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FACULTY OF SCIENCES

MATHEMATICS DEPARTMENT

On the one-dimensional Schrödinger operator with singular perturbations

EDISON JAIR LEGUIZAMON QUINCHE

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Thesis Advisor:

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Contents

INTRODUCTION

The Schrödinger equation is the basic equation in quantum theory. The study of this equation plays an exceptional role in modern physics. From a mathematician's point of view the Schrödinger equation is as inexhaustible as mathematics itself. The time-independent equation of a one-dimensional non-relativistic particle is given by

$$\left(-\frac{h}{2\mu}\frac{d^2}{dx^2} + q(x)\right) f = Ef$$

where h is the Planck constant and μ is the reduced mass of the particle, E is the energy of the state and $q(x)$ the potential. f is known as the *wave function*. When the potential q is regular (that is $q \in L^1_{loc}(\mathbb{R})$) the equation is mathematically well-defined. For instance, when $q = 0$, it is well known (see [AE04]) that the operator

$$Hf := -\frac{d^2}{dx^2} f; \quad D(H) := W_2^2(\mathbb{R}),$$

is self-adjoint, positive and its spectrum is $\sigma(H) = \sigma_{\text{ess}}[0, \infty)$.

Singular potentials have been studied for years. They provide important solvable models with a wide variety of applications in atomic physics, such as the Lieb-Liniger model for a one dimensional gas of bosons interacting by means of a δ potential (see [LL63] and [Lie63]). For other applications see e.g., [Exn95] and [Kun99].

The δ and δ' potentials have been studied by S. Albeverio and Exner in [AE04] using the von Neumann theory of self-adjoint extensions of symmetric operators. They find that the differential expressions

$$-\frac{d^2}{dx^2} + \alpha\delta(x) \quad \text{and} \quad -\frac{d^2}{dx^2} + \alpha\delta'(x), \qquad \text{with } \alpha \in \mathbb{R}, \tag{1}$$

can be defined as self-adjoint operators

$$T_\alpha f := -\frac{d^2}{dx^2} f; \quad D(T_\alpha) := \left\{x \in W_2^2(\mathbb{R} - \{0\}) : f'(0+) - f'(0-) = \alpha f(0)\right\},$$
$$T'_\alpha f := -\frac{d^2}{dx^2} f; \quad D(T'_\alpha) := \left\{x \in W_2^2(\mathbb{R} - \{0\}) : f(0+) - f(0-) = \alpha f'(0)\right\}.$$

Moreover they find that the spectrum of T_α and T'_α has one negative eigenvalue when $\alpha < 0$. They prove that T_α and T'_α have the same essential spectrum as H. The effect of the δ and δ' perturbations is that a negative eigenvalue may appear.

In [Kur96], Kurasov works with singular potentials based on an alternative theory of distributions defined on spaces of discontinuous test functions. Both Kurasov and Albeverio and Exner define rigorously the differential expressions (1).

Based on these two previous research works the following questions emerge: Suppose $q(x)$ is a regular potential and let $\{x_k\}_{k=1}^n \subset \mathbb{R}$.

(Q1) Can the differential expressions

$$-\frac{d^2}{dx^2} + q(x) + \sum_{k=1}^{n} \alpha_i \delta(x - x_k), \quad \text{and} \quad -\frac{d^2}{dx^2} + q(x) + \sum_{k=1}^{n} \alpha_i \delta'(x - x_k), \tag{2}$$

be defined as self-adjoint operators? If so, what can be said about their spectra?

(Q2) Can singular potentials be defined rigorously using the classical distribution theory?

Recent works such [AN03a],[AN03b] and [GO10], by Albeverio, Nizhnik, Goloschapova and Oridoroga reveal that the differential expression

$$-\frac{d^2}{dx^2} + \sum_{k=1}^{n} \alpha_k \delta(x - x_k)$$

can be defined rigorously as a self-adjoint operator such that the positive spectrum coincides with the spectrum of H and the negative spectrum are only eigenvalues of finite multiplicity with at most n negative eigenvalues. Also M. Calcada, T. Lunardi, A. Manzoni, and W. Monteiro in [CLMM14] give a distributional approach to the expressions above using physical principles. In [SW16], V. Strauss and M. Winklmeier prove that the differential expressions

$$-\frac{d^2}{dx^2} + x^2 + \alpha\delta(x); \quad -\frac{d^2}{dx^2} + x^2 + \alpha\delta'(x),$$

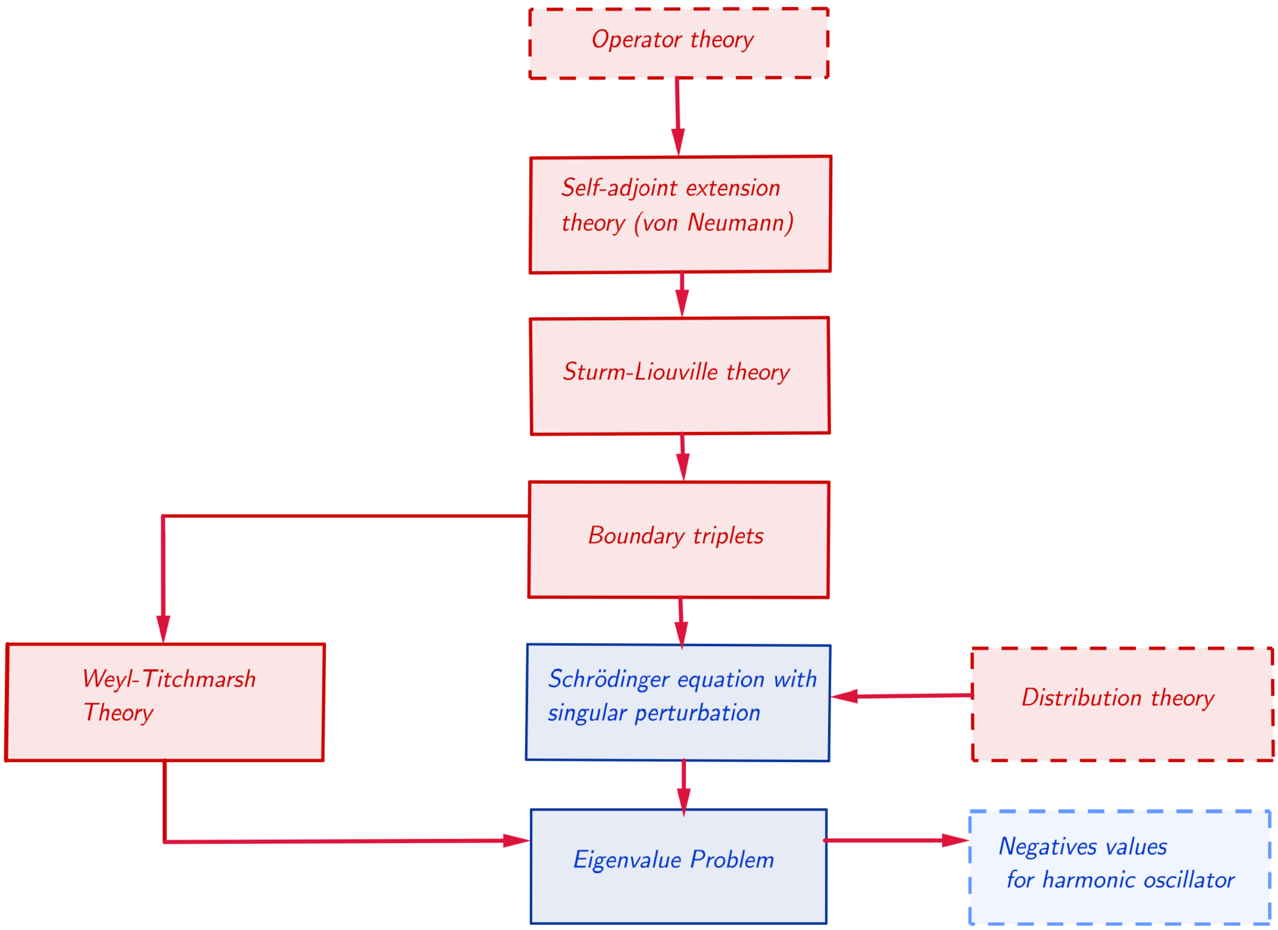
can be interpreted as self-adjoint operators such that the spectrum are only eigenvalues of finite multiplicity with at most one negative eigenvalue that exists when α is less than a negative constant.

In this document we will answer the questions (Q1) and (Q2) for continuous potentials q which are bounded from below and satisfy $q(x) \to \infty$ when $|x| \to \infty$. Moreover we give a meaning to (2) as self-adjoint operators with purely discrete spectrum using the self-adjoint extensions theory, boundary triplets and Sturm-Liouville theory. We will show that for potentials $q \geq 0$ the number of negative eigenvalues is the same as that of a Hermitian matrix using the method used in [GO10] for the case $q = 0$. For the case of the harmonic oscillator (i.e. $q(x) = x^2$) we find an algorithm for the number of negative eigenvalues in terms of the strength of the interactions α_i and the solutions of the differential equation $-y'' + x^2 y = 0$. Also we find an upper bound for the strength of the interaction α_i that works as a sufficient condition for the number of negative eigenvalues to be equal to the number of point interactions. We analyze the behavior of the bounds in terms of the interactions and for the harmonic oscillator case we find that if the interactions are near to $\pm\infty$, then the first or the last interactions must be less than some negative value in order to generate a negative eigenvalue.

In Theorem [GO10, Theorem 3.7] we show that the negative eigenvalues of the Schrödinger operator with singular perturbations are given as the negative eigenvalues of a certain associated matrix. In Theorem [GO10, Theorem 3.8] we associate a recursively defined sequence determined by the strengths α_i and the distances between the point interactions to the operator; the number of negative terms of this sequence is equal to the number of its negative eigenvalues.

For the case $q = 0$ we made two programs in Python to calculate the number of negative eigenvalues of the perturbed operator. The first program uses Theorem [GO10, Theorem 3.7] to compute the eigenvalues of the perturbed operator T_α by computing the eigenvalues of the associated matrix. The second program calculates the terms of the sequence defined in Theorem [GO10, Theorem 3.8] and counts the number of its negative terms.

The computational time of the second program grows linearly with respect to the number of perturbations n and is less than the computational time of the first one. On the other hand, the first program lets us conclude that the condition given in [GO10, Theorem 3.3] is necessary when the number of perturbations tends to infinity.


