial_x G_\to g(x)| \leq \Big(|u'(x)|\|v\|_x + |v'(x)|\|u\|_x\Big)\|g\|_x, \tag{7.10}$$

where $\|g\|_x := \Big(\int_a^x |g(y)|^2 \mathrm{d}y\Big)^{\frac{1}{2}}$*. If* $\chi \in C_\mathrm{c}^\infty[a,b[$*,* $\chi = 1$ *around* a*, then every* $f \in \mathcal{D}(L_{\max})$ *has a unique decomposition as*

$$f = \alpha\chi u + \beta\chi v + f_a, \quad f_a \in \mathcal{D}(L_a). \tag{7.11}$$

Proof. Let $a < d < b$. Then we can restrict our problem to $]a,d[$. Now $\dim \mathcal{U}_a(0) = \dim \mathcal{U}_d(0) = 2$. Therefore, we can apply Prop. 7.3, using the fact that $G_\to$ restricted to $L^2]a,d[$ is an L^2 Green's operator of $L^{a,d}$. □

The main assertion of Theorem 6.15 is, technically speaking, that $\dim \mathcal{U}_a(0) = 2$ if $\nu_a(L) = 2$. We may state an improved version of this assertion as a boundary value problem and this is of a certain interest: it says that if $\nu_a(L) = 2$ then the endpoint a behaves almost as if it were a regular end (in the regular case one works with L^1 instead of L^2). Note that since only the behavior near a of the solutions matters, we may assume b a regular endpoint.

Proposition 7.6. *Suppose that* $\nu_a(L) = 2$ *and* b *is a regular endpoint for* L*. Let* $\phi, \psi \in \mathcal{B}_a(L)$ *be a pair of linearly independent boundary value functionals. Then the linear continuous map*

$$\mathcal{D}(L_{\max}) \ni f \mapsto (Lf, \phi(f), \psi(f)) \in L^2]a,b[\times\mathbb{C}\times\mathbb{C} \tag{7.12}$$

is bounded and invertible. In particular, for any $g \in L^2]a,b[$ *and any* $\alpha, \beta \in \mathbb{C}$*, there is a unique* $f \in \mathcal{D}(L_{\max})$ *such that* $Lf = g$*,* $\phi(f) = \alpha$*, and* $\psi(f) = \beta$*.*

Proof. By Proposition 7.3, the operator $L_a : \mathcal{D}(L_a) \to L^2]a,b[$ is bijective hence the map (7.12) is injective. Since the map is clearly continuous, by the open mapping theorem it suffices to prove its surjectivity. Let $g \in L^2]a,b[$ and $\alpha, \beta \in \mathbb{C}$. Since L_a is surjective, there is $h \in \mathcal{D}(L_a)$ such that $Lh = g$. Now it suffices to show that there is $k \in \mathcal{N}(L_{\max})$ such that $\phi(k) = \alpha, \psi(k) = \beta$ because then $f = h + k \in \mathcal{D}(L_{\max})$ will satisfy $Lf = g$, $\phi(f) = \alpha$, and $\psi(f) = \beta$. Clearly, it suffices to prove this just for one couple ϕ, ψ. Since $\mathcal{N}(L_{\max})$ is two dimensional, there are $u, v \in \mathcal{N}(L_{\max})$ with $W(u,v) = 1$ and we may take $\phi = \vec{u}_a$ and $\psi = \vec{v}_a$ since, by Theorem 5.5 the boundary value functionals $\vec{u}_a, \vec{v}_a \in \mathcal{B}_a(L)$ are linearly independent. Then it suffices to take $k = -\beta u + \alpha v$. □

7.3. **Green's operators with two-sided boundary conditions.** Recall from Def. 5.11 that if $\phi \in \mathcal{B}_a$ and $\psi \in \mathcal{B}_b$ be are nonzero functionals, then $L_{\phi,\psi}$ is the operator $L_{\phi,\psi} \subset L_{\max}$ with

$$\mathcal{D}(L_{\phi,\psi}) := \{f \in \mathcal{D}(L_{\max}) \ \mid \phi(f) = \psi(f) = 0\}.$$

Note that $L_{\phi,\psi}^\# = L_{\phi,\psi}$.

Recall also that, if u, v are solutions of the equation $Lf = 0$ with $W(v,u) = 1$, we defined in Def. 2.10 the two-sided Green's operator $G_{u,v}$

$$G_{u,v}g(x) := \int_x^b u(x)v(y)g(y)\mathrm{d}y + \int_a^x v(x)u(y)g(y)\mathrm{d}y.$$

Clearly, there exists a close relationship between realizations of L of the form $L_{\phi,\psi}$ and Green's operators of the form $G_{u,v}$.

Proposition 7.7. *Suppose $\phi \in \mathcal{B}_a$, $\psi \in \mathcal{B}_b$ and $0 \in \mathrm{rs}(L_{\phi,\psi})$. Then there exists $u \in \mathcal{U}_a(0)$ and $v \in \mathcal{U}_b(0)$ with $W(v,u) \neq 0$ such that, in the notation of Def. 5.4,*

$$\phi = \vec{u}_a, \quad \psi = \vec{v}_b, \tag{7.13}$$

Proof. Let us prove the existence of u. Note that by Proposition 7.2 we have $\dim \mathcal{U}_a(0) \geq 1$. Then, by Proposition 7.1, the operator $L_{\phi,\psi}^{-1}$ has an integral kernel $G_{\phi,\psi}(\cdot,\cdot)$ such that for any $a < c < b$ the restriction of $G_{\phi,\psi}(c,\cdot)$ to $]a,c[$ belongs to $\mathcal{D}(L_{\max}^{a,c})$ and satisfies $LG_{\phi,\psi}(c,\cdot) = 0$. If $f \in \mathcal{D}(L_{\phi,\psi})$ the relation (7.1) gives

$$f(x) = \int_a^b G_{\phi,\psi}(x,y)(L_{\phi,\psi}f)(y)\mathrm{d}y$$

hence if $a < x < c$ and $f(x) = 0$ for $x > c$ we have

$$0 = \int_a^c G_{\phi,\psi}(c,y)(L_{\phi,\psi}f)(y)\mathrm{d}y. \tag{7.14}$$

Denote $L_{\phi,c}^{a,c}$ the operator in $L^2]a,c[$ defined by L and the boundary conditions $\phi(f) = 0$ and $f(c) = f'(c) = 0$. Clearly, any function f satisfying such conditions extends to a function in $\mathcal{D}(L_{\phi,\psi})$ if we set $f(x) = 0$ for $x > c$ hence (7.14) is equivalent to

$$\int_a^c G_{\phi,\psi}(c,\cdot)L_{\phi,c}^{a,c}f\mathrm{d}x = 0 \quad \forall f \in \mathcal{D}(L_{\phi,c}^{a,c}).$$

We noted above that $L_{\phi,\psi}^{\#} = L_{\phi,\psi}$ and by a simple argument this implies $(L_{\phi,c}^{a,c})^{\#} = L_{\phi,0}^{a,c} \equiv L_{\phi}^{a,c}$ hence the preceding relation means $G_{\phi,\psi}(c,\cdot)|_{]a,c[} \in \mathcal{N}(L_{\phi}^{a,c})$. Now recall that during the proof of Proposition 7.2 we have seen that c may be chosen such that $G_{\phi,\psi}(c,\cdot)|_{]a,c[} \neq 0$. Finally, if we fix such a c and denote $u = G_{\phi,\psi}(c,\cdot)$ then we get a nonzero element $u \in \mathcal{U}_a(0)$ such that $\phi(u) = 0$ which, since $u \neq 0$, is equivalent to $\phi = \alpha\vec{u}_a$.

