ON 1-DIMENSIONAL SCHRÖDINGER OPERATORS WITH COMPLEX POTENTIALS

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Some time ago together with Vladimir we decided to write a review about 1-dimensional Schrödinger operators

$$L = -\partial_x^2 + V(x)$$

on $L^2]a,b[$.

We wanted to answer rather basic and classical questions:

How to describe closed realizations $L_\bullet$ of the formal operator L?

How to compute their resolvents $(L_\bullet - \lambda)^{-1}$ or Green's operators?

We wanted to be as general as possible:

- a can be $-\infty$, b can be $+\infty$.
- V can be complex.
- V can be very singular
- V can have an arbitrary behavior close to the endpoints.

Our main motivation were exactly solvable Hamiltonians such as

$$-\partial_x^2 + \Big(\alpha - \frac{1}{4}\Big)\frac{1}{x^2} - \frac{\beta}{x},$$

on $L^2(\mathbb{R}_+)$ or $L^2(\mathbb{R})$. In exactly solvable Hamiltonians complex potentials appear naturally. Moreover, their potentials are often singular, especially at the endpoints, but also in the midle of the domain. Recently, I studied such problems together with Serge Richard and Jeremy Faupin. We thought it would be nice to have a paper describing the general framework.

Of course, 1-dimensional Schrödinger operators have a huge literature. Many of my and Vladimir's discoveries turned out to be rediscoveries. This does not mean they were easy or not interesting.

Most textbooks assume that V is real. It is also convenient to suppose that $V \in L^2_{\mathrm{loc}}$. Denote the closure of L restricted to $C_{\mathrm{c}}^\infty\big(]a,b[\big)$ by $L_{\min}$. Then $L_{\min}$ is a Hermitian operator (commonly called symmetric). This means $L_{\min} \subset L_{\max} := L_{\min}^*$. One is mostly interested in self-adjoint extensions $L_\bullet$ of L. They satisfy

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

and $L_\bullet^* = L_\bullet$.

There exists a well-known abstract theory going back to von Neumann about self-adjoint extensions. One defines the deficiency spaces and indices

$$\mathcal{N}_\pm := \mathcal{N}(L_{\max} \mp \mathrm{i}), \quad d_\pm := \dim \mathcal{N}_\pm.$$

$L_{\min}$ possesses self-adjoint extensions iff $d_+ = d_-$. Self-adjoint extensions of $L_{\min}$ are parametrized by maximal subspaces of $\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) \simeq \mathcal{N}_+ \oplus \mathcal{N}_-$ on which the anti-Hermitian form

$$(L_{\max} f|g) - (f|L_{\max} g)$$

is zero.

For Schrödinger operators $\overline{\mathcal{N}_+} = \mathcal{N}_-$, hence $d_+ = d_-$ and self-adjoint extensions exist. In one dimension we have 3 possibilities: $d_+ = d_- = 0, 1, 2$. More precisely, we can naturally split the boundary space

$$\mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}) \simeq \mathcal{G}_a \oplus \mathcal{G}_b$$

where $\mathcal{G}_a$ describes the boundary condition at a and $\mathcal{G}_b$ describes the boundary conditions at b.

Let us describe the classic theory of regular boundary coditions. For simplicity we assume that $\mathcal{G}_b = \{0\}$. Suppose that $V \in L^1$ in a neighborhood of a. Then one can show that for $f \in \mathcal{D}(L_{\max})$ the values $f(a)$ and $f'(a)$ are well-defined continuous functionals on $\mathcal{G}_a$. Self-adjoint extensions are L_μ with $\mu \in \mathbb{R} \cup \{\infty\}$ and

$$\mathcal{D}(L_\mu) := \{f \in \mathcal{D}(L_{\max}) \mid f'(a) = \mu f(a)\}.$$

This was essentially known to Sturm and Liouville.

Now assume that V is complex. We define $L_{\max}$ as the operator $-\partial_x^2+V(x)$ (appropriately understood—more about this later) on

$$\mathcal{D}(L_{\max}) := \{f \in L^2]a,b[\mid (-\partial_x^2 + V(x))f \in L^2]a,b[\}.$$

Then we define $L_{\min}$ to be the closure of $L_{\max}$ restricted to functions compactly supported in $]a,b[$. We are looking for closed operators $L_\bullet$ such that

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

The most interesting are those that have a nonempty resolvent set. Such operators are sometimes called well-posed (see e.g. Edmunds-Evans).

What is a natural condition for V? If we want that V is a densely defined closable operator, then we need to assume that $V \in L^2_{\rm loc}$. This is however much too restrictive.

Let AC denote the space of absolutely continuous functions. More precisely, $f \in AC]a,b[$ iff $f' \in L^1_{\rm loc}]a,b[$. Similarly, $f \in AC^1]a,b[$ iff $f'' \in L^1_{\rm loc}]a,b[$.