Operator theory
Self-adjoint extension theory (von Neumann)
Sturm-Liouville theory
Boundary triplets
Weyl-Titchmarsh Theory
Schrödinger equation with singular perturbation
Distribution theory
Eigenvalue Problem
Negatives values for harmonic oscillator

1 PRELIMINARIES

1.1 Basic notions of operator theory

We start with some basic definitions of functional analysis and operator theory. Let H be a Hilbert space. We denote an operator defined on a subspace of H by $T(H \to H)$ and we write $D(T)$, $\text{Ran}(T)$, $\text{Ker}(T)$ for the domain of T, range of T and kernel of T respectively.

Definition 1.1. Let H be a complex Hilbert space and $T : D(T) \subset H \to H$ a closed densely defined linear operator . We define the *resolvent set* and the *spectrum* of the operator T by

$$\rho(T) := \{z \in \mathbb{C} : T - z \text{ is bijective } \},$$
$$\sigma(T) := \{z \in \mathbb{C} : T - z \text{ is not bijective } \}.$$

The spectrum $\sigma(T)$ can be divided in three disjoint subsets:

$$\sigma_p(T) := \{z \in \mathbb{C} : T - z \text{ is not injective } \},$$
$$\sigma_c(T) := \{z \in \mathbb{C} : T - z \text{ is injective}, \overline{\text{Ran}(T - z)} = H\},$$
$$\sigma_r(T) := \{z \in \mathbb{C} : T - z \text{ is injective}, \overline{\text{Ran}(T - z)} \neq H\}.$$

The sets $\sigma_p(T), \sigma_c(T)$ and $\sigma_r(T)$ are known as the *point spectrum, continuos spectrum* and *residual spectrum.*

The elements of σ_p are called *eigenvalues* of T. For $z \in \sigma_p(T)$, the subspace $\text{Ker}(T - z)$ is called *eigenspace* of z, the dimension of $\text{Ker}(T - z)$ is called the *multiplicity* of the eigenvalue. If $f \in \text{Ker}(T - z)$, it is called an *eigenvector* of T belonging to the eigenvalue z.
For $z \in \rho(T)$ the operator

$$R(z, T) := (T - z)^{-1} : H \to H$$

is called the *resolvent* of T.
Let $T(H \to H)$ be a densely defined linear operator on a Hilbert space H. Fix $y \in H$ and consider the map $D(T) \to \mathbb{C}$, $x \mapsto \langle Tx, y\rangle$. If the map is continuous on $D(T)$ we can extend it to a unique linear continuous functional $\phi_y \in H$ and by the Riesz representation theorem there exists exactly one element $y^* \in H$ such that

$$\phi_y(x) = \langle Tx, y\rangle = \langle x, y^*\rangle \,; \quad x \in D(T).$$

Definition 1.2. Let H be a Hilbert space and $T(H \to H)$ a densely defined linear operator. Its Hilbert *space adjoint* T^* is defined by

$$\begin{aligned} D(T^*) &:= \{z \in H : x \mapsto \langle Tx, z\rangle \text{ is continuous on } D(T)\}, \\ T^* : D(T^*) &\longrightarrow H, \\ z &\mapsto T^* z = z^* \end{aligned}$$

where z^* is the unique element in H such that $\langle Tx, z\rangle = \langle x, z^*\rangle$.

We give some properties of the adjoint operator taken from [Wei80].

Proposition 1.3. *Let H be a Hilbert space and $T(H \to H)$ a densely defined linear operator. Then*

(a) *T^* is closed.*
(b) *T^* is bounded if and only if T is bounded.*
(c) *If T is closable then T^* is densely defined and $\overline{T} = T^{**}$.*

Definition 1.4. Let H be a Hilbert space and $T(H \to H)$ a densely defined linear operator. Then

(a) T is *symmetric* if $T \subseteq T^*$.
(b) T is *self-adjoint* if $T = T^*$.
(c) T is *essentially self-adjoint* if $\overline{T}$ is self-adjoint.

Theorem 1.5. *Let H be a Hilbert space and $T(H \to H)$ a densely defined linear operator. Then*

(a) $\text{Ran}(T)^\perp = \text{Ker}(T^*)$.
(b) $\overline{\text{Ran}(T)} = \text{Ker}(T^*)^\perp$.
(c) $\text{Ran}(T^*)^\perp = \text{Ker}(T)$.
(d) $\overline{\text{Ran}(T^*)} = \text{Ker}(T)^\perp$.

We give some basic properties of the spectrum of self-adjoint operators.

Lemma 1.6 ([Tri92, Lemma 4.2.2]). *Let H be a Hilbert space and $T(H \to H)$ a self-adjoint operator. Then $\sigma(T) \subset \mathbb{R}$ and*

$$\|R(z,T)\| \le \frac{1}{|\text{Im } z|}, \quad \text{for Im } z \neq 0.$$

In addition $\text{Ran}(T - z)$ *is closed when* $\text{Im } z \neq 0$.

Proposition 1.7 ([Wei80, Section 7.4]). *Any isolated point z of the spectrum of a self-adjoint operator $T(H \to H)$ on a complex Hilbert space H is an eigenvalue of T.*

Let us denote by $\sigma'(T)$ as the accumulation points of $\sigma(T)$. Define the sets

$$\begin{aligned} \sigma_{\text{ess}}(T) &:= \sigma'(T) \cup \{z \in \sigma_p(T) : \dim(\text{Ker}(T - z)) = \infty\}, \\ \sigma_d(T) &:= \sigma(T) - \sigma_{\text{ess}}(T). \end{aligned}$$

The sets $\sigma_{ess}(T)$ and $\sigma_d(T)$ are known as the *essential spectrum* and *discrete spectrum* of T respectively.

An immediate consequence of 1.7 is the following corollary.

Corollary 1.8. *Let $T(H \to H)$ be a self-adjoint spectrum on a complex Hilbert space H, then*

$$\sigma_d(T) := \{z \in \sigma_p(T) : \dim(\text{Ker}(T - z)) < \infty, \text{ and } z \notin \sigma'(T)\}.$$

For a self-adjoint operator T we say that T has *purely discrete spectrum* if $\sigma_{ess}(T) = \emptyset$.

1.2 Self-adjoint extensions of symmetric operators

Now we are going to give a review of the principal results of the von Neumann theory on self-adjoint extensions of symmetric operators. For this we define the *Cayley transform* of a symmetric linear operator.

Definition 1.9. Let H be a complex Hilbert space and $T(H \to H)$ a densely defined symmetric operator. Then the *Cayley transform* of T is defined by

$$U_T : \text{Ran}(T + i) \longrightarrow H, \qquad U_T := (T - i)(T + i)^{-1}.$$

By [Wei80, Theorem 5.18] we know that $T + i$ is boundedly invertible in $\text{Ran}(T + i)$ and $\text{Ran}((T + i)^{-1}) = D(T + i) = D(T - i)$. Therefore U_T is well defined.

Proposition 1.10 (Properties of the Cayley transformation). *Let H be a complex Hilbert space and $T(H \to H)$ a symmetric operator with Cayley transform U_T. Then*

(a) *U_T is isometric and* $\text{Ran}(U_T) = \text{Ran}(T - i)$. *If T is closed, so is U_T.*
(b) $1 \neq \sigma_p(U_T)$, $\text{Ran}(I - U_T)$ *is dense in H and the map*

$$(I - U_T)^{-1} : D(T) \longrightarrow D(U_T)$$

exists and is surjective.
(c) $T = i(I + U_T)(I - U_T)^{-1}$.
(d) *T is self-adjoint if and only if U_T is unitary.*

For a closed symmetric operator T on a complex Hilbert space H we set

$$N_+ = \text{Ker}(T^* + i) = \text{Ran}(T - i)^\perp,$$
$$N_- = \text{Ker}(T^* - i) = \text{Ran}(T + i)^\perp.$$

The second equality in both lines is due to Theorem 1.5. The numbers

$$\eta_+ := \dim(N_+),$$
$$\eta_- := \dim(N_-),$$

are known as the *deficiency indices* of T.
The most important result about the Cayley transform is its relation with symmetric extensions of a given symmetric operator [Wei80, Theorem 8.6].

Theorem 1.11. *Let H be a complex Hilbert space, $T(H \to H)$ a closed symmetric operator, and U its Cayley transform. Then*

(a) *U' is the Cayley transform of a closed symmetric extension T' of T if and only if the following holds: There exist closed subspaces F_- of N_- and F_+ of N_+ and an isometric mapping $\widehat{U}$ of F_+ onto F_- for which*

$$\begin{aligned} D(U') &= \operatorname{Ran}(T'-i) = \operatorname{Ran}(T-i) \oplus F_+, \\ U'(f+g) &= Uf + \widehat{U}g \quad \text{for } f \in \operatorname{Ran}(T-i), g \in F_+, \\ \operatorname{Ran}(U') &= \operatorname{Ran}(T'+i) = \operatorname{Ran}(T+i) \oplus F_-. \end{aligned}$$

The spaces F_- and F_+ have the same dimension.

(b) *The operator U' in part (a) is unitary if and only if $F_- = N_-$ and $F_+ = N_+$.*

(c) T possesses self-adjoint extensions if and only if its deficiency indices are equal.

We give the von Neumann formulas taken from [Wei80, theorem 8.11 and 8.12].