In an analogous way we prove the existence of v. Both are nonzero. If u is proportional to v, then they are eigenvectors of $L_{\phi,\psi}$ for the eigenvalue 0, which contradicts $0 \in \mathrm{rs}(L_{\phi,\psi})$. Hence they are not proportional to one another, so that $W(v,u) \neq 0$. □

Note that in the above proposition we can have $\phi = 0$ or $\psi = 0$, or both. However, u and v are always non-zero.

Suppose now that we start from a two-sided Green's operator.

Proposition 7.8. *Let $G_{u,v}$ be bounded on $L^2]a,b[$. Then $u \in \mathcal{U}_a(0)$ and $v \in \mathcal{U}_b(0)$.*

Proof. Let $a < d < b$. If $G_{u,v}$ is bounded, then so is $1\!\!1_{]a,d]}(x)G_{u,v}1\!\!1_{]d,b]}(x)$, where x denotes the operator of multiplication by the variable in $]a,b[$. But its integral kernel is

$$u(x)1\!\!1_{]a,d]}(x)v(y)1\!\!1_{]d,b]}(y)$$

where x and y denote the variables in $]a,b[$. This is a rank one operator with the norm

$$\Big(\int_a^d |u|^2(x)\mathrm{d}x\Big)^{\frac{1}{2}}\Big(\int_d^b |v|^2(x)\mathrm{d}x\Big)^{\frac{1}{2}}. \qquad \square$$

Until the end of this subsection we assume that $u \in \mathcal{U}_a(0)$ and $v \in \mathcal{U}_b(0)$ and the functionals ϕ, ψ are given by (7.13). Thus we have both Green's operator $G_{u,v}$ and the operator $L_{\phi,\psi}$.

Let $\chi \in C^\infty]a,b[$ such that $\chi = 1$ close to a and $\chi = 0$ close to b. Clearly,

$$\mathcal{D}(L_{\phi,\psi}) = \mathcal{D}(L_{\min}) + \mathrm{Span}\{\chi u, (1-\chi)v\}. \tag{7.15}$$

We will show that $G_{u,v}$ is bounded iff and only if $0 \in \mathrm{rs}(L_{\phi,\psi})$. However, it seems that there is no guarantee that $G_{u,v}$ is bounded.

Proposition 7.9.

$$G_{u,v}L_{\mathrm{c}}^2]a,b[\subset \mathcal{D}(L_{\phi,\psi}), \tag{7.16}$$

$$G_{u,v}L^2]a,b[\subset AC^1]a,b[. \tag{7.17}$$

Moreover, $G_{u,v}$ is bounded if and only if there exists $c > 0$ such that

$$\|L_{\phi,\psi}f\| \geq c\|f\|, \quad f \in \mathcal{D}(L_{\phi,\psi}). \tag{7.18}$$

If this is the case, then 0 belongs to the resolvent set of $L_{\phi,\psi}$, we have $G_{u,v} = L_{\phi,\psi}^{-1}$, $G_{u,v}^{\#} = G_{u,v}$ and

$$\mathcal{D}(L_{\phi,\psi}) = G_{u,v}L^2]a,b[. \tag{7.19}$$

Proof. It is easy to see that

$$G_{u,v}L_{\rm c}^2]a,b[\subset \mathcal{D}(L_{\rm c}) + \mathrm{Span}\{\chi u, (1-\chi)v\},$$

which implies (7.16).

Let $g \in L^2]a,b[$. For $a < x < b$ we compute:

$$\partial_x G_{u,v}g(x) = u'(x)\int_x^b v(y)g(y)\mathrm{d}y + v'(x)\int_a^x u(y)g(y)\mathrm{d}y. \tag{7.20}$$

Now, $x \mapsto u'(x), v'(x), \int_x^b v(y)g(y)\mathrm{d}y$, $\int_a^x u(y)g(y)\mathrm{d}y$ belong to $AC]a,b[$. Hence (7.20) belongs to $AC]a,b[$. Therefore, (7.17) is true. Next, let

$$f = f_{\rm c} + \alpha\chi u + \beta(1-\chi)v, \quad f_{\rm c} \in \mathcal{D}(L_{\rm c}). \tag{7.21}$$

We compute, integrating by parts,

$$G_{u,v}L_{\phi,\psi}f(x) = \int_a^b \Big(\big(-\partial_y^2 + V(y)\big)G_{u,v}(x,y)\Big)f(y)\mathrm{d}y \tag{7.22}$$

$$+\lim_{y\to a}\big(G_{u,v}(x,y)f'(y) - \partial_y G_{u,v}(x,y)f(y)\big) \tag{7.23}$$

$$-\lim_{y\to b}\big(G_{u,v}(x,y)f'(y) - \partial_y G_{u,v}(x,y)f(y)\big) \tag{7.24}$$

$$= f(x) + v(x)W(u,f;a) - u(x)W(v,f;b) \quad = \quad f(x). \tag{7.25}$$

Moreover, functions of the form (7.21) are dense in $\mathcal{D}(L_{\phi,\psi})$. Therefore, if $G_{u,v}$ is bounded, then (7.25) extends to

$$G_{u,v}L_{\phi,\psi}f = f, \quad f \in \mathcal{D}(L_{\phi,\psi}). \tag{7.26}$$

Hence $\|f\| = \|G_{u,v}L_{\phi,\psi}f\| \leq \|G_{u,v}\|\|L_{\phi,\psi}f\|$ which gives (7.18).

Assume that $G_{u,v}$ is bounded in the sense of $L^2]a,b[$. By Prop. 3.12, $G_{u,v}$ is an L^2 Green's operator. By Prop. 3.9, it is also bounded from $L^2]a,b[$ to $\mathcal{D}(L_{\max})$. Therefore (7.16) extends then to

$$G_{u,v}L^2]a,b[\subset \mathcal{D}(L_{\phi,\psi}), \tag{7.27}$$

so that

$$L_{\phi,\psi}G_{u,v}g = g, \quad g \in L^2]a,b[. \tag{7.28}$$

By (7.26) and (7.28), $G_{u,v}$ is a (bounded) inverse of $L_{\phi,\psi}$ so that (7.18) and (7.19) are true.

Now assume that (7.18) holds. By (7.16), we then have

$$g = L_{\phi,\psi}G_{u,v}g, \quad g \in L_{\rm c}^2]a,b[. \tag{7.29}$$

Hence,

$$\|g\| = \|L_{\phi,\psi}G_{u,v}g\| \geq c\|G_{u,v}g\| \tag{7.30}$$

on $L_{\rm c}^2]a,b[$, which is dense in $L^2]a,b[$. Therefore, $G_{u,v}$ is bounded. □

7.4. **Classification of realizations possessing non-empty resolvent set.** In applications well posed operators (possessing non-empty resolvent set) are by far the most useful. The following theorem describes a classification of realizations of L with this property.

Theorem 7.10. *Suppose that $L_\bullet$ is a realization of L with a non-empty resolvent set. Then exactly one of the following statements is true.*

(1) $L_\bullet = L_{\max}$.
Then also $L_{\min} = L_\bullet$, so that L possesses a unique realization. We have $\nu(L) = 0$.
If $\lambda \in \mathrm{rs}(L_\bullet)$, then $\dim \mathcal{N}(L_{\max} - \lambda) = 0$, $\dim \mathcal{U}_a(\lambda) = \dim \mathcal{U}_b(\lambda) = 1$ and $\mathcal{U}_a(\lambda) \neq \mathcal{U}_b(\lambda)$. If $u \in \mathcal{U}_a(\lambda)$ and $v \in \mathcal{U}_b(\lambda)$ with $W(v,u) = 1$, then
$$(L_\bullet - \lambda)^{-1} = G_{u,v}.$$
$L_\bullet$ is self-transposed and has separated boundary conditions. (See Def. 5.10 for separated boundary conditions.)