A natural class of potentials (considered often in the literature) is $V \in L^1_{\mathrm{loc}}$. If $f \in AC^1$, then both $-\partial_x^2 f$ and Vf are well defined as elements of L^1_{loc}. We can define

$$\mathcal{D}(L_{\max}) := \{f \in AC^1 \cap L^2 \mid (-\partial_x^2 + V(x))f \in L^2\}.$$

We can rewrite

$$(-\partial_x^2 + V(x) - \lambda)f = g \qquad (*)$$

as a first order equation with L^1_{loc} coefficients:

$$\partial_x \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ V - \lambda & 0 \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} + \begin{bmatrix} 0 \\ g \end{bmatrix}.$$

One can do much better. As noticed by Savchuk-Shkalikov, one can assume that $V = G'$ where $G \in L^2_{\mathrm{loc}}$. Indeed, formally

$$-\partial_x^2 + G'(x) = -\partial_x(\partial_x - G) - G(\partial_x - G) - G^2.$$

We can again rewrite $(*)$ as as a first order equation with L^1_{loc} coefficients:

$$\partial_x \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} G & 1 \\ G^2-\lambda & -G \end{bmatrix} \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} + \begin{bmatrix} 0 \\ g \end{bmatrix}.$$

Clearly, if V is complex, then $L_{\min}$ is not Hermitian, so the theory of self-adjoint extensions does not apply. But there is a different theory.

$L^2]a,b[$ is equipped with a natural conjugation and a bilinear product

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

If A is bounded, we say that $A^{\#}$ is the transpose of A (J-conjugate of A) if

$$\langle f|Ag\rangle = \langle A^{\#}f|g\rangle.$$

Let A have dense domain $\mathcal{D}(A)$. We say that $f \in \mathcal{D}(A^{\#})$ if there exists h such that

$$\langle f|Ag\rangle = \langle h|g\rangle, \quad g \in \mathcal{D}(A),$$

and then $A^{\#}f := h$. We say that A is symmetric (J-symmetric) if $A \subset A^{\#}$ and self-transposed if $A = A^{\#}$ (J-self-adjoint).

Note that $\sigma(A) = \sigma(A^{\#})$. Besides

$$\left((z-A)^{-1}\right)^{\#} = (z-A^{\#})^{-1}, \quad (\mathrm{e}^{\mathrm{i}tA})^{\#} = \mathrm{e}^{\mathrm{i}tA^{\#}}.$$

(Not true for Hermitian conjugation!).

Let $L_{\min} \subset L_{\min}^{\#} =: L_{\max}$.

Theorem. There always exist a self-transposed $L_\bullet$ such that

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

Proof.

$$[\![f|g]\!] := \langle L_{\max} f|g\rangle - \langle f|L_{\max} g\rangle$$

defines a continuous symplectic form on the boundary space

$$\mathcal{G} := \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min}).$$

Lagrangian subspaces correspond to self-transposed extensions. Lagrangian subspaces alway exist.

Theorem. Suppose that $L_\bullet$ satisfies

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

If $L_\bullet$ is well-posed or self-transposed, then

$$\dim \mathcal{D}(L_\bullet)/\mathcal{D}(L_{\min}) = \dim \mathcal{D}(L_{\max})/\mathcal{D}(L_\bullet).$$

Consider again $-\partial_x^2 + V(x)$ and the corresponding $L_{\min}, L_{\max}$. We have $L_{\min} \subset L_{\min}^{\#} = L_{\max}$. The boundary space

$$\mathcal{G} := \mathcal{D}(L_{\max})/\mathcal{D}(L_{\min})$$

naturally splits in two subspaces $\mathcal{G} = \mathcal{G}_a \oplus \mathcal{G}_b$. In order to describe $\mathcal{G}_a$ and $\mathcal{G}_b$, for $\lambda \in \mathbb{C}$ we define

$$\mathcal{U}_a(\lambda) := \{f \mid (L-\lambda)f = 0,\ f \text{ square integrable around } \ a\}.$$

Similarly we define $\mathcal{U}_b(\lambda)$.

Theorem. $\dim \mathcal{G}_a = 0$ or 2.

1) The following are equivalent:

a) $\dim \mathcal{G}_a = 2$.

b) $\dim \mathcal{U}_a(\lambda) = 2$ for all $\lambda \in \mathbb{C}$.

c) $\dim \mathcal{U}_a(\lambda) = 2$ for some $\lambda \in \mathbb{C}$.

2) The following are equivalent:

a) $\dim \mathcal{G}_a = 0$.

b) $\dim \mathcal{U}_a(\lambda) \leq 1$ for all $\lambda \in \mathbb{C}$.

c) $\dim \mathcal{U}_a(\lambda) \leq 1$ for some $\lambda \in \mathbb{C}$.