Theorem 1.12 (1st von Neumann formula). *Let H be a complex Hilbert space and $T(H \to H)$ a closed symmetric operator. Then*

$$D(T^*) = D(T) \dotplus N_+ \dotplus N_-,$$

$$T^*(f_0 + g_+ + g_-) = Tf_0 - ig_+ + ig_- \quad \text{for} \quad f_0 \in D(T), g_+ \in N_+, g_- \in N_-.$$

Theorem 1.13 (2nd von Neumann formula). *Let H be a complex Hilbert space and $T(H \to H)$ a closed symmetric operator. Then*

(a) *T' is a closed symmetric extension of T if and only if the following holds: There are closed subspaces F_+ of N_+ and F_- of N_- and an isometric mapping $\widehat{V}$ of F_+ onto F_- such that*

$$D(T') = D(T) \dotplus \{g + \widehat{V}g : g \in F_+\}$$

and

$$T'(f_0 + g + \widehat{V}g) = Tf_0 - ig + i\widehat{V}g \quad \text{for} \quad f_0 \in D(T), g \in F_+.$$

(b) *T' is selfadjoint if and only if $F_+ = N_+$ and $F_- = N_-$.*

Proof. We only have to show that the operator T' of the Theorem 1.11 can be represented in the above form. Let U' the Cayley transform of T'. By Theorem 1.11

$$\begin{aligned} D(T') &= \operatorname{Ran}(I - U') = (I - U')D(U') = (I - U')(D(U) \oplus F_+) \\ &= (I - U)D(U) \dotplus (I - \widehat{U})F_+ \\ &= D(T) \dotplus \{g - \widehat{U}g : g \in F_+\}. \end{aligned}$$

The sum is direct, as $\{g - \widehat{U}g : g \in F_+\} \subset F_+ \dot{+} F_- \subset N_+ \dot{+} N_-$. Since $T' \subset T^*$, we have in addition that

$$T'(f_0 + g - \widehat{U}g) = T^*(f_0 + g - \widehat{U}g) = Tf_0 - ig - i\widehat{U}g$$

for all $f_0 \in D(T)$ and $g \in F_+$. The assertion follows if we take $\widehat{V} = -\widehat{U}$. QED

Example 1.14. Let $H = L^2(a,b)$ with $a, b \in \mathbb{R}$ and let $\mathrm{AC}[\alpha,\beta]$ be the set of absolutely continuous functions in the interval $[\alpha,\beta]$. We define T by

$$\begin{aligned} D(T) &:= \{f \in L^2(a,b) : f \in \mathrm{AC}[\alpha,\beta],\ \text{for all } [\alpha,\beta] \subset (a,b),\ f' \in L^2(a,b),\ f(a) = f(b) = 0\}, \\ Tf &:= -if'. \end{aligned}$$

T is a closed symmetric operator and

$$\begin{aligned} T^*f &= -if' \\ D(T^*) &= \{f \in L^2(a,b) : f \in \mathrm{AC}[\alpha,\beta],\ \text{for all } [\alpha,\beta] \subset (a,b),\ f' \in L^2(a,b)\}. \end{aligned}$$

After some calculations we find that

$$N_+ = \mathrm{Ker}(T^* + i) = \mathrm{span}\{e^t\}, \quad N_- = \mathrm{Ker}(T^* - i) = \mathrm{span}\{e^{-t}\}.$$

Hence $\eta_+ = \eta_- = 1$, so T admits self-adjoint extensions.
To find them we have to calculate all unitary maps $N_+ \to N_-$, that is, find all U such that

$$\langle Ue^t, Ue^t \rangle_{L^2} = \langle e^t, e^t \rangle_{L^2}.$$

Since $Ue^t = ze^{-t}$, this problem reduces to find all $z \in \mathbb{C}$ such that

$$|z|^2 = \frac{\langle e^t, e^t \rangle_{L^2}}{\langle e^{-t}, e^{-t} \rangle_{L^2}} = \left(\frac{e^{2b} - e^{2a}}{e^{-2a} - e^{-2b}} \right),$$

therefore

$$z = e^{i\theta} \left(\frac{e^{2b} - e^{2a}}{e^{-2a} - e^{-2b}} \right)^{1/2}, \quad \text{for } \theta \in \mathbb{R}.$$

Hence all self-adjoint extensions of T are of the form

$$D(T'_\theta) = D(T) + \mathrm{span}\left\{ e^t + e^{i\theta} \left(\frac{e^b - e^a}{e^{-a} - e^{-b}} \right)^{1/2} e^{-t} \right\},$$

$$T'_\theta \left(f_0 + \alpha \left(e^t + e^{i\theta} \left(\frac{e^{2b} - e^{2a}}{e^{-2a} - e^{-2b}} \right)^{1/2} e^{-t} \right) \right) = f'_0 + i\alpha e^t - i\alpha e^{i\theta} \left(\frac{e^{2b} - e^{2a}}{e^{-2a} - e^{-2b}} \right)^{1/2} e^{-t}.$$

Definition 1.15. Let T and T' be linear operators such that $T \subset T'$; then we say that T' is an $m-$*dimensional extension* of T if the quotient space $D(T')/D(T)$ has dimension m. We also say that T is an $m-$*dimensional restriction* of T'.

Theorem 1.16. *Let H be a complex Hilbert space, $T(H \to H)$ a closed symmetric operator, and T' a symmetric extension of T. Then*

- *T' is an $m-$dimensional extension of T if and only if* $\dim(F_+) = m$.
- *If T has deficiency indices (m, m), then a symmetric extension T' of T is selfadjoint if and only if T' is an $m-$dimensional symmetric extension of T.*

We need to define the set known as the *numerical range.*

Definition 1.17. *Let H a complex Hilbert space and $T(H \to H)$ a linear operator on H. We define the numerical range of T*

$$W(T) := \{\langle Tx, x\rangle : x \in D(T),\ \|x\| = 1\}.$$

For a densely defined symmetric operator $T(H \to H)$ we say that T is *lower semibounded* if there exists $\gamma \in \mathbb{R}$ such that

$$W(T) \subset [\gamma, \infty).$$

Remark 1.18. It is well known that the deficiency indices are constant in the complement of the numerical range [Kat95, Ch. V, Theorem 3.2].

Corollary 1.19. *If T is symmetric and $W(T) \subset [\gamma, \infty)$ for some $\gamma \in \mathbb{R}$, then T has equal deficiency indices and therefore it has self-adjoint extensions.*

Now we introduce two results about the spectrum of the self-ajoint extensions of a closed symmetric operator.

Theorem 1.20 ([Wei80, Theorem 8.18]). *Let $T(H \to H)$ be a closed symmetric operator on a complex Hilbert space with equal finite defect indices. Then all self-adjoint extensions of T have the same essential spectrum. If some self-adjoint extension of T has a purely discrete spectrum, then all self-adjoint extensions of T do, too.*

Corollary 1.21 ([Wei80, Chapter 8 Corollary 2]). *If $T(H \to H)$ is a closed symmetric operator on a complex Hilbert space, lower semibounded with lower bound γ and finite defect indices (m, m), and T' is a self-adjoint extension of T, then $\sigma(T') \cap (-\infty, \gamma)$ consists of isolated eigenvalues only with total multiplicity $\leq m$.*

1.2.1 Friedrichs extension of a semibounded symmetric operator

In this section we introduce a a distinguished self-adjoint extension, called the *Friedrichs extension*, of a densely defined lower semibounded symmetric operator. That construction is based on the theory of sesquilinear forms and their relation with symmetric operators.

Definition 1.22. A *sesquilinear form* (or briefly, a *form*) on a linear subspace $D(t)$ of a Hilbert space H is a mapping $t[\cdot, \cdot] : D(t) \times D(t) \to \mathbb{C}$ such that

$$t[\alpha x + \beta y, z] = \alpha t[x, z] + \beta t[y, z], \qquad t[z, \alpha x + \beta y] = \bar{\alpha} t[z, x] + \bar{\beta} t[z, y]$$

for $\alpha, \beta \in \mathbb{C}$, $x, y, z \in D(t)$. The subspace $D(t)$ is called the *domain* of t.

The *quadratic form* $t[\cdot] : D(t) \to \mathbb{C}$ associated with a form t is defined by

$$t[x] := t[x, x].$$

Recall that the *graph norm* generated by a linear operator $T(H \to H)$ is defined by

$$\|x\| := \|x\| + \|Tx\|, \quad \text{for all } x \in D(T).$$

Definition 1.23. Let $t : D(t) \times D(t) \to \mathbb{C}$ be a sesquilinear form.

(a) t is called *symmetric,* or *Hermitian,* if

$$t[x, y] = \overline{t[y, x]} \qquad \text{for } x, y \in D(t).$$

(b) If t is symmetric, it is called *lower semibounded* if there is an $\gamma \in \mathbb{R}$ such that

$$t[x] \geq \gamma \|x\|^2 \qquad \text{for } x \in D(t).$$

(c) If t is lower semibounded, we say that t is *closed* if $(D(t), \|\cdot\|_t)$ is complete, and t is *closable* if there exists a closed lower semibounded form which is an extension of t.

The next proposition gives us a characterization of closable forms.

Proposition 1.24 ([Sch12, Proposition 10.3]). *The following statements are equivalent:*

(a) *t is closable.*

(b) *For any sequence of vectors $(x_n)_{n\in\mathbb{N}} \subset D(t)$ such that $\lim_{n\to\infty} x_n = 0$ in H and $\lim_{n,k\to\infty} t[x_n - x_k] = 0$, we have $\lim_{n\to\infty} t[x_n] = 0$.*

We define the *closure* of a closable quadratic form t, $\bar{t}$ as the closed extension of t such that

$$\bar{t}[x] = \lim_{n\to\infty} t[x_n],$$

where $\{x_n\}$ is a sequence in $D(t)$ such that $x_n \to x$, and

$$D(\bar{t}) := \{x \in H, \lim_{n\to\infty} x_n = x, \ (x_n)_{n\in\mathbb{N}} \subset D(t), \ \lim_{n,k\to\infty} t[x_n - x_k] = 0\}. \tag{1.1}$$

The next theorem establishes a direct relation between densely defined lower semibounded closed forms and the self-adjoint operators on a Hilbert space.

Theorem 1.25 ([Sch12, Theorem 10.7]). *If t is a densely defined lower semibounded closed form on H, then the operator A_t defined as $A_t x := u_x$ for $x \in D(A_t)$, where*

$$D(A_t) = \{x \in D(t) : \text{ exists } u_x \in H \text{ such that } t[x, y] = \langle u_x, y\rangle \text{ for } y \in D(t)\},$$

is self-adjoint.

Given a lower semibounded symmetric operator T we define the form

$$s_T[x,y] := \langle Tx, y\rangle, \quad D(s_T) := D(T). \tag{1.2}$$

It is clear that s_T is symmetric and lower semibounded. The fact that s_T is closable is the following lemma.

Lemma 1.26 ([Sch12, Lemma 10.16]). *If T is a densely defined lower semibounded symmetric operator, then the form s_T defined as in* (1.1)*, is closable.*

The closure $t := \overline{s_T}$ is a densely defined lower semibounded closed form. By Theorem 1.25 the operator A_t associated with this form is self-adjoint.

Definition 1.27. The operator A_t is called the *Friedrich extension* of T and is denoted by T_F.

Theorem 1.28 ([Sch12, Theorem 10.17]). *Let T be a densely defined lower semibounded symmetric operator on a Hilbert space H.*

(a) *T_F is a lower semibounded self-adjoint extension of T which has the same greatest lower bound as T.*
(b) *$D(T_F) = D(T^*) \cap D(\overline{s_T})$ and $T_F = T^*|_{D(\overline{s_T})}$. Moreover, T_F is the only self-adjoint extension of T with domain contained in $D(\overline{s_T})$.*
(c) *$(T + \lambda I)_F = T_F + \lambda I$ for $\lambda \in \mathbb{R}$.*

Remark 1.29. If T is symmetric and densely defined but not closed, it is not difficult to see that $\overline{s_T} = \overline{s_{\overline{T}}}$.