(2) The inclusion $\mathcal{D}(L_\bullet) \subset \mathcal{D}(L_{\max})$ is of codimension 1.
Then the inclusion $\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_\bullet)$ is of codimension 1 and we have $\nu(L) = 2$.
If $\lambda \in \mathrm{rs}(L_\bullet)$, then $\dim \mathcal{N}(L_{\max} - \lambda) = 1$, $\dim \mathcal{U}_a(\lambda) = 2$ and $\dim \mathcal{U}_b(\lambda) = 1$, or $\dim \mathcal{U}_a(\lambda) = 1$ and $\dim \mathcal{U}_b(\lambda) = 2$. We can find $u \in \mathcal{U}_a(\lambda)$ and $v \in \mathcal{U}_b(\lambda)$ with $W(v,u) = 1$ such that
$$(L_\bullet - \lambda)^{-1} = G_{u,v}.$$
$L_\bullet$ is self-transposed and has separated boundary conditions.

(3) The inclusion $\mathcal{D}(L_\bullet) \subset \mathcal{D}(L_{\max})$ is of codimension 2.
Then the inclusion $\mathcal{D}(L_{\min}) \subset \mathcal{D}(L_\bullet)$ is of codimension 2. We have $\nu(L) = 4$.
The spectrum of $L_\bullet$ is discrete and its resolvents are Hilbert-Schmidt. For any $\lambda \in \mathbb{C}$ we have $\dim \mathcal{N}(L_{\max} - \lambda) = 2$, $\dim \mathcal{U}_a(\lambda) = 2$ and $\dim \mathcal{U}_b(\lambda) = 2$.
If in addition $L_\bullet$ is self-transposed, has separated boundary conditions, and $\lambda \in \mathrm{rs}(L_\bullet)$, then we can find $u \in \mathcal{U}_a(\lambda)$ and $v \in \mathcal{U}_b(\lambda)$ with $W(v,u) = 1$ such that
$$(L_\bullet - \lambda)^{-1} = G_{u,v}.$$
If, instead, $L_\bullet$ is not self-transposed and has separated boundary conditions, then it has empty spectrum and one of the following possibilities hold:
(i) *$L_\bullet = L_a$ and $(L_\bullet - \lambda)^{-1}$ is given by the forward Green's operator.*
(ii) *$L_\bullet = L_b$ and $(L_\bullet - \lambda)^{-1}$ is given by the backward Green's operator.*
We have $L_a^{\#} = L_b$, and both (i) and (ii) are described in Prop. 7.5.

7.5. **Existence of realizations with non-empty resolvent set.** $\mathbb{C}\backslash\mathbb{R}$ is contained in the resolvent set of all self-adjoint operators. The following proposition gives a generalization of this fact.

Proposition 7.11. *Let V_{R} and V_{I} be the real and imaginary part of V. Let $\|V_{\mathrm{I}}\|_\infty =: \beta < \infty$. Then*
$$\{\lambda \in \mathbb{C} \mid |\operatorname{Im} \lambda| > \beta\} \tag{7.31}$$
is contained in the resolvent set of some realizations of L. All realizations of L possess only discrete spectrum in (7.31).

Proof. Let $L_{\mathrm{R}} := -\partial_x^2 + V_{\mathrm{R}}$. By Theorem 4.4, $L_{\mathrm{R},\min}$ is densely defined and $L_{\mathrm{R},\min}^{\#} = L_{\mathrm{R},\max} \supset L_{\mathrm{R},\min}$. By the reality of V_{R}, $L_{\mathrm{R},\min}^{*} = L_{\mathrm{R},\min}^{\#}$. Therefore, $L_{\mathrm{R},\min}^{*} \supset L_{\mathrm{R},\min}$. This means that $L_{\mathrm{R},\min}$ is Hermitian (symmetric). Let us now apply the well-known theory of self-adjoint extensions of Hermitian operators. Let $d_\pm := \mathcal{N}\big(L_{\mathrm{R},\min}^{*} \mp \mathrm{i}\big)$ be the deficiency indices. Using the fact that $L_{\mathrm{R},\min}$ is real we conclude that $d_+ = d_-$. Therefore, $L_{\mathrm{R},\min}$ possesses at least one self-adjoint extension, which we denote $L_{\mathrm{R},\bullet}$. By the self-adjointness of $L_{\mathrm{R},\bullet}$ we have $\|(L_{\mathrm{R},\bullet} - \lambda)^{-1}\| \leq |\operatorname{Im} \lambda|^{-1}$ for all $\lambda \notin \mathbb{R}$. Set $L_\bullet := L_{\mathrm{R},\bullet} + \mathrm{i}V_{\mathrm{I}}$. Clearly,
$$L_{\max} \supset L_\bullet \supset L_{\min}. \tag{7.32}$$

For $|\operatorname{Im}\lambda| > \beta$, λ belongs to the resolvent set of $L_\bullet$, and its resolvent is given by

$$(L_\bullet - \lambda)^{-1} = (L_{\mathrm{R},\bullet} - \lambda)^{-1}\big(\mathbb{1} + \mathrm{i}V_{\mathrm{I}}(L_{\mathrm{R},\bullet} - \lambda)^{-1}\big)^{-1}.$$

□

Note that the above proposition can be improved to cover some singularities of V_{I}. In fact, if there are numbers α, β with $0 \le \alpha < 1$ such that

$$\|V_{\mathrm{I}}f\|^2 \le \alpha^2\big(\|L_{\mathrm{R},\bullet}f\|^2 + \beta^2\|f\|^2\big), \quad \forall f \in \mathcal{D}(L_{\mathrm{R},\bullet}),$$

then still

$$\|V_{\mathrm{I}}(L_{\mathrm{R},\bullet} - \lambda)^{-1}\| \le \alpha < 1,$$

and the conclusion of Prop. 7.11 holds.

7.6. **"Pathological" spectral properties.** We construct now 1d Schrödinger operators whose realizations have an empty resolvent set. Such operators seem to be rather pathological and not very interesting for applications.

Proposition 7.12. *There is $V \in L^\infty_{\mathrm{loc}}[0,\infty[$ such that if $L = -\partial^2 + V$ then any operator $L_\bullet$ on $L^2]0,\infty[$ with $L_{\min} \subset L_\bullet \subset L_{\max}$ has empty resolvent set, hence $\sigma(L_\bullet) = \mathbb{C}$.*