If V is real then the above theorem is well-known and easy. $\dim \mathcal{G}_a = 2$ goes under the name of the limit circle case and $\dim \mathcal{G}_a = 0$ goes under the name of the limit point case. (These names are no longer justified if V is complex).

If V is real, we know much more in the limit point case: The following are equivalent:

a) $\dim \mathcal{G}_a = 0$.

b) $\dim \mathcal{U}_a(\lambda) = 1$ for $\lambda \in \mathbb{C} \backslash \mathbb{R}$ and $\dim \mathcal{U}_a(\lambda) \leq 1$ for $\lambda \in \mathbb{R}$.

The usual proof for the real case does not generalize to the complex case. The main idea for the proof in the complex case is to reduce the problem to a system of 4 1st order ODE's and to use the following result due to Atkinson:

Theorem. 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

$$J\partial_x \phi(x) = \lambda A(x)\phi(x) + B(x)\phi(x) \qquad (\mathbf{a})$$

satisfy

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

then for all $\lambda \in \mathbb{C}$ all solutions of (a) satisfy (b).

Consider the Bessel operator given by the formal expression

$$L_\alpha = -\partial_x^2 + \big(-\frac{1}{4} + \alpha \big) \frac{1}{x^2}.$$

We will see that it is often natural to write $\alpha = m^2$

Theorem 0.0.1. .

1. *For* $1 \leq \operatorname{Re} m$, $L_{m^2}^{\min} = L_{m^2}^{\max}$.
2. *For* $-1 < \operatorname{Re} m < 1$, $L_{m^2}^{\min} \subsetneq L_{m^2}^{\max}$, *and the codimension of their domains is* 2.
3. $(L_\alpha^{\min})^* = L_{\overline{\alpha}}^{\max}$. *Hence, for* $\alpha \in \mathbb{R}$, $L_\alpha^{\min}$ *is Hermitian.*
4. $L_\alpha^{\min}$ *and* $L_\alpha^{\max}$ *are homogeneous of degree* -2.

Notice that

$$Lx^{\frac12 \pm m} = 0.$$

Let ξ be a compactly supported cutoff equal 1 around 0.

Let $-1 < \operatorname{Re} m$. Note that $x^{\frac12 + m}\xi$ belongs to $\operatorname{Dom} L_{m^2}^{\max}$.

This suggests to define the operator H_m to be the restriction of $L_{m^2}^{\max}$ to

$$\operatorname{Dom} L_{m^2}^{\min} + \mathbb{C} x^{\frac12 + m}\xi.$$

Theorem 0.0.2. .

1. *For* $1 \leq \operatorname{Re} m$, $L_{m^2}^{\min} = H_m = L_{m^2}^{\max}$.
2. *For* $-1 < \operatorname{Re} m < 1$, $L_{m^2}^{\min} \subsetneq H_m \subsetneq L_{m^2}^{\max}$ *and the codimension of the domains is* 1.
3. $H_m^* = H_{\overline{m}}$. *Hence, for* $m \in]-1, \infty[$, H_m *is self-adjoint.*
4. H_m *is homogeneous of degree* -2.
5. $\sigma(H_m) = [0, \infty[$.
6. $\{\operatorname{Re} m > -1\} \ni m \mapsto H_m$ *is a holomorphic family of closed operators.*

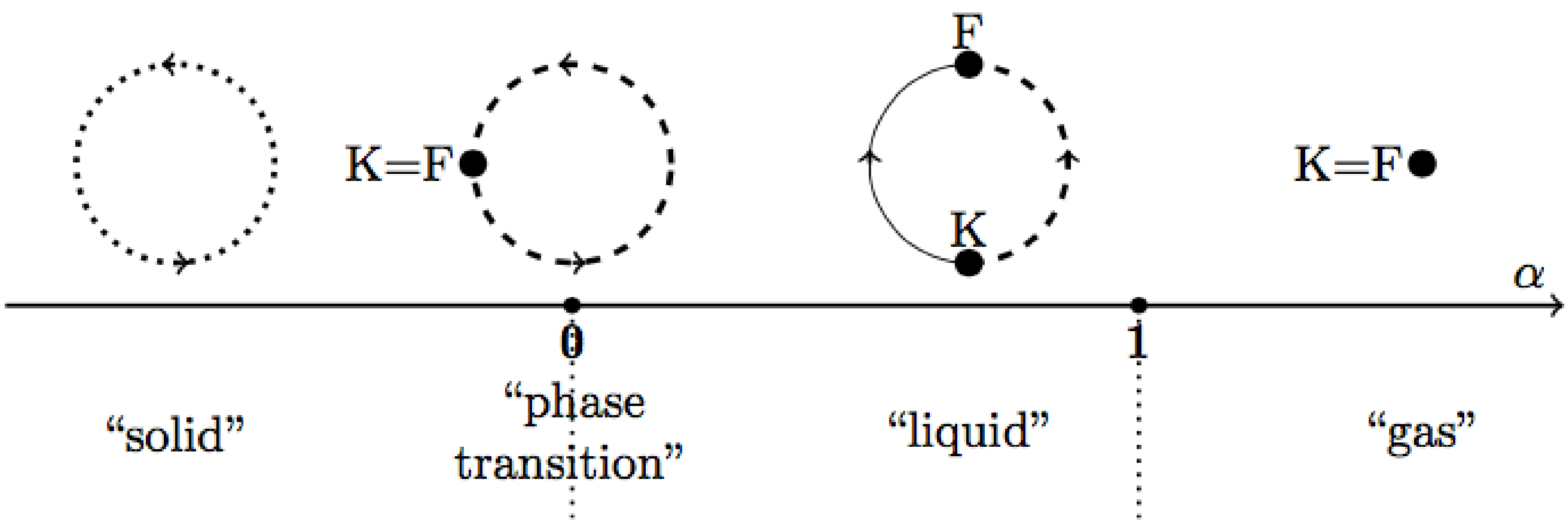
Theorem 0.0.3. .