Example 1.30. Let $H = L^2(a,b)$ with $-\infty \leq a < b \leq \infty$ and

$$Tf := -\frac{d^2 f}{dx^2},$$
$$D(T) := C_c^\infty(a,b)$$

with adjoint ([Bre10, Chapter 8])

$$T^* f := -\frac{d^2 f}{dx^2},$$
$$D(T^*) := H^2(a,b) := \{f \in L^2(a,b) : f,\ f' \in \mathrm{AC}[\alpha,\beta],\ \text{for all } [\alpha,\beta] \subset (a,b),\ f'' \in L^2(a,b)\}.$$

The associated form is given by

$$s_T[f,g] := \langle Tf, g\rangle = -\int_a^b f'' g\, dx.$$

Integration by parts shows that

$$s_T[f] = \|f'\|^2.$$

It is well known from [Bre10, Chapter 8] that the closure of $(C_c^\infty(a,b), \|\cdot\|_{s_T})$ on $L^2(a,b)$ is $H_0^1(a,b)$. By Theorem 1.28

$$D(T_F) = H^2(a,b) \cap H_0^1(a,b) = H_0^2(a,b).$$

1.2.2 Boundary triplets

In this section we will use so-called boundary triplets to parametrize all self-adjoint extensions of a given symmetric operator.

Definition 1.31. Let $T(H \to H)$ be a densely defined symmetric operator on a Hilbert space H. A *boundary triplet* for T^* is a triplet $(\mathcal{K}, \Gamma_0, \Gamma_1)$ of a Hilbert space $(\mathcal{K}, \langle\cdot,\cdot\rangle)$ and linear mappings $\Gamma_0 : D(T^*) \to \mathcal{K}$ and $\Gamma_1 : D(T^*) \to \mathcal{K}$ such that:

(a) $[x,y]_{T^*} \equiv \langle T^*x, y\rangle - \langle x, T^*y\rangle = \langle \Gamma_1 x, \Gamma_0 y\rangle - \langle \Gamma_0 x, \Gamma_1 y\rangle$ for $x, y \in D(T^*)$.
(b) The following map is surjective

$$\begin{aligned} D(T^*) &\longrightarrow \mathcal{K} \oplus \mathcal{K}, \\ x &\longmapsto (\Gamma_1 x, \Gamma_0 x). \end{aligned}$$

The question whether a boundary triplet for T^* exists is answered by the following:

Proposition 1.32. [Sch12, Proposition 14.5] *There exists a boundary triplet $(\mathcal{K}, \Gamma_0, \Gamma_1)$ for T^* if and only if the symmetric operator T has equal deficiency indices. In this case we have $\eta_+ = \eta_- =$* $\dim(\mathcal{K})$.

It is not difficult to see that

$$T_0 := T^*\big|_{D(T_0)}; \quad D(T_0) := D(T^*) \cap \mathrm{Ker}(\Gamma_0), \tag{1.3}$$
$$T_1 := T^*\big|_{D(T_1)}; \quad D(T_1) := D(T^*) \cap \mathrm{Ker}(\Gamma_1), \tag{1.4}$$

are self-adjoint restrictions of T^*.
Define $S(\mathcal{K})$ as the set of all self-adjoint operators B acting on a closed subspace $\mathcal{K}_B$ of $\mathcal{K}$ and let P_B be the orthogonal projection onto $\mathcal{K}_B$. For any $B \in S(\mathcal{K})$, we define T_B to be the restriction of T^* to the domain

$$D(T_B) := \{x \in D(T^*) : \ \Gamma_0 x \in D(B) \text{ and } B\Gamma_0 x = P_B \Gamma_1 x\}. \tag{1.5}$$

Another type of restrictions is described by the unitary operators on $\mathcal{K}$. Let V be a unitary operator on $\mathcal{K}$ and let T^V be the restriction of T^* to

$$D(T^V) := \{x \in D(T^*) : V\Gamma_+ x = \Gamma_- x\}, \tag{1.6}$$

where $\Gamma_\pm := \Gamma_1 \pm i\Gamma_0$. The question of how the boundary triplets describe the self-adjoint extensions is answered by the following theorem taken from [Sch12, Theorem 14.10].

Theorem 1.33. *Let $T(H \to H)$ be a densely defined closed symmetric operator on a complex Hilbert space H and suppose that $(\mathcal{K}, \Gamma_0, \Gamma_1)$ is a boundary triplet for T^*. For any operator S on H, the following are equivalent:*

(a) *S is a self-adjoint extension of T on H.*

(b) *There is a self-adjoint operator* B *acting on a closed subspace* $\mathcal{K}_B$ *of* $\mathcal{K}$ *such that* $S = T_B$.
(c) *There is a unitary operator* V *on* $\mathcal{K}$ *such that* $S = T^V$.

The operators V *and* B *are uniquely determined by* S.

Futher, any proper extension of T admits the representation (see [DHMdS00])

$$D(T_{G,D}) := D(T^*) \cap \mathrm{Ker}(D\Gamma_1 - G\Gamma_0), \tag{1.7}$$

where G, D are bounded operators on $\mathcal{K}$ such that $GD^* = DC^*$ and $0 \in \rho(D \pm iC)$.

Suppose that for a densely defined closed symmetric operator $T(H \to H)$ there are linear functionals $\phi_1, \dots, \phi_d, \psi_1, \dots, \psi_d$, $d \in \mathbb{N}$, on $D(T^*)$ such that

$$\langle T^* x, y\rangle - \langle x, T^* y\rangle = \sum_{k=1}^{d} \left(\psi_k(x)\overline{\phi_k(y)} - \phi_k(x)\overline{\psi_k(y)}\right), \quad x, y \in D(T^*) \tag{1.8}$$

with

$$\{(\phi(x), \psi(x)) : \ x \in D(T^*)\} = \mathbb{C}^{2d},$$

where $\phi(x) := (\phi_1(x), \dots, \phi_d(x))$ and $\psi(x) := (\psi_1(x), \dots, \psi_d(x))$.
Is not difficult to see that there is a boundary triplet $(\mathcal{K}, \Gamma_0, \Gamma_1)$ for T^* defined by

$$\mathcal{K} = \mathbb{C}^d, \quad \Gamma_0(x) = \phi(x), \quad \Gamma(x) = \psi(x). \tag{1.9}$$

Let $B \in S(\mathcal{K})$. We choose an orthonormal basis $\{e_1, \dots, e_n\}$ of $\mathcal{K}_B$ and a basis $\{\hat{e}_{n+1}, \dots, \hat{e}_d\}$ of $(\mathcal{K}_B)^\perp$. Since B is a self-adjoint operator on $\mathcal{K}_B$, B is a hermitian $n \times n$ matrix (B_{kl}) such that

$$Be_l = \sum_{k=1}^{n} B_{kl} e_k.$$

It is clear that

$$P_B\Gamma_1(x) = \sum_{k=1}^{n} \langle \Gamma_1(x), e_k\rangle\, e_k.$$

If $\Gamma_0(x) \in \mathcal{K}_B$, then we have

$$B\Gamma_0(x) = B\sum_{l=1}^{n} \langle \Gamma_0(x), e_l\rangle\, e_l = \sum_{k,l} \langle \Gamma_0(x), e_l\rangle\, B_{kl} e_k.$$

Recall that $x \in D(T_B)$ if and only if $\Gamma_0 x \in \mathcal{K}_B$ and $P_B\Gamma_1(x) = B\Gamma_0(x)$. Therefore, $x \in D(T^*)$ belongs to $D(T_B)$ if and only if

$$\langle \Gamma_0(x), \hat{e}_j\rangle = 0 \quad j = n+1, \dots, d, \tag{1.10}$$

$$\langle \Gamma_1(x), e_k\rangle = \sum_{l=1}^{n} B_{kl} \langle \Gamma_0(x), e_l\rangle \quad k = 1, \dots, n. \tag{1.11}$$

In the chapter 2 we will to see some differential operators such that holds (1.8).

Example 1.34. Let H and T be as in Example 1.14. Integration by parts gives

$$\begin{aligned}\langle T^*f,g\rangle - \langle f,T^*g\rangle &= -i\int_a^b f'\bar{g}\,\mathrm{d}x - i\int_a^b f\bar{g}'\,\mathrm{d}x\\ &= -if\bar{g}|_a^b + i\int_a^b f\bar{g}'\,\mathrm{d}x - i\int_a^b f\bar{g}'\,\mathrm{d}x\\ &= if(a)\overline{g(a)} - if(b)\overline{g(b)}\\ &= \frac{i}{2}\left[(f(a)+f(b))(\overline{g(a)}-\overline{g(b)}) + (f(a)-f(b))(\overline{g(a)}+\overline{g(b)})\right].\end{aligned}$$

We define

$$\Gamma_0 f = \frac{\sqrt{2}}{2}\left(f(a)+f(b)\right), \quad \Gamma_1 f = -\frac{\sqrt{2}i}{2}\left(f(a)-f(b)\right).$$

Given that

$$\{(f(a),f(b)) : f\in H^2(a,b)\} = \mathbb{C}^2,$$

then $(\mathbb{C},\Gamma_0,\Gamma_1)$ is a boundary triplet for T^*. By Theorem 1.32 (b), T has self-adjoint extensions and deficiency indices $(1,1)$. By Theorem 1.33 (b), in order to find all self-adjoint extensions of T, we only have to find $S(\mathbb{C})$. Clearly, it consists of all $B_\nu : \mathbb{C}\to\mathbb{C}$, $B_\nu z = \nu z$ with $\nu\in\mathbb{R}$ and $\widetilde{B} : \{0\}\to\{0\}$, $\widetilde{B}0 = 0$. Hence all self-adjoint extensions of T are

$$\begin{aligned}T_{B_\nu} f = T^*f;\quad D(T_{B_\nu}) : &= \{f\in D(T^*) : \nu\left(f(a)+f(b)\right) = -i\left(f(a)-f(b)\right)\}\\ &= \left\{f\in D(T^*) : f(b) = f(a)\frac{i+\nu}{i-\nu}\right\}\end{aligned}$$

and

$$T_{\widehat{B}} f := T^*f;\quad D(T_{\widehat{B}}) := \{f\in D(T^*) : f(b) = -f(a)\}.$$

Notice that

$$\Gamma_+ f = \sqrt{2}f(a),\quad \Gamma_- f = \sqrt{2}f(b).$$

Using the Theorem 1.33 (c) we obtain

$$T_z f = T^*f;\quad D(T_z) : = \{f\in D(T^*) : zf(a) = f(b)\}$$

with $|z| = 1$. Now using the representation described by the equation (1.7) obtain

$$\begin{aligned}T_{G,D} f = T^*f;\quad D(T_\nu) : &= \{f\in D(T^*) : G\left(f(a)+f(b)\right) = -iD\left(f(a)-f(b)\right)\}\\ &= \left\{f\in D(T^*) : f(b) = f(a)\frac{G+iD}{iD-G}\right\}\end{aligned}$$

with $G,D\in\mathbb{C}$ such that $G\overline{D} = D\overline{C}$ and $iD\pm C\neq 0$. We can see that the above representations are equivalent.