Proof. Let $I_n =]n^2 - n, n^2 + n[$ with $n \ge 1$ integer. Then I_n is an open interval of length $|I_n| = 2n$ and I_{n+1} starts with the point $n^2 + n$ which is the endpoint of I_n. Thus $\cup_n I_n$ is a disjoint union equal to $]0,\infty[\setminus\{n^2+n \mid n \ge 1\}$. Let $\mathbb{P}$ be the set prime numbers $\mathbb{P} = \{2,3,5,\dots\}$ and for each prime p denote $J_p = \cup_{k\ge1} I_{p^k}$. We get a family of open subsets J_p of $]0,\infty[$ which are pairwise disjoint and each of them contains intervals of length as large as we wish. Now let $p \mapsto c_p$ be a bijective map from $\mathbb{P}$ to the set of complex rational numbers and let us define a function $V : [0,\infty[\to \mathbb{C}$ by the following rules: if $x \in J_p$ for some prime p then $V(x) = c_p$ and $V(x) = 0$ if $x \notin \cup_p J_p$. Then V is a locally bounded function whose range contains all the complex rational numbers. We set $L = -\partial^2 + V(x)$ and we prove that the spectrum of any $L_\bullet$ with $L_{\min} \subset L_\bullet \subset L_{\max}$ is equal to $\mathbb{C}$. Since the spectrum is closed, it suffices to show that any complex rational number c belongs to the spectrum of any $L_\bullet$. If not, there is a number $\alpha > 0$ such that $\|(L_\bullet - c)\phi\| \ge \alpha\|\phi\|$ for any $\phi \in \mathcal{D}(L_\bullet)$. If r is a (large) positive number then there is an open interval I of length $\ge r$ such that $V(x) = c$ on I. Let $\phi \in C^\infty_{\mathrm{c}}(I)$ such that $\phi(x) = 1$ for x at distance ≥ 1 from the boundary of I and with $|\phi''| \le \beta$ with a constant β independent of r (take $r > 3$ for example). Then $\phi \in \mathcal{D}(L_{\min})$ and $(L - c)\phi = -\phi'' + V\phi - c\phi = -\phi''$ hence $\|\phi''\| = \|(L_\bullet - c)\phi\| \ge \alpha\|\phi\|$ so $\alpha\|\phi\| \le 2\beta$ which is impossible because the left hand side is of order $\sqrt{r}$. One may choose V of class C^∞ by a simple modification of this construction. □

8. Potentials with a negative imaginary part

8.1. **Dissipative 1d Schrödinger operators.** Recall that an operator A is called *dissipative* if

$$\operatorname{Im}(f|Af) \le 0, \quad f \in \mathcal{D}(A), \tag{8.1}$$

that is, if its numerical range is contained in $\{\lambda \in \mathbb{C} \mid \operatorname{Im}\lambda \le 0\}$. It is called *maximal dissipative* if in addition its spectrum is contained in $\{\lambda \in \mathbb{C} \mid \operatorname{Im}\lambda \le 0\}$. The following criterion is well-known [18].

Proposition 8.1. *Assume A is closed, densely defined and dissipative. Then A is maximal dissipative if and only if $-A^*$ is dissipative, and then $-A^*$ is maximal dissipative.*

Let us now consider $L = -\partial_x^2 + V(x)$ with $V \in L^1_{\mathrm{loc}}]a,b[$.

Proposition 8.2. *The operator $L_{\min}$ is dissipative if and only if $\operatorname{Im}V \le 0$. It is maximal dissipative if in addition $L_{\min} = L_{\max}$.*

Proof. If $f \in \mathcal{D}(L_{\max})$ then

$$\begin{aligned}(f|L_{\max}f) &= \int_a^b \left(\overline{f}'f' - (\overline{f}f')' + V\overline{f}f\right.\\ &= \lim_{\substack{a_1\to a\\ b_1\to b}} \left(\overline{f}(a_1)f'(a_1) - \overline{f}(b_1)f'(b_1) + \int_{a_1}^{b_1} \left(|f'|^2 + V|f|^2\right)\right)\end{aligned}$$

hence

$$\operatorname{Im}(f|L_{\max}f) = \lim_{\substack{a_1\to a\\ b_1\to b}} \left(\int_{a_1}^{b_1} \operatorname{Im}(V)|f|^2 + \operatorname{Im}(\overline{f}(a_1)f'(a_1)) - \operatorname{Im}(\overline{f}(b_1)f'(b_1))\right). \tag{8.2}$$

Thus

$$\operatorname{Im}(f|L_{\min}f) = \int_a^b \operatorname{Im}(V)|f|^2 \geq 0, \quad f \in \mathcal{D}(L_{\mathrm{c}}). \tag{8.3}$$

By continuity, (8.3) extends to $f \in \mathcal{D}(L_{\min})$, which clearly implies that $L_{\min}$ is dissipative. The same argument as above shows that $-\overline{L}_{\min}$ is dissipative

If $L_{\min} = L_{\max}$, then $\overline{L}_{\min} = \overline{L}_{\max}$. But $L^*_{\min} = \overline{L}_{\max}$. Hence $-L^*_{\min}$ is dissipative. This proves maximal dissipativity of $L_{\min}$.

If $L_{\min} \neq L_{\max}$, then the spectrum of $L_{\min}$ is $\mathbb{C}$, so $L_{\min}$ is not maximally dissipative. □

A convenient criterion for dissipativity holds if $\mathcal{D}(A) \subset \mathcal{D}(A^*)$: then A is dissipative if and only if $\frac{1}{\mathrm{i}2}(A - A^*) \geq 0$. Unfortunately, an operator A can be dissipative even if $\mathcal{D}(A) \cap \mathcal{D}(A^*) = \{0\}$. This is related to a certain difficulty when one tries to study the dissipativity of Schrödinger operators with singular complex potentials. Suppose that we want to check that $L_\bullet$ is dissipative using this criterion. If $L_{\min} \subset L_\bullet \subset L_{\max}$, then $\overline{L}_{\min} \subset L^*_\bullet \subset \overline{L}_{\max}$. But we may have $\mathcal{D}(\overline{L}_{\max}) \cap \mathcal{D}(L_{\max}) = \{0\}$ (Lemma 4.10), hence we could have $\mathcal{D}(L_\bullet) \cap \mathcal{D}(L^*_\bullet) = \{0\}$ which is annoying. Indeed, although $W_x(\overline{f}, f) = 2\mathrm{i}\operatorname{Im}(\overline{f}(x)f'(x))$, we cannot use in (8.2) the existence of the limits (4.4) and (4.5) because in general $\overline{f} \notin \mathcal{D}(L_{\max})$.

Let us describe the action of conjugation on boundary conditions. The *conjugate* of $\alpha \in \mathcal{B}(L)$ is the boundary functional $\overline{\alpha} \in \mathcal{B}(\overline{L})$ given by

$$\overline{\alpha}(f) := \overline{\alpha(\overline{f})}. \tag{8.4}$$

Clearly $\alpha \mapsto \overline{\alpha}$ is a bijective anti-linear map $\mathcal{B}(L) \to \mathcal{B}(\overline{L})$ which sends $\mathcal{B}_a(L)$ into $\mathcal{B}_a(\overline{L})$ and $\mathcal{B}_b(L)$ into $\mathcal{B}_b(\overline{L})$. Then if $g \in \mathcal{D}(L_{\max})$ is a representative of $\alpha \in \mathcal{B}_a$, so that

$$\alpha(f) = W_a(g, f), \quad f \in \mathcal{D}(L_{\max}), \tag{8.5}$$

then

$$\overline{\alpha}(f) = W_a(\overline{g}, f), \quad f \in \mathcal{D}(\overline{L}_{\max}). \tag{8.6}$$

Recall that $\mathcal{B}_a$ and $\mathcal{B}_b$ are equipped with symplectic forms $[\![\cdot|\cdot]\!]_a$ and $[\![\cdot|\cdot]\!]_b$, see (5.13).

Fix $\alpha \in \mathcal{B}_a$ and $\beta \in \mathcal{B}_b$. Consider $L_{\alpha,\beta}$, the realizations of L introduced in Definition 5.11. Recall that it is the restriction of $L_{\max}$ to $\mathcal{D}(L_{\alpha\beta}) = \{f \in \mathcal{D}(L_{\max}) \mid \alpha(f) = \beta(f) = 0\}$.

Proposition 8.3. $L^*_{\alpha\beta} = \overline{L}_{\overline{\alpha}\,\overline{\beta}}$.