1. *For* $\alpha \geq 1$, $L_\alpha^{\min} = H_{\sqrt{\alpha}}$ *is essentially self-adjoint on* $C_c^\infty]0,\infty[$.
2. *For* $\alpha < 1$, $L_\alpha^{\min}$ *is not essentially self-adjoint on* $C_c^\infty]0,\infty[$.
3. *For* $0 \leq \alpha < 1$, *the operator* $H_{\sqrt{\alpha}}$ *is the Friedrichs extension and* $H_{-\sqrt{\alpha}}$ *is the Krein extension of* $L_\alpha^{\min}$.
4. $H_{\frac{1}{2}}$ *is the Dirichlet Laplacian and* $H_{-\frac{1}{2}}$ *is the Neumann Laplacian on halfline.*
5. *For* $\alpha < 0$, $L_\alpha^{\min}$ *has no homogeneous selfadjoint extensions.*

Self-adjoint extensions of the Hermitian operator

$$L_\alpha = -\partial_x^2 + \Big(-\frac{1}{4} + \alpha \Big) \frac{1}{x^2}.$$

K—Krein, F—Friedrichs, dashed line—single bound state, dotted line—infinite sequence of bound states.



Consider now the Whittaker operator given by the formal expression

$$L_{\beta,\alpha} := -\partial_x^2 + \Big(\alpha - \frac{1}{4}\Big)\frac{1}{x^2} - \frac{\beta}{x},$$

where the parameters β, α are complex numbers. It is natural to write $\alpha = m^2$.

For any $m \in \mathbb{C}$ with $\mathrm{Re}(m) > -1$ we introduce the closed operator $H_{\beta,m}$ that equals L_{β,m^2} on functions that behave as

$$x^{\frac{1}{2}+m}\left(1 - \frac{\beta}{1+2m}x\right)$$

near zero. We obtain a family

$$\mathbb{C} \times \{m \in \mathbb{C} \mid \mathrm{Re}(m) > -1\} \ni (\beta, m) \mapsto H_{\beta,m},$$

which is holomorphic except for a singularity at $(0, -\frac{1}{2})$.

The singularity at $(\beta, m) = (0, -\frac{1}{2})$ is quite curious: it is invisible when we consider just the variable m. In fact,

$$m \mapsto H_m = H_{0,m}$$

is holomorphic around $m = -\frac{1}{2}$, and $H_{-\frac{1}{2}}$ has the Neumann boundary condition. It is also holomorphic around $m = \frac{1}{2}$, and $H_{\frac{1}{2}}$ has the Dirichlet boundary condition. Thus one has

$$H_{0,-\frac{1}{2}} \neq H_{0,\frac{1}{2}}.$$

If we introduce the Coulomb potential, then

$$\text{whenever } \beta \neq 0, \quad H_{\beta,-\frac{1}{2}} = H_{\beta,\frac{1}{2}}.$$

The function

$$(\beta, m) \mapsto H_{\beta,m} \qquad (*)$$

is holomorphic around $(0, \frac{1}{2})$, in particular,

$$\lim_{\beta \to 0} (\mathbb{1} + H_{\beta,\frac{1}{2}})^{-1} = (\mathbb{1} + H_{0,\frac{1}{2}})^{-1}.$$

But $\lim\limits_{\beta \to 0} (\mathbb{1} + H_{\beta,-\frac{1}{2}})^{-1} = (\mathbb{1} + H_{0,\frac{1}{2}})^{-1} \neq (\mathbb{1} + H_{0,-\frac{1}{2}})^{-1}$. Thus $(*)$ is not even continuous near $(0, -\frac{1}{2})$.