Now we define a holomorphic family and give one technical result.

Definition 1.35. *Let $T(H \to H)$ be a closed symmetric linear operator on a Hilbert space H and $\Pi = (\mathcal{K}, \Gamma_0, \Gamma_1)$ a boundary triplet for T^* and let T_0 be defined as in* (1.3). *The Weyl function corresponding to Π is the unique mapping $M : \rho(T_0) \to \mathcal{B}(\mathcal{K})$ such that*

$$\Gamma_1 f_z = M(z)\Gamma_0 f_z, \quad \text{for } f_z \in N_z := \text{Ker}(T^* - z), \quad z \in \rho(T_0).$$

For the detection of the spectrum of the self-adjoint realizations we give the next proposition taken from [Sch12, Proposition 14.17]

Proposition 1.36. *Suppose that $B \in S(\mathcal{K})$ and $z \in \rho(T_0)$. Then $B - M(z)$ is closed and we have:*

(a) $\dim \text{Ker}(T_B - z) = \dim(B - M(z))$. *In particular, z is an eigenvalue of T_B if and only if* $\text{Ker}(B - M(z)) \neq \{0\}$.
(b) $z \in \rho(T_B)$ *if and only if* $0 \in \rho(B - M(z))$.

Definition 1.37. Let $T(H \to H)$ be a self-adjoint operator on a complex Hilbert space H, and let E_T be its spectral resolution. We define the *negative squares* of T as the number $k_-(T) = \dim(E(-\infty, 0))$.

The Weyl function M enables us to describe the number of negative squares of self-adjoint extensions of a non-negative symmetric operator T

Theorem 1.38 ([DHMdS12]). *Let T be a closed densely defined non-negative symmetric operator in H with equal deficiency indices, and let $T_{C,D}$ be a self-adjoint extension defined as in* (1.7). *Assume that $(\mathcal{K}, \Gamma_0, \Gamma_1)$ is a boundary triplet for T^* such that $T_0 = T_F$. Then the following assertions hold.*

(a) *The strong resolvent limit $M(0) := \text{s} - \text{R} - \lim_{x \uparrow 0} M(x)$ (see [Kat95, Chapter 8]) exists.*
(b) *If $M(0)$ is bounded, then*

$$k_-(T_{C,D}) = k_-\left(CD^* - DM(0)D^*\right). \tag{1.12}$$

1.3 Basic notions of distribution theory

To define the δ and δ' as potentials we need some concepts of distribution theory.

Definition 1.39. We define the space of *test functions* J as $C_c^\infty(\mathbb{R})$

We say that a sequence $\phi_n \to \phi$ in J if and only if all supports of the ϕ_n are contained in a common compact set K and $\phi_n^{(m)} \to \phi^{(m)}$ for all $m \in \mathbb{N}$ uniformly on K for $n \to \infty$.

Definition 1.40. A *distribution* Ψ is a linear functional on J such that, if $\phi_n \to \phi$ in J then $\Psi(\phi_n) \to \Psi(\phi)$ for $n \to \infty$.

We denote its action on $\phi \in$ J by $\langle \Psi | \phi \rangle$.

Note that every $f \in L^1_{loc}(\mathbb{R})$ defines a distribution in a natural way by

$$\langle f|\phi\rangle := \int_{-\infty}^{\infty} f(t)\phi(t)\,\mathrm{d}t.$$

If for a distribution Ψ there exists a function $f \in L^1_{loc}(\mathbb{R})$ such that:

$$\langle \Psi|\phi\rangle = \langle f|\phi\rangle, \quad \text{for all } \phi \in \mathrm{J},$$

then we say that Ψ is *regular*. Otherwise we say that Ψ is *singular*. The most well-known example of a singular distribution is the δ distribution (see details in [Zem87, Section 1.3]) given by the action

$$\langle \delta|\phi\rangle := \phi(0).$$

and we take as a definition

$$\langle \delta_\tau|\phi\rangle := \phi(\tau).$$

Let $\Psi \in \mathrm{J}'$ be a distribution and $f \in \mathrm{J}$. We define the product of a distribution and a function $f\Psi$, as

$$\langle f\Psi|\phi\rangle = \langle \Psi f|\phi\rangle = \langle \Psi|f\phi\rangle, \quad \text{for all } \phi \in \mathrm{J}.$$

Similarly if $f, g \in L^1_{loc}(\mathbb{R})$ then their product as distributions is defined by

$$\langle fg|\phi\rangle = \langle g|f\phi\rangle = \langle f|g\phi\rangle, \quad \text{for all } \phi \in \mathrm{J}.$$

Let $\Psi, \Phi \in \mathrm{J}'$ be two distributions and let I be an interval such that

$$\langle \Psi|\phi\rangle = \langle \Phi|\phi\rangle, \quad \text{for all } \phi \in C_c^\infty(I).$$

Then we say that Ψ and Φ *are equal on* I.

Definition 1.41. The *null set* $\mathrm{null}(\Psi) \subset \mathbb{R}$ of a distribution Ψ is the union of all open sets N_i such that

$$\langle \Psi|\phi\rangle = 0, \quad \text{for all } \phi \in \mathrm{J}, \text{ with } \mathrm{supp}(\phi) \subseteq N_i.$$

The complement of the null set, $\mathrm{null}(\Psi)^c =: \mathrm{supp}(\Psi)$ is known as the *support of* Ψ.

Definition 1.42. Let $\Psi \in \mathrm{J}'$ be a distribution. We define its *first derivative* ψ' by the functional

$$\langle \Psi'|\phi\rangle = \langle \Psi|-\phi'\rangle, \quad \text{for all } \phi \in \mathrm{J}.$$

Iterating we obtain a formula for the nth-derivative:

$$\left\langle \Psi^{(n)}|\phi\right\rangle = \left\langle \Psi|(-1)^n\phi^{(n)}\right\rangle, \quad \text{for all } \phi \in \mathrm{J}.$$

Theorem 1.43 ([Zem87, Theorem 2.4-1]). *The derivative of a distribution is again a distribution.*

Example 1.44. The derivative of the distribution δ is defined by

$$\langle \delta' | \phi \rangle = \langle \delta | - \phi' \rangle = -\phi'(0),$$

for $\phi \in \mathrm{J}$.

Remark 1.45. Notice that for a function f which is continuous at 0 the action $\langle \delta | f \rangle$ is well defined and moreover the product satisfies

$$\langle \delta f | \phi \rangle = \langle \delta | f \rangle \langle \delta | \phi \rangle$$

so $\delta f = \langle \delta | f \rangle \delta = f(0)\delta$. Analogously for a continuous function f whose derivative f' is continuous at 0 we have $-\delta' f = f'(0)\delta + f(0)\delta'$.

Similarly, we can define the integral of a distribution.

Definition 1.46. Let $\Psi \in \mathrm{J}'$ be a distribution. A *primitive (or indefinite integral)* of Ψ is a functional g such that

$$\langle g | \phi' \rangle = \langle \Psi | - \phi \rangle, \quad \text{for all } \phi \in \mathrm{J}.$$

In this case we write $g = \Psi^{(-1)}$.

However this existence is not trivial. This fact is the following theorem.

Theorem 1.47 ([Zem87, Theorem 2.6-1]). *Every distribution has an infinity of primitives. Each primitive is also a distribution. The difference between two primitives of a given distribution is a constant distribution.*

Example 1.48. Note that for $\phi \in \mathrm{J}$

$$\langle \delta | - \phi \rangle = -\phi(0) = -\int_{-\infty}^{0} \phi'(t)\, \mathrm{d}t = \int_{-\infty}^{\infty} \theta(t)\phi'(t)\, \mathrm{d}t \tag{1.13}$$

where

$$\theta(t) := \begin{cases} 1 & \text{if } t > 0 \\ 0 & \text{else,} \end{cases}$$

is the so called *Heaviside function*. From (1.13) is clear that the distribution defined by θ is a primitive of δ.

Definition 1.49. Let $\Psi \in \mathrm{J}'$ be a distribution. The *order* of Ψ in a closed interval I is the smallest non-negative integer r for which

$$\langle \Psi | \phi \rangle = \left\langle \nu^{(r+2)}, \phi \right\rangle, \quad \phi \in C_c^\infty(I),$$

for some continuous function ν on I.

Example 1.50. Integration by parts gives

$$\langle\theta| - \phi\rangle = \int_0^\infty t\phi'(t)\mathrm{d}t = \int_{-\infty}^\infty \psi(t)\phi'(t)\mathrm{d}t \tag{1.14}$$

where

$$\psi(t) := \begin{cases} t & \text{if } t \geq 0 \\ 0 & \text{else,} \end{cases}$$

From (1.14) the distribution defined by the continuous function $\psi(t)$ is a primitive of θ. This implies that δ and δ' have order 0 and 1 respectively.

Remark 1.51. We can extend the above notation to negative integers. We shall say that Ψ is of order -1 if it is the first derivate of a continuous function but is not itself a continuous function on I. Also, we shall say that Ψ is of order r ($r = -2, -3, \ldots$) on I if it and its derivatives up to and including the order $-r-2$ are continuous functions and its $(-r-1)-$order derivative is not a continuous function on I. So, with this notation Ψ is a singular distribution on I if $r \geq 0$ and it is a regular distribution on I if $r \leq -2$. If the order is $r = -1$, the distribution can be regular or singular.

Notice that if $\Psi \in \mathrm{J}'$ has order r then Ψ' and $\Psi^{(-1)}$ have order $r+1$ and $r-1$ respectively.