Proof. By Proposition 7.9, $L^{\#}_{\alpha\beta} = L_{\alpha\,\beta}$. Clearly, $\overline{L_{\alpha\beta}} = \overline{L}_{\overline{\alpha}\,\overline{\beta}}$. Therefore, the proposition follows from $L^*_{\alpha\beta} = \overline{L^{\#}_{\alpha\,\beta}}$. □

In the following two subsections we will describe boundary conditions that guarantee the dissipativity of $L_{\alpha,\beta}$. We will consider separately two classes of potentials: $V \in L^2_{\mathrm{loc}}]a,b[$ and $V \in L^1]a,b[$.

8.2. **Dissipative boundary conditions for locally square integrable potentials.** Note first the following sesquilinear version of Green's identity (4.6).

Lemma 8.4. *Suppose that* $f, \overline{f}, g \in \mathcal{D}(L_{\max})$. *Then* $\mathrm{Im}(V)f \in L^2]a,b[$ *and*

$$(L_{\max} f|g) - (f|L_{\max} g) = -2\mathrm{i}\int_a^b \mathrm{Im}(V)\overline{f}g + W_b(\overline{f},g) - W_a(\overline{f},g). \tag{8.7}$$

Proof. The left hand side of (8.7) is

$$\begin{aligned}\langle\overline{L_{\max} f}|g\rangle - \langle\overline{f}|L_{\max} g\rangle &= \langle\overline{L_{\max} f}|g\rangle - \langle L_{\max}\overline{f}|g\rangle & (8.8)\\ &+ \langle L_{\max}\overline{f}|g\rangle - \langle\overline{f}|L_{\max} g\rangle. & (8.9)\end{aligned}$$

Then we apply $\overline{L_{\max}} - L_{\max} = -2\mathrm{i}\,\mathrm{Im}(V)$ to (8.8) and Green's identity (4.6) to (8.9). □

For the rest of the argument we need the equality of the domains $\mathcal{D}(\overline{L}_{\max}) = \mathcal{D}(L_{\max})$ which, by Lemma 4.10, is equivalent to $\mathrm{Im}\, V \in L^2_{\mathrm{loc}}]a,b[$. Then we have $\mathcal{B}(L) = \mathcal{B}(\overline{L})$, hence $\alpha \mapsto \overline{\alpha}$ is a conjugation in $\mathcal{B}(L)$ which leaves invariant the subspaces $\mathcal{B}_a(L)$ and $\mathcal{B}_b(L)$. Recall that in (5.13) we equiped $\mathcal{B}_a(L)$ in a symplectic form $[\![\cdot|\cdot]\!]_a$. Note that $[\![\overline{\alpha}|\alpha]\!]_a$ is well defined for any $\alpha \in \mathcal{B}_a(L)$.

Lemma 8.5. *If* $\mathrm{Im}\, V \in L^2_{\mathrm{loc}}]a,b[$ *and* $\alpha \in \mathcal{B}_a$ *then the number* $[\![\overline{\alpha}|\alpha]\!]_a$ *is purely imaginary and*

$$\frac{1}{2\mathrm{i}}[\![\overline{\alpha}|\alpha]\!]_a \geq 0 \iff \frac{1}{2\mathrm{i}}W_a(\overline{f},f) \geq 0\ \forall f \in \mathcal{D}(L_{\max}) \text{ with } \alpha(f) = 0.$$

Proof. Let $g \in \mathcal{D}(L_{\max})$ be a representative of α, so that (8.5) and (8.6) are true. Then

$$[\![\overline{\alpha}|\alpha]\!]_a = W_a(\overline{g},g) = \lim_{c\searrow a}\big(\overline{g}(c)g'(c) - \overline{g}'(c)g(c)\big),$$

which proves that $[\![\overline{\alpha}|\alpha]\!]_a$ is purely imaginary. Now, by the Kodaira identity

$$W_a(\overline{g},g)W_a(\overline{f},f) = |W_a(g,f)|^2 - |W_a(\overline{g},f)|^2.$$

But $\alpha(f) = 0$ means $W_a(g,f) = 0$. Therefore, $[\![(\overline{\alpha}|\alpha]\!]_a W_a(\overline{f},f) \leq 0$. □

Theorem 8.6. *Let* $\alpha \in \mathcal{B}_a$ *and* $\beta \in \mathcal{B}_b$. *If* $\mathrm{Im}\, V \in L^2_{\mathrm{loc}}]a,b[$, *we have*

$$L_{\alpha\beta} \text{ is dissipative } \iff \mathrm{Im}\, V \leq 0,\ \frac{1}{2\mathrm{i}}[\![\overline{\alpha}|\alpha]\!]_a \leq 0, \text{ and } \frac{1}{2\mathrm{i}}[\![\overline{\beta}|\beta]\!]_b \geq 0. \tag{8.10}$$

And then $L_{\alpha\beta}$ *is maximal dissipative.*

Proof. We consider only the case $\alpha \neq 0, \beta \neq 0$. Lemma 8.4 gives

$$\mathrm{Im}(f|L_{\max} f) = \int_a^b \mathrm{Im}(V)|f|^2 + \frac{1}{2\mathrm{i}}W_a(\overline{f},f) - \frac{1}{2\mathrm{i}}W_b(\overline{f},f) \quad \forall f \in \mathcal{D}(L_{\max}) \tag{8.11}$$

and this implies that $L_{\alpha\beta}$ is dissipative if and only if

$$\frac{1}{2\mathrm{i}}W_a(\overline{f},f) - \frac{1}{2\mathrm{i}}W_b(\overline{f},f) \leq \int_a^b \mathrm{Im}(-V)|f|^2 \quad \forall f \in \mathcal{D}(L_{\alpha\beta}). \tag{8.12}$$

If $L_{\alpha\beta}$ is dissipative, by taking $f \in \mathcal{D}(L_{\mathrm{c}})$ in (8.12) we get $\mathrm{Im}(-V) \geq 0$. Then by choosing $f \in \mathcal{D}(L_{\alpha\beta})$ equal to zero near b we get $\frac{1}{2\mathrm{i}}W_a(\overline{f},f) \leq \int_a^b \mathrm{Im}(-V)|f|^2$. If we fix such an f and replace it in this estimate by $f\theta$ where $\theta \in C^\infty(\mathbb{R})$ with $0 \leq \theta \leq 1$ and $\theta(x) = 1$ on a neighborhood of a the we get $\frac{1}{2\mathrm{i}}W_a(\overline{f},f) \leq \int_a^b \mathrm{Im}(-V)|f\theta|^2$. Since the right hand side here can be made as small as we wish by taking θ equal to zero for $x > d > a$ with d close to a, we see that we must have $\frac{1}{2\mathrm{i}}W_a(\overline{f},f) \leq 0$ and this clearly implies the same inequality for any $f \in \mathcal{D}(L_{\alpha\beta})$. Then we get $\frac{1}{2\mathrm{i}}[\![\overline{\alpha}|\alpha]\!]_a \leq 0$ by Lemma 8.5. We similarly prove $\frac{1}{2\mathrm{i}}[\![\overline{\beta}|\beta]\!]_b \geq 0$.