Finally we characterize distributions whose support is only a point.

Theorem 1.52. *Let $\Psi \in \mathrm{J}'$ be a distribution with finite order r on a closed interval I. Then* $\mathrm{supp}(\Psi) = \{\tau\}$ *if and only if there exist constants $a_0, a_1, \ldots, a_r$ such that*

$$\Psi = \sum_{k=0}^{r} a_k \delta^{(k)}(t-\tau)$$

on I.

Remark 1.53. Given that $\mathrm{supp}(\delta) = \{0\}$

$$\langle\delta|\phi\rangle = 0,$$

for all $\phi \in C_c^\infty(\mathbb{R} - \{0\})$. So, abusing notation we, say that $\delta(t) = 0$ for $t \neq 0$.

1.4 Sturm-Liouville operators

We consider the differential expression:

$$\mathcal{U} = -\frac{d^2}{dx^2} + q(x), \tag{1.15}$$

on the interval (a, b), where $-\infty \leq a < b \leq \infty$ and $q \in C(a, b)$. It is known from [AE04] that

$$Af := \mathcal{U}f; \qquad D(A) := C_c^\infty(a, b) \tag{1.16}$$

is not closed, but closable because it is symmetric. We denote $\overline{A} =: T$. It is clear that T is symmetric. In [Sch12, 15.1] it is shown that T is densely defined and

$$T^* f = \mathcal{U} f,$$
$$D(T^*) := \{f \in L^2(a,b) : f,\ f' \in \mathrm{AC}[\alpha,\beta], \text{ for all } [\alpha,\beta] \subset (a,b),\ \mathcal{U} f \in L^2(a,b)\}.$$

If $f, g \in D(T^*)$ and $c \in (a,b)$, we abbreviate:

$$[f,g]_c := f(c)\overline{g'(c)} - g(c)\overline{f'(c)}.$$

This expresion is known as the *Lagrange bracket.*

Definition 1.54. The expresion $\mathcal{U}$ is *regular* at a if $a \in \mathbb{R}$ and $q \in L^1(a,c)$ for some $c \in (a,b)$. Otherwise $\mathcal{U}$ is said to be *singular* at a. In the same way, we say that $\mathcal{U}$ is *regular* at b if $b \in \mathbb{R}$ and $q \in L^1(c,b)$ for some $c \in (a,b)$. Otherwise $\mathcal{U}$ is said to be *singular* at b.

Definition 1.55. Let f be a function on (a,b). We say that f is *in* L^2 *near* a if there is a number $c \in (a,b)$ such that $f \in L^2(a,c)$. In the same way, we say that f is *in* L^2 *near* b if there is a number $c \in (a,b)$ such that $f \in L^2(c,b)$.

Proposition 1.56 ([Sch12, Proposition 15.5]). *Suppose that the end point a is regular for $\mathcal{U}$. Then*

(a) *If $f \in D(T^*)$, then f, f' can be extended to continuous functions on $[a,b)$.*
(b) *Let f be a solution of*

$$\mathcal{U} f = \lambda f \quad \text{on } (a,b) \tag{1.17}$$

where $\lambda \in \mathbb{C}$. Then f and f' extend to continuous functions on $[a,b)$. In particular, f is in L^2 near a.
(c) *The vector space $\{(f(a), f'(a)) : f \in D(T^*)\}$ is equal to $\mathbb{C}^2$.*
(d) *If $f \in D(\overline{T})$, then $f(a) = f'(a) = 0$.*
(e) *If $\mathcal{U}$ is regular at a and b, then*

$$f(a) = f'(a) = f(b) = f'(b) = 0,$$

for any $f \in D(\overline{T})$.

To determine the defect indices of T we need the next theorem known as *Weyl's alternative* taken from [Sch12, Theorem 15.8].

Theorem 1.57 (Weyl alternative). *Let d denote an end point of the interval (a,b). Then precisely one of the following two possibilities is valid:*

(a) *For each $\lambda \in \mathbb{C}$, all solutions of (1.17) are in L^2 near d.*
(b) *For each $\lambda \in \mathbb{C}$, there exists one solution of (1.17) which is not in L^2 near d.*

In case (b), for any $\lambda \in \mathbb{C} - \mathbb{R}$, there is a unique (up to a constant factor) nonzero solution of (1.17) which is in L^2 near d.

We introduce the following terminology

Definition 1.58. If case (a) holds, then we say that T is in the *limit circle case* at d. If the case (b) holds, then we say that T is in the *limit point case at* d.

Remark 1.59. Note that if d is regular for $\mathcal{U}$, then T is in the limit circle case by Proposition 1.56.

Before the next theorem we state the following lemma taken from [Sch12, Lemma 15.9].

Lemma 1.60. *If T is in the limit point case at a (or b), then $[f,g]_a = 0$ (or $[f,g]_b = 0$) for all $f,g \in D(T^*)$.*

We give a caracterization of the defect indices of T.

Theorem 1.61. *The Sturm-Liouville operator T has deficiency indices*

- *(2,2) if T is in the limit circle case at both end points.*
- *(1,1) if T is in the limit circle case at one end point and in the limit circle case at the other.*
- *(0,0) if T is in the limit point case at both end points.*

Proof. If T is in the limit circle case at both end points, all solutions of (1.17) are in L^2 near a and b; hence, they are in $L^2(a,b)$, because if f is solution of (1.17), f and f' are in $[\alpha,\beta]$ for $a<\alpha<\beta<b$. So T has deficiency indices $(2,2)$.
Now, without loss of generality, suppose that T is in the limit point case at a and in the limit circle case at b. Then, by the assertion (b) of the Theorem 1.57, for any $\lambda \in \mathbb{C}-\mathbb{R}$, there is a unique nonzero solution of (1.17) which is in L^2 near b. Since T is in the limit circle case at a, this solution is in L^2 near a and hence in $L^2(a,b)$. Therefore, the deficiency indices of T are $(1,1)$.
Assume that T is in the limit point case at both end points. Then, by Lemma 1.60,

$$[f,g]_a = [f,g]_b = 0 \qquad \text{for } f,g \in D(T^*).$$

So

$$\langle T^* f, g\rangle - \langle f, T^*, g\rangle = [f,g]_a - [f,g]_b = 0,$$

wich implies that T^* is symmetric. Therefore T is essentially self-adjoint and has deficiency indices (0,0). QED

The next two propositions contain two useful criteria that allow us to decide which of the two cases happens.

Proposition 1.62 ([Sch12, Proposition 15.11]). *Let $b=+\infty$ and suppose that there are numbers $\gamma > a$ and $\lambda \in \mathbb{R}$ such that $q(x) \geq \gamma$ for all $x \geq c$ (q is bounded from below on (c,∞)). Then T is in the limit point case at $b=+\infty$.*

Proof. It is well known that there is a unique solution of the differential equation

$$-f'' + qf = \lambda f \quad \text{ on } (a,\infty)$$

satisfying $u(c)=1$, $u'(c)=0$. Since $\overline{u}$ is a solution with the same initial data, u is real-valued by the uniqueness of solutions. Then

$$\left(u^2\right)'' = 2\left(u'\right)^2 + 2u''u = 2\left(u'\right)^2 + 2(q-\gamma)u^2 \geq 0 \quad \text{ on } (c,+\infty).$$

Therefore, since $\left(u^2\right)'(c) = 2u'(c)u(c) = 0$, we obtain

$$\left(u^2\right)'(x) = \int_c^x 2\left(u^2\right)''(t)dt \geq 0 \quad \text{for } x \in (c, +\infty).$$

Hence, the function u^2 is increasing on $(c, +\infty)$. Since $u(\gamma) = 1$, it follows that u is not in L^2 near $b = +\infty$, so T is in the limit point case at $b = +\infty$. QED

Remark 1.63. In the same way, for the case $a = -\infty$ we have the following criteria:
Let $a = -\infty$ and suppose that there are numbers $\gamma < b$ and $\gamma \in \mathbb{R}$ such that $q(x) \geq \gamma$ for all $x \leq c$ (q is bounded from below on $(-\infty, c)$). Then T is in the point limit case at $a = -\infty$.

Proposition 1.64 ([Sch12, Proposition 15.12]). *Suppose that $a = 0$ and $b \in (0, +\infty]$.*

(a) *If there exists a positive number γ such that $\gamma < b$ and $q(x) \geq \frac{3}{4}x^{-2}$ for all $x \in (0, \gamma)$, then T is in the limit point case at $a = 0$.*
(b) *If there are positive numbers ϵ and γ such that $\gamma < b$ and $|q(x)| \leq \left(\frac{3}{4} - \epsilon\right)x^{-2}$ for all $x \in (0, \gamma)$, then T is in the limit circle case at $a = 0$.*

Remark 1.65. Consider $q \in C(\mathbb{R})$ such that $q \geq \gamma$ for some $\gamma \in \mathbb{R}$ and $q(x) \to \infty$, if $|x| \to \infty$.

- If $a \in \mathbb{R}$ then T is regular at a and by Remark 1.59 it is in the limit circle case at a. By Proposition 1.62, T is in the limit point case at $b = +\infty$. Hence by Theorem 1.61 the deficiency indices of T on $(a, +\infty)$ are $(1, 1)$. In the same way we have that if $b \in \mathbb{R}$ and $a = -\infty$ then T has deficiency indices $(1, 1)$.
- If $a, b \in \mathbb{R}$, then both are regular points and by Remark 1.59 T is in the limit circle case at both end points. Hence, by Theorem 1.61, T has deficiency indices $(2, 2)$.
- If $a = -\infty$ and $b = \infty$ then T is essentially self-adjoint as shown in [Tri92, Section 5.2]. Therefore T has deficiency indices $(0, 0)$.

2 SCHRÖDINGER OPERATORS WITH SINGULAR PERTURBATIONS

The goal of this chapter is to describe the spectrum of the Schrödinger operator under finite δ and δ' perturbations. In particular, we are interested in the existence of negative eigenvalues.

2.1 Perturbations δ and δ' as self-adjoint extensions

Let $\{a_i\}_{i=1}^n \subset \mathbb{R}$ where with $a_0 = -\infty$, $a_{n+1} = \infty$ and $a_i < a_{i+1}$ por $i = 1, \dots, n$. Recall that in (1.15) we defined the differential expression

$$\mathcal{U} = -\frac{d^2}{dx^2} + q \qquad \text{on } \mathbb{R}.$$

In this section we will associate several operators with it and its restrictions to intervals of the form (a_i, a_{i+1}). Note that for an interval I and $f \in C_c^\infty(I)$, f can be extended to $\mathbb{R}$ by the function:

$$\widehat{f}(x) = \begin{cases} f(x) & \text{if } x \in I \\ 0 & \text{otherwise.} \end{cases}$$

$C_c^\infty(I)$ can be viewed as subspace of $L^2(\mathbb{R})$ through the inclusion

$$\begin{aligned} i : C_c^\infty(I) &\to L^2(\mathbb{R}) \\ f &\to \overline{\widehat{f}}. \end{aligned}$$

Define the symmetric densely defined operators

$$\mathbf{E}_i f = \mathcal{U} f; \quad D(\mathbf{E}_i) := C_c^\infty(a_i, a_{i+1}), \tag{2.1}$$

$$\mathbf{E} f = \mathcal{U} f; \quad D(\mathbf{E}) := C_c^\infty(\mathbb{R}). \tag{2.2}$$

Notice that all $\mathbf{E}_i$ are closable (because they are symmetric), so we denote $\overline{\mathbf{E}}_i = \mathbf{T}_i$. We define the closed symmetric operators

$$\mathbf{A} f = \mathcal{U} f; \quad D(\mathbf{A}) := \oplus_{i=0}^n D(\overline{\mathbf{E}}_i) =: \oplus_{i=0}^n D(\mathbf{T}_i), \tag{2.3}$$

$$\mathbf{T} f = \mathcal{U} f; \quad D(\mathbf{T}) := D(\overline{\mathbf{E}}). \tag{2.4}$$

By the Remark 1.65 we know that $\mathbf{T}$ has deficiency index $(0,0)$, therefore $\mathbf{T}$ is self-adjoint, $\mathbf{T}_0$ and $\mathbf{T}_n$ have deficiency indices $(1,1)$ and, for $1 \le i \le n-1$, $\mathbf{T}_i$ has deficiency indices $(2,2)$. Moreover, we know that

$$D(\mathbf{T}) = \{f \in L^2(\mathbb{R}) : f,\ f' \in \mathrm{AC}[\alpha,\beta], \text{ for all } [\alpha,\beta] \subset (a,b), \mathcal{U}f \in L^2(\mathbb{R})\}.$$

We define the closed symmetric operators based in the above operators

$$\mathbf{B}f := \mathcal{U}f, \quad D(\mathbf{B}) := \{f \in D(\mathbf{T}) :\ f(a_i) = 0;\ i = 1,\dots,n\}, \tag{2.5}$$

$$\mathbf{C}f := \mathcal{U}f, \quad D(\mathbf{C}) := \{f \in D(\mathbf{T}) :\ f(a_i) = f'(a_i) = 0;\ i = 1,\dots,n\}. \tag{2.6}$$

Note that $\mathbf{A}^*$ is given by

$$\mathbf{A}^* f(t) = \{\mathbf{T}_i^* f(t),\ a_i < t < a_{i+1},\ i = 0,\dots,n\},$$
$$D(\mathbf{A}^*) = \oplus_{i=0}^n D(\mathbf{T}_i^*).$$

We compute the adjoint of $\mathbf{B}$ and $\mathbf{C}$ arguing as in [SW16, Lemma 8].

Lemma 2.1. *We have the chain of extensions $\boldsymbol{A} \subset \boldsymbol{C} \subset \boldsymbol{B} \subset \boldsymbol{T} \subset \boldsymbol{B}^* \subset \boldsymbol{C}^* = \boldsymbol{A}^*$ and*

$$\boldsymbol{B}^* f = \boldsymbol{A}^* f; \quad D(\boldsymbol{B}^*) := \{f_\pm \in D(\boldsymbol{A}^*),\ f(a_i+) = f(a_i-),\ i = 1,\dots,n\}.$$

Proof. The chain of extensions follows directly from the definitions of the operators and the fact that $\mathbf{T}$ is self-adjoint. Let $f \in D(\mathbf{B})$ and $g \in D(\mathbf{A}^*)$. Integration by parts gives

$$\begin{aligned}
\langle \mathbf{B}f, g\rangle - \langle f, \mathbf{A}^* g\rangle &= \sum_{i=0}^n \int_{a_i}^{a_{i+1}} -f''\bar{g} + qf\bar{g}\,\mathrm{d}x + \int_{a_i}^{a_{i+1}} f\bar{g}'' - qf\bar{g}\,\mathrm{d}x \\
&= \sum_{i=0}^n -f'\bar{g}\ \Big|_{a_i}^{a_{i+1}} + f\bar{g}'\ \Big|_{a_i}^{a_{i+1}} \\
&= -f'(a_1)\overline{g(a_1-)} - \sum_{i=1}^{n-1}\left(f'(a_{i+1})\overline{g(a_{i+1}-)} - f'(a_i)\overline{g(a_i+)}\right) + f'(a_n)\overline{g(a_n+)} \\
&= \sum_{i=1}^n f'(a_i)\left(\overline{g(a_i+) - g(a_i-)}\right).
\end{aligned}$$

Note that $\lim_{x\to\infty} f'(x)g(x) = \lim_{x\to-\infty} f'(x)g(x) = 0$ because g is in L^2 and g' is absolutely continuous in (a_n,∞) and $(-\infty,a_1)$. Now $g \in D(\mathbf{B}^*)$, if and only if $\langle \mathbf{B}f, g\rangle - \langle f, \mathbf{A}^* g\rangle = 0$ for all $f \in D(\mathbf{B})$. For $i = 1,\dots,n$ we can choose $f_i \in D(\mathbf{B})$ such that $f_i'(a_i) = 1$ and $f_i'(a_j) = 0$ for $i \ne j$. Therefore, $g \in D(\mathbf{B}^*)$ if and only if $g \in D(\mathbf{A}^*)$ and $g(a_i+) = g(a_i-)$ for $i = 1,\dots,n$. Now for all $f \in D(\mathbf{C})$ and $g \in \mathbf{A}^*$ we obtain that

$$\langle \mathbf{C}f, g\rangle - \langle f, \mathbf{A}^* g\rangle = \sum_{i=1}^n f'(a_i)\left(\overline{g(a_i+) - g(a_i-)}\right) = 0,$$

therefore $\mathbf{A}^* = \mathbf{C}^*$. QED

Now we calculate the defect indices of **B** and **C** and give some of their self-adjoint realizations.

Proposition 2.2. *The deficiency indices of* **B** *and* **C** *are* (n,n) *and* $(2n,2n)$ *respectively and the following operators are self-adjoint extensions of* **B** *and* **C**, *respectively.*

$$\boldsymbol{B}_\alpha f = \boldsymbol{B}^* f; \quad D(\boldsymbol{B}_\alpha) := \{f \in D(\boldsymbol{B}^*) : \alpha_i f(a_i) = f'(a_i+) - f'(a_i-);\ k = 1, \dots, n\}, \tag{2.7}$$

$$\boldsymbol{C}_\alpha f = \boldsymbol{C}^* f; \quad D(\boldsymbol{C}_\alpha) := \left\{ f \in D(\boldsymbol{C}^*) : \begin{array}{c} f(a_i-) = f(a_i+), \\ \alpha_i f(a_i) = f'(a_i+) - f'(a_i-) \end{array}; k = 1, \dots, n \right\}, \tag{2.8}$$

$$\boldsymbol{C}_\beta f = \boldsymbol{C}^* f; \quad D(\boldsymbol{C}_\beta) := \left\{ f \in D(\boldsymbol{C}^*) : \begin{array}{c} f'(a_i-) = f'(a_i+), \\ \beta_i f'(a_i) = f'(a_i+) - f'(a_i-) \end{array}; k = 1, \dots, n \right\}, \tag{2.9}$$

where $\alpha = \{\alpha_i\}_{i=1}^n$ *and* $\beta = \{\beta_i\}_{i=1}^n$ *are subsets of* $\mathbb{R}$.

Proof. By Theorem 1.32 we have to compute appropriate boundary triplets for **B** and **C** . For $f, g \in D(\mathbf{B}^*)$ we obtain

$$\begin{aligned} \langle \mathbf{B}^* f, g \rangle - \langle f, \mathbf{B}^* g \rangle &= \sum_{i=1}^n f(a_i)\big(\bar{g}'(a_i-) - \bar{g}'(a_i+)\big) - \bar{g}(a_i)\big(f'(a_i-) - f'(a_i+)\big) \\ &= \langle \psi(f), \phi(g) \rangle - \langle \phi(f), \psi(g) \rangle \end{aligned}$$

where

$$\phi(f) = \big(f'(a_1-) - f'(a_1+),\ \dots,\ f'(a_n-) - f'(a_n+)\big); \qquad \psi(f) = \big(f(a_1), \dots, f(a_n)\big).$$

Note that $(\mathbb{C}^n, \phi, \psi)$ is a boundary triplet for $\mathbf{B}^*$ and by Theorem 1.32 **B** has deficiency indices (n,n) and therefore admits self-adjoint extensions. Define the self-adjoint operator in $\mathbb{C}^n$

$$F_\alpha = - \begin{pmatrix} \alpha_1^{-1} & 0 & \dots & 0 \\ 0 & \alpha_2^{-1} & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \alpha_n^{-1} \end{pmatrix}.$$

By Theorem 1.33 the operator $\mathbf{B}_\alpha := \mathbf{B}_{F_\alpha}$ defined as in (2.7) is a self-adjoint extension of **B**.