We proved the implication $\Rightarrow$ in (8.10) and $\Leftarrow$ is clear by (8.12). It remains to show the maximal dissipativity assertion. Due to Propositions 8.1 and 8.3 it suffices to prove that the operator $-L_{\alpha\beta}^* = -\overline{L}_{\overline{\alpha}\,\overline{\beta}}$ is dissipative. Observe first that the relation $\mathcal{D}(\overline{L}_{\max}) = \mathcal{D}(L_{\max})$ implies $\mathcal{D}(\overline{L}_{\overline{\alpha}\,\overline{\beta}}) = \mathcal{D}(L_{\overline{\alpha}\,\overline{\beta}})$. Then (8.11) gives

$$\operatorname{Im}(f| - \overline{L}_{\max} f) = \int_a^b \operatorname{Im}(V)|f|^2 - \frac{1}{2\mathrm{i}} W_a(\overline{f}, f) + \frac{1}{2\mathrm{i}} W_b(\overline{f}, f) \quad \forall f \in \mathcal{D}(L_{\max}) \tag{8.13}$$

hence instead of (8.12) we get the condition

$$-\frac{1}{2\mathrm{i}} W_a(\overline{f}, f) + \frac{1}{2\mathrm{i}} W_b(\overline{f}, f) \le \int_a^b \operatorname{Im}(-V)|f|^2 \quad \forall f \in \mathcal{D}(L_{\overline{\alpha}\,\overline{\beta}}).$$

As above we get $\frac{1}{2\mathrm{i}} W_a(\overline{f}, f) \ge 0$ and $\frac{1}{2\mathrm{i}} W_b(\overline{f}, f) \le 0$ for any $f \in \mathcal{D}(L_{\overline{\alpha}\,\overline{\beta}})$. Thus, if $f \in \mathcal{D}(L_{\max})$ and $\overline{\alpha}(f) = 0$ then $\frac{1}{2\mathrm{i}} W_a(\overline{f}, f) \ge 0$ and by Lemma 8.5 this means $\frac{1}{2\mathrm{i}} [\![\alpha|\overline{\alpha}]\!]_a \ge 0$ which is equivalent to $\frac{1}{2\mathrm{i}} [\![\overline{\alpha}|\alpha]\!] \le 0$. Similarly we get $\frac{1}{2\mathrm{i}} [\![\overline{\beta}|\beta]\!]_b \ge 0$ and the last two conditions are satisfied by the assumptions in the right hand side of (8.10). Hence $-L_{\alpha\beta}^*$ is dissipative. □

8.3. **Dissipative regular boundary conditions.** Suppose that the operator L has a regular left endpoint at a. As we noted several times, for regular boundary conditions $\mathcal{B}_a$ can be identified with $\mathbb{C}^2$. Indeed,

$$\alpha(f) = \alpha_0 f'(a) - \alpha_1 f(a),$$

is a general form of a boundary functional, with $\alpha = (\alpha_0, \alpha_1) \in \mathbb{C}^2$ and $f \in \mathcal{D}(L_{\max})$.

The space $\mathcal{B}_a$ is equipped with the symplectic form $[\![\,\cdot\,|\,\cdot\,]\!]_a$, which coincides with the usual (two-dimensional) vector product:

$$[\![\alpha|\beta]\!]_a = \alpha_0\beta_1 - \alpha_1\beta_0 = \alpha \times \beta.$$

Thus, if we write $\vec{f}_a := \big(f(a), f'(a)\big)$, an alternative notation for $\alpha(f)$ is

$$\alpha(f) = \alpha \times \vec{f}_a.$$

Note that there is no guarantee that $\mathcal{D}(L_{\min})$ and $\mathcal{D}(L_{\max})$ are invariant wrt the complex conjugation. However the space $\mathcal{B}_a \simeq \mathbb{C}^2$ is equipped with the obvious complex conjugation:

$$\overline{\alpha}(f) = \overline{\alpha}_0 f'(a) - \overline{\alpha}_1 f(a) = \overline{\alpha} \times \vec{f}_a.$$

Lemma 8.7. *(1) $\alpha \times \beta = 0$ if and only if the vectors α, β are collinear.*
(2) $\overline{\alpha} \times \alpha \in \mathrm{i}\mathbb{R}$ and $\overline{\alpha} \times \alpha = 0$ if and only if α is proportional to a real vector.
(3) $(\overline{\alpha} \times \alpha)(\overline{\beta} \times \beta) = |\alpha \times \beta|^2 - |\overline{\alpha} \times \beta|^2$

Proof. (1): If $\alpha_0\beta_1 = \alpha_1\beta_0$ and $\beta \ne 0$ then $\beta_k = 0 \Rightarrow \alpha_k = 0$ and if $\beta_0 \ne 0 \ne \beta_1$ then $\alpha_0/\beta_0 = \alpha_1/\beta_1$. (2): If $\overline{\alpha} \times \alpha = 0$ we get $\overline{\alpha} = c^2\alpha$ for some complex c with $|c| = 1$ which implies $(c\alpha)^* = c\alpha$. (3) follows by the Kodaira identity. □

Here is a version of Lemma 8.4 for the regular case.

Lemma 8.8. *Let $V \in L^1]a, b[$. Suppose that $f, g \in \mathcal{D}(L_{\max})$. Then*

$$(L_{\max} f|g) - (f|L_{\max} g) = -2\mathrm{i} \int_a^b \operatorname{Im}(V)\overline{f}g + W_b(\overline{f}, g) - W_a(\overline{f}, g). \tag{8.14}$$

Next we have a version of Thm 8.6 for the regular case. Fix *nonzero vectors* α, β and define $L_{\alpha\beta}$ by imposing the boundary conditions at a and b:

$$f(a)\alpha_1 - f'(a)\alpha_0 = 0, \quad f(b)\beta_1 - f'(b)\beta_0 = 0.$$

In this context it is quite easy to prove that $L_{\alpha\beta}^* = \overline{L}_{\overline{\alpha}\,\overline{\beta}}$.

Theorem 8.9. *Suppose that a, b are finite and $V \in L^1]a, b[$. Then*

$$L_{\alpha\beta} \text{ is dissipative } \Leftrightarrow \operatorname{Im} V \le 0, \quad \operatorname{Im}(\overline{\alpha}_0\alpha_1) \le 0, \text{ and } \operatorname{Im}(\overline{\beta}_0\beta_1) \ge 0.$$

And in this case $L_{\alpha\beta}$ is maximal dissipative.

Proof. The proof is similar to that of Theorem 8.6, but much simpler. We use Lemma 8.8 instead of Lemma 8.4 and get the same relation (8.12) as necessary and sufficient condition for dissipativity. Then we use

$$\frac{1}{2\mathrm{i}}[\![\overline{\alpha}|\alpha]\!]_a = \frac{1}{2\mathrm{i}}(\overline{\alpha}_0\alpha_1 - \overline{\alpha}_1\alpha_0) = \mathrm{Im}(\overline{\alpha}_0\alpha_1)$$

and a similar relation for β. Finally, when checking the dissipativity of $-L^*_{\alpha\beta}$, note that this operator is associated to the differential expression $\partial^2 - \overline{V}$, which explains a difference of sign. □

8.4. **Weyl circle in the regular case.** In this subsection we fix a regular operator L whose potential has a negative imaginary part. We study solutions of $(L-\lambda)f = 0$ for $\mathrm{Im}\,\lambda > 0$ with real boundary conditions. In Theorem 8.10 we show that they define a certain circle in the complex plane called the *Weyl circle*. This result will be needed in the next subsection §8.5, where general boundary conditions are studied.

We will use an argument essentially due to H. Weyl in the real case, cf. [5, 20, 21] for example. The Weyl circle for potentials with semi-bounded imaginary part were first treated in [24], see [3] for more recent results.

Let us denote $U = \mathrm{Im}(\lambda - V)$ and

$$(f|g)_U = \int_a^b \overline{f} g U. \tag{8.15}$$

We set $\|f\|_U^2 = (f|f)_U$ and note that if $U \geq 0$, then $(\cdot|\cdot)_U$ is a positive hermitian form and we denote $\|\cdot\|_U$ is the corresponding seminorm. Now if $f, g \in \mathcal{D}(L_{\max})$ and $Lf = \lambda f$, $Lg = \lambda g$ for some complex number λ then (8.7) can be rewritten as

$$2\mathrm{i}(f|g)_U = W_a(\overline{f}, g) - W_b(f, g). \tag{8.16}$$

Theorem 8.10. *Assume that* $\mathrm{Im}\,V \leq 0$ *and* $\mathrm{Im}\,\lambda > 0$. *Let* u, v *be solutions of the equation* $Lf = \lambda f$ *with real boundary condition at* a *and satisfying* $W(v, u) = 1$. *If* w *is a solution of* $Lf = \lambda f$ *with a real boundary condition at* b*, then there is a unique* $m \in \mathbb{C}$ *such that* $w = mu + v$*; this number is on the circle*

$$\int_a^b |mu + v|^2 \,\mathrm{Im}(\lambda - V) = \mathrm{Im}\,m, \tag{8.17}$$

which has

$$\text{center } c = \frac{\mathrm{i}/2 - (u|v)_U}{\|u\|_U^2} = \frac{W_b(\overline{u}, v)}{2\mathrm{i}\|u\|_U^2} \quad \text{and radius } r = \frac{1}{2\|u\|_U^2}. \tag{8.18}$$

Conversely, let m *be a complex number on the circle* (8.17)*, and define* w *by* $w = mu + v$. *Then* w *has a real boundary condition at* b *and* $W(w, u) = 1$.

Proof. From Lemma 8.7 (2) and the reality of the boundary conditions at a we get

$$W_a(\overline{u}, u) = 0, \quad W_a(\overline{v}, v) = 0. \tag{8.19}$$

This implies

$$\|u\|_U^2 = \frac{\mathrm{i}}{2} W_b(\overline{u}, u), \quad \|v\|_U^2 = \frac{\mathrm{i}}{2} W_b(\overline{v}, v), \tag{8.20}$$

due to (8.16). And if w is as in the first part of the theorem then the same argument gives

$$\|w\|_U^2 = \frac{1}{2\mathrm{i}} W_a(\overline{w}, w). \tag{8.21}$$

Since u, v are linearly independent solutions of $Lf = \lambda f$, if w is another solution then we have $w = mu + nv$ for uniquely determined complex numbers m, n. Since $W(v, u) = 1$ we see that $n = 1$.

Now fix $w = mu + v$. Using (8.19) and $W_a(u, v) = -1$, we get

$$W(\overline{w}, w)_a = |m|^2 W_a(\overline{u}, u) + \overline{m} W_a(\overline{u}, v) + m W_a(\overline{v}, u) + W_a(\overline{v}, v) = 2\mathrm{i}\,\mathrm{Im}\,m. \tag{8.22}$$

From (8.21) and (8.22) we get

$$\|w\|_U^2 = \mathrm{Im}\,m. \tag{8.23}$$

From this relation we get

$$\operatorname{Im} m = \|mu + v\|_U^2 = |m|^2\|u\|_U^2 + 2\operatorname{Re}\big(\overline{m}(u|v)_U\big) + \|v\|_U^2 \tag{8.24}$$

and since $\operatorname{Im} m = 2\operatorname{Re}(\overline{m}\,\mathrm{i}/2)$ we may rewrite this as

$$|m|^2\|u\|_U^2 - 2\operatorname{Re}\big(\overline{m}(\mathrm{i}/2 - (u|v)_U)\big) + \|v\|_U^2 = 0. \tag{8.25}$$

Clearly, $\|w\|_U > 0$ hence $\operatorname{Im} m > 0$ by (8.23) so (8.25) may be rewritten

$$|m|^2 - 2\operatorname{Re}\left(\overline{m}\frac{\mathrm{i}/2 - (u|v)_U}{\|u\|_U^2}\right) + \frac{\|v\|_U^2}{\|u\|_U^2} = 0. \tag{8.26}$$

If $c \in \mathbb{C}$ and $d \in \mathbb{R}$ then $|m|^2 - 2\operatorname{Re}(\overline{m}c) + d = |m - c|^2 - (|c|^2 - d)$. Hence there is m such that $|m|^2 - 2\operatorname{Re}(\overline{m}c) + d = 0$ if and only if $d \le |c|^2$, and then $|m|^2 - 2\operatorname{Re}(\overline{m}c) + d = 0$ is the equation of a circle with center c and radius $\sqrt{|c|^2 - d}$. Thus (8.26) is the equation of the circle with

$$\text{center} \quad c = \frac{\mathrm{i}/2 - (u|v)_U}{\|u\|_U^2} \quad \text{and square of radius} \quad r^2 = \frac{|\mathrm{i}/2 - (u|v)_U|^2 - \|u\|_U^2\|v\|_U^2}{\|u\|_U^4}.$$

From (8.16) we get $2\mathrm{i}(u|v)_U = W_a(\overline{u}, v) - W_b(\overline{u}, v) = -1 - W_b(\overline{u}, v)$, hence $\mathrm{i}/2 - (u|v)_U = W_b(\overline{u}, v)/2\mathrm{i}$. Then (8.20) implies

$$\|u\|_U^2\|v\|_U^2 = -\frac{1}{4}W_b(\overline{u}, u)W_b(\overline{v}, v),$$

hence

$$|\mathrm{i}/2 - (u|v)_U|^2 - \|u\|_U^2\|v\|_U^2 = \big(|W_b(\overline{u}, v)|^2 + W_b(\overline{u}, u)W_b(\overline{v}, v)\big)/4.$$

But by the Kodaira identity $W_b(\overline{u}, u)W_b(\overline{v}, v) = 1 - |W_b(\overline{u}, v)|^2$, hence we get

$$|\mathrm{i}/2 - (u|v)_U|^2 - \|u\|_U^2\|v\|_U^2 = 1/4$$

so (8.26) is just the circle described by (8.18).

To prove the reciprocal part of the theorem, consider a point m on this circle and let $w = mu + v$. Clearly $Lw = \lambda w$ and $W(w, u) = 1$ and the computation (8.22) gives us $W_a(\overline{w}, w) = 2\mathrm{i}\operatorname{Im} m$. We also have (8.24) because this just says that m is on the circle (8.18). Thus we have

$$\|w\|_U^2 = \operatorname{Im} m = W_a(\overline{w}, w)/2\mathrm{i},$$

and then (8.16) implies $W_b(\overline{w}, w) = 0$. Therefore, by Lemma 8.16 w has a real boundary condition at b. This proves the final assertion of the theorem. □

8.5. **Limit point/circle.** In this section we again assume that $\operatorname{Im} V \le 0$ and $\operatorname{Im}\lambda > 0$. We allow b to be an irregular endpoint. We also assume that a is a regular endpoint. Thus we assume that $V \in L^1_{\mathrm{loc}}[a, b[$. This class of potentials has first been considered in [24]; see [3] for more general conditions.

Using Theorem 8.10, we will obtain a classification of the properties of L around b into three categories. This classification can be called the *Weyl trichotomy*. It replaces the *Weyl dichotomy*, well known classification of irregular endpoints for real potentials.

Note that this classifiction depends only on the behaviour of V close to b. In particular, the assumption of regularity of a is made only for convenience. If a is also irregular, then the analysis should be done separately on intervals $]a, a_1]$ and $[b_1, b[$.

Let u, v be solutions of $Lf = \lambda f$ on $]a, b[$ with real boundary conditions at a and such that $W(v, u) = 1$.

Definition 8.11. *For any $d \in]a,b[$ we define*

$$\text{\textit{the} Weyl circle} \quad \mathscr{C}_d := \Big\{ m \in \mathbb{C} \mid \int_a^d |mu+v|^2 \operatorname{Im}(\lambda - V) = \operatorname{Im} m \Big\},$$

$$\text{\textit{the} open Weyl disk} \quad \mathscr{C}_d^\circ := \Big\{ m \in \mathbb{C} \mid \int_a^d |mu+v|^2 \operatorname{Im}(\lambda - V) < \operatorname{Im} m \Big\},$$

$$\text{\textit{the} closed Weyl disk} \quad \mathscr{C}_d^\bullet := \Big\{ m \in \mathbb{C} \mid \int_a^d |mu+v|^2 \operatorname{Im}(\lambda - V) \leq \operatorname{Im} m \Big\} = \mathscr{C}_d^\circ \cup \mathscr{C}_d.$$

Thus the Weyl circle is given by the condition (8.17) with b replaced by d. Since the left hand side of (8.17) growth like $|m|^2$ when $m \to \infty$, it follows that $\mathscr{C}_d^\circ$ is inside $\mathscr{C}_d$. If $d_1 < d_2$ then

$$\int_a^{d_2} |mu+v|^2 \operatorname{Im}(\lambda - V) \leq \operatorname{Im} m \Rightarrow \int_a^{d_1} |mu+v|^2 \operatorname{Im}(\lambda - V) < \operatorname{Im} m.$$

Hence $\mathscr{C}_{d_2}^\bullet \subset \mathscr{C}_{d_1}^\circ$ strictly if $d_1 < d_2 < b$.

Definition 8.12. *We set*

$$\mathscr{C}_b^\bullet := \bigcap_{d<b} \mathscr{C}_d^\bullet,$$
$$\mathscr{C}_b := \text{the boundary of } \mathscr{C}_b^\bullet.$$

It follows that either $\mathscr{C}_b^\bullet = \mathscr{C}_b$ is a point, or $\mathscr{C}_b^\bullet$ is a disk and $\mathscr{C}_b$ is a circle of radius > 0.

Definition 8.13. *We say that b is* limit point *if $\mathscr{C}_b$ is a point. We say that b is* limit circle *if $\mathscr{C}_b$ is a circle of a positive radius.*

Lemma 8.14. *Let $m \in \mathscr{C}_b^\bullet$. Then*

$$\int_a^b |w|^2 \operatorname{Im}(\lambda - V) \leq \operatorname{Im}(m). \tag{8.27}$$

If b is limit point then $\int_a^b |u|^2 \operatorname{Im}(\lambda - V) = \infty$.

Proof. For any $d \in]a,b[$, we have $\mathscr{C}_b^\bullet \subset \mathscr{C}_d^\bullet$. Therefore,

$$\int_a^d |w|^2 \operatorname{Im}(\lambda - V) \leq \operatorname{Im}(m). \tag{8.28}$$

Then we take the limit $d \nearrow b$. If b is limit point then the radius of the Weyl circle $\mathscr{C}_d$ tends to zero as $d \to b$ hence $\lim_{d \to b} \int_a^d |u|^2 \operatorname{Im}(\lambda - V) = \infty$ by the last relation in (8.18). □

The above lemma implies immediately the following theorem:

Theorem 8.15. *If b is limit circle, then all solutions of $(L - \lambda)f - 0$ satisfy*

$$\int_a^b |w|^2 \operatorname{Im}(\lambda - V) \quad \textit{is bounded.} \tag{8.29}$$

If b is limit point, then there exists only one (modulo a complex factor) solution of $(L - \lambda)f = 0$ satisfying (8.29).

Note that $\operatorname{Im}(\lambda - V) \geq \operatorname{Im}\lambda > 0$. Therefore, (8.29) implies the square integrability of w.

Thus, for potentials with a negative imaginary part instead of Weyl's dichotomy we have three possibilities for solutions of $(L - \lambda)f = 0$ (we consider solutions modulo a complex factor):

(1) limit point case, only one solution satisfies (8.29), only one solution is square integrable;
(2) limit point case, only one solution satisfies (8.29), all solutions are square integrable;
(3) limit circle, all solutions satisfy (8.29), and hence all solutions are square integrable.

If V is real, then the case (2) is absent and we have the usual Weyl's dichotomy. Then L is limit point at b iff for any λ there is at most one solution of $Lf = \lambda f$ which is square integrable near b. But this is not the case if V is complex.

We emphasize that *the limit point/circle terminology is interpreted here in the geometric sense described above* (based on Theorem 8.10).

There exist examples of (2) in the literature. *In the limit point case, it is possible that we have only one nonzero solution satisfying* (8.29)*, whereas all solutions are square integrable with respect to the Lebesgue measure.* Indeed, Sims [24, p. 257] has shown that this happens in simple examples like $V(x) = x^6 - 3\mathrm{i}x^2/2$ on $]1,\infty[$. See also the discussion in [3].

Remark 8.16. *We also note that if V is real then for any non-real λ there is at least one nonzero solution of $Lf = \lambda f$ which is square integrable near b. But it does not seem to be known whether for arbitrary complex V there is λ such that $Lf = \lambda f$ has a nonzero solution which is square integrable near b.*

Appendix A. Symplectic spaces

Let $\mathcal{V}$ be a vector space. A bilinear form $[\![\cdot|\cdot]\!]$ on $\mathcal{V}$ is called *symplectic* if it is antisymmetric and nondegenerate, i.e. $[\![\phi|\psi]\!] = -[\![\phi|\psi]\!]$ and for any $\phi \in \mathcal{V}$ there exists $\psi \in \mathcal{V}$ such that $[\![\phi|\psi]\!] \neq 0$. For a subspace $\mathcal{W}$ in $\mathcal{V}$ we define its *symplectic orthogonal complement*

$$\mathcal{W}^{\mathrm{s}\perp} := \{\phi \mid [\![\phi|\psi]\!] = 0, \quad \psi \in \mathcal{W}\}.$$

$\mathcal{W}$ is called *isotropic* if $\mathcal{W} \subset \mathcal{W}^{\mathrm{s}\perp}$ and Lagrangian if $\mathcal{W} = \mathcal{W}^{\mathrm{s}\perp}$.

The following proposition is well-known and easy to prove. Perhaps the only nontrivial point is (4) for infinite-dimensional $\mathcal{V}$, where the usual induction argument needs to use the Zorn Lemma.

Proposition A.1.

(1) If $\mathcal{V}$ is a symplectic space, then $\dim \mathcal{V}$ *is even or infinite.*
(2) If $\mathcal{W}$ is a subspace of $\mathcal{V}$, then $\dim \mathcal{W} = \dim \mathcal{V}/\mathcal{W}^{\mathrm{s}\perp}$.
(3) If $\mathcal{W}$ is a Lagrangian subspace, then $\dim \mathcal{W} = \frac{1}{2}\dim \mathcal{V}$.
(4) There exist Lagrangian subspaces in $\mathcal{V}$.

Assume in addition that $\mathcal{V}$ is a Banach space with norm $\|\cdot\|$. We say that the symplectic form is continuous if

$$|[\![\phi|\psi]\!]| \leq c\|\phi\|\|\psi\|. \tag{A.1}$$

Proposition A.2. *If $\mathcal{V}$ is a Banach space and the symplectic form is continuous, then:*

(1) If $\mathcal{W}$ is a subspace of $\mathcal{V}$, then $\mathcal{W}^{\mathrm{s}\perp}$ is closed.
(2) Every Lagrangian subspace of $\mathcal{V}$ is closed.

Proof. (1) is obvious. It implies (2). □

Let $\mathcal{V}'$ denote the dual space of $\mathcal{V}$. We have the map

$$\mathcal{V} \ni v \mapsto v' := [\![v|\cdot]\!] \in \mathcal{V}'. \tag{A.2}$$

If $\dim \mathcal{V}$ is finite, then this is an isomorphism. $\mathcal{V}'$ is then equipped with a symplectic form

$$[\![v'|w']\!] := [\![v|w]\!]. \tag{A.3}$$

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