For $f, g \in D(\mathbf{C}_n^*)$ we have that

$$\begin{aligned}
\langle \mathbf{C}_n^* f, g\rangle - \langle f, \mathbf{C}_n^* g\rangle &= \sum_{i=1}^{n} f(a_i+)\bar{g}'(a_i+) - \bar{g}(a_i+)f'(a_i+) \\
&\quad + \sum_{i=1}^{n} -f(a_i-)\bar{g}'(a_i-) + \bar{g}(a_i-)f'(a_i-) \\
&= \sum_{i=1}^{n} f(a_i+)\bar{g}'(a_i+) - \bar{g}(a_i+)f'(a_i+) \\
&\quad + \sum_{i=1}^{n} \big(-f(a_i-)\big)\bar{g}'(a_i-) - \big(-\bar{g}(a_i-)\big)f'(a_i-) \\
&= \langle \Gamma_0(f), \Gamma_1(g)\rangle - \langle \Gamma_1(f), \Gamma_0(g)\rangle,
\end{aligned}$$

where

$$\Gamma_0(f) = \big(-f(a_1-), f(a_1+), \ldots, -f(a_n-), f(a_n+)\big) \tag{2.10}$$
$$\Gamma_1(f) = \big(f'(a_1-), f'(a_1+), \ldots, f'(a_n-), f'(a_n+)\big). \tag{2.11}$$

Note that $(\mathbb{C}^{2n}, \Gamma_0, \Gamma_1)$ is a boundary triplet for $\mathbf{C}^*$, and by Theorem 1.32, $\mathbf{C}$ has self-adjoint extensions with deficiency indices $(2n, 2n)$. Define the self-adjoint operator in $\mathbb{C}^{2n}$

$$R_\alpha = \frac{1}{2}\begin{pmatrix} \alpha_1 & -\alpha_1 & 0 & 0 & \ldots & 0 & 0 \\ -\alpha_1 & \alpha_1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \alpha_2 & -\alpha_2 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & \alpha_n & -\alpha_n \\ 0 & 0 & 0 & 0 & \ldots & -\alpha_n & \alpha_n \end{pmatrix},$$

acting on the closed subspace $\{(x_1, \ldots, x_{2n}) \in \mathbb{C}^{2n} : x_{2i} = -x_{2i-1},\ i = 1, \ldots, n.\} =: D(R_\alpha)$. By Theorem 1.33 (b) the operator $\mathbf{C}_\alpha := \mathbf{C}_{R_\alpha}$ defined as in (2.8) is a self-adjoint extension of $\mathbf{C}$.

In the same way define the Hermitian matrix on $\mathbb{C}^{2n}$

$$W_\beta = \begin{pmatrix} \beta_1^{-1} & \beta_1^{-1} & 0 & 0 & \ldots & 0 & 0 \\ \beta_1^{-1} & \beta_1^{-1} & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & \beta_2^{-1} & \beta_2^{-1} & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & \beta_n^{-1} & \beta_n^{-1} \\ 0 & 0 & 0 & 0 & \ldots & \beta_n^{-1} & \beta_n^{-1} \end{pmatrix},$$

with $D(W_\beta) = \mathbb{C}^{2n}$. By Theorem 1.33 (b) the operator $\mathbf{C}_\beta := \mathbf{C}_{W_\beta}$ defined as in (2.9) is a self-adjoint extension of $\mathbf{C}$. QED

Remark 2.3. (a) In the above proposition we did not calculate all self-adjoint extensions, we only calculated 3 special self-adjoint extensions. In addition $\mathbf{C}_\alpha$ and $\mathbf{C}_\beta$ can be interpreted as a formal definition for the differential expressions

$$\mathcal{V} := -\frac{d^2}{dx^2} + q(x) + \sum_{i=1}^{n} \alpha_i \delta_{a_i},$$

and

$$\mathcal{W} := -\frac{d^2}{dx^2} + q(x) + \sum_{i=1}^{n} \beta_i \delta'_{a_i},$$

respectively. Also, note that if $f \in D(\mathbf{C}_\alpha)$ then f is continuous in all a_i, so $f \in D(\mathbf{B}^*)$. This implies that $\mathbf{B}_\alpha = \mathbf{C}_\alpha$.

(b) Note that for the case $n = 1$, a boundary triplet for $\mathbf{C}$ is $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$ where

$$\Gamma_0 = \begin{pmatrix} -f(a_1-) \\ f(a_1+) \end{pmatrix}; \quad \Gamma_1 = \begin{pmatrix} f'(a_1-) \\ f'(a_1+) \end{pmatrix}.$$

By Theorem 1.33 all self-adjoint extensions are determined by the equation

$$V \begin{pmatrix} f'(a_1-) - if(a_1-) \\ f'(a_1+) + if(a_1+) \end{pmatrix} = \begin{pmatrix} f'(a_1-) + if(a_1-) \\ f'(a_1+) - if(a_1+) \end{pmatrix},$$

where $V \in \mathbb{M}(2 \times 2)$ is a unitary matrix. The above equation coincides with the condition obtained in [SW16] for the harmonic oscillator case.

(c) By the Lemma 2.1 we know that $\mathbf{T}$ is a self-adjoint extension of $\mathbf{B}$ and $\mathbf{C}$, and by Theorem 1.20 we obtain that $\mathbf{T}, \mathbf{C}_\alpha$ and $\mathbf{C}_\beta$ have the same essential spectrum. Moreover by [Tri92, Theorem 5.2.1] $\mathbf{T}$ has purely discrete spectrum, so $\mathbf{C}_\alpha$ and $\mathbf{C}_\beta$ have purely discrete spectrum.

(d) Let $\{e_j\}_{j=1}^{2n}$ be the canonical basis on $\mathbb{C}^{2n}$. Define the orthonormal basis $\{e_i^*\}_{i=1}^{2n}$ by

$$e_{2k-1}^* = \frac{1}{\sqrt{2}}(e_{2k-1} + e_{2k}), \quad e_{2k}^* = \frac{1}{\sqrt{2}}(e_{2k} - e_{2k-1}),$$

for $k = 1, \dots, n$.

We can obtain $\mathbf{C}_\alpha$ as self-adjoint extension of $\mathbf{C}$ using the equations (1.10)-(1.11) for the self-adjoint operator

$$R'_\alpha = \begin{pmatrix} \alpha_1 & 0 & \cdots & 0 & 0 \\ 0 & \alpha_2 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & \alpha_{n-1} & 0 \\ 0 & 0 & \cdots & 0 & \alpha_n \end{pmatrix},$$

acting on the closed subspace $\{e_{2k}^*\}_{k=1}^{n}$.

2.2 Negative squares of $\mathbf{C}^*$

Taking the boundary triplet $(\mathbb{C}^{2n}, \Gamma_0, \Gamma_1)$ for $\mathbf{C}^*$ defined by (2.10) and (2.11) and the operators on $\mathbb{C}^{2n}$:

$$G = \begin{pmatrix} 0 & \alpha_1 & \dots & 0 & 0 \\ 1 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & \alpha_n \\ 0 & 0 & \dots & 1 & 1 \end{pmatrix}, \quad D = \begin{pmatrix} -1 & 1 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & -1 & 1 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \tag{2.12}$$

it is clear that $\mathbf{C}_\alpha = \mathbf{C}_{G,D}$. Notice that if the potential satisfies $q(x) \geq 0$ for all $x \in \mathbb{R}$ then $\mathbf{C}$ is positive. We want to apply the Proposition 1.38 to $\mathbf{C}$, so we have to prove that $\mathbf{C}_0 = \mathbf{C}^*|_{\ker \Gamma_0}$ is the Friedrich extension of $\mathbf{C}$.

Proposition 2.4. *If q is continuous lower bounded on $\mathbb{R}$ (i.e. $q(x) \geq \gamma$ for all $x \in \mathbb{R}$ for some $\gamma \in \mathbb{R}$), then we have for the Friedrichs extension $\boldsymbol{C}_F$*

$$\boldsymbol{C}_F f = \boldsymbol{C}^* f; \quad D(\boldsymbol{C}_F) = D(\boldsymbol{C}_0) = D(\boldsymbol{C}^*) \cap \{f \in L^2(\mathbb{R}) : f(a_i) = 0,\ i = 1, \dots, n\}.$$

Proof. By the Proposition 1.28 we only have to prove the assertion for $q \geq 0$. The boundary triplet $(\mathbb{C}^{2n}, \Gamma_0, \Gamma_1)$ defined by (2.10) and (2.11), has the form

$$\mathcal{K} = \oplus_{i=0}^n \mathcal{K}_i, \quad \Gamma_0 = \oplus_{i=0}^n \Gamma_0^i; \quad \Gamma_1 = \oplus_{i=0}^n \Gamma_1^i, \tag{2.13}$$

where:

$$\mathcal{K}_0 = \mathbb{C}, \quad \Gamma_0^0 f = -f(a_1-), \quad \Gamma_1^0 f = f'(a_1-),$$

$$K_i = \mathbb{C}^2, \quad \Gamma_0^i f = \begin{pmatrix} f(a_i+) \\ -f(a_{i+1}-) \end{pmatrix}, \quad \Gamma_1^i f = \begin{pmatrix} f'(a_i+) \\ f'(a_{i+1}-) \end{pmatrix}, \quad \text{for } i = 1, \dots n-1, \tag{2.14}$$

and

$$\mathcal{K}_n = \mathbb{C}, \quad \Gamma_0^n f = f(a_n+), \quad \Gamma_1^n f = f'(a_n+).$$

Let us denote the Friedrichs extension of $\mathbf{T}_i$ by $\mathbf{T}_{i,F}$ and let $\mathbf{T}_{i,0} = \mathbf{T}_i^*|_{\ker(\Gamma_0^i)}$. Since $\mathbf{A}^* = \mathbf{C}^*$, we only have to prove that $\mathbf{T}_{i,F} = \mathbf{T}_{i,0}$ for $i = 0, \dots, n$. By the Remark 1.29 we have that $\overline{s_{\mathbf{T}_i}} = \overline{s_{\mathbf{E}_i}}$. Now if $f \in C_c^\infty(a_i, a_{i+1})$, integration by parts gives:

$$s_{\mathbf{E}_i}[f] = \langle \mathbf{E}_i f, f \rangle = \|f'\|^2 + \|\sqrt{q} f\|^2.$$

If $i = 1, \dots, n-1$, then the closure of $(C_c^\infty, \|\cdot\|_{s_{\mathbf{E}_i}})$ is $H_0^1(a_i, a_{i+1})$. Because q is continuous in $\mathbb{R}$, we have that $q \in L^2(a_i, a_{i+1})$ and

$$D(\mathbf{T}_{i,F}) = D(\mathbf{T}_i^*) \cap H_0^1(a_i, a_{i+1}) = D(\mathbf{T}_i^*) \cap \text{Ker}(\Gamma_0).$$

For $i = 0$ we have that

$$D(\overline{s_{\mathbf{T}_i}}) = H_0^1 \cap \{f \in L^2(-\infty, a_1) : \ \sqrt{q} f \in L^2(-\infty, a_1)\} \subset \text{Ker}(\Gamma_0),$$

therefore $\mathbf{T}_{0,F} \subset \mathbf{T}_{0,0}$, and by definition $\mathbf{T}_{0,F}$ and $\mathbf{T}_{0,0}$ are self-adjoint, which implies that $\mathbf{T}_{0,F} = \mathbf{T}_{0,0}$. In the same way we obtain that $\mathbf{T}_{n,F} = \mathbf{T}_{n,0}$. QED

Recall that for a self-adjoint operator T the number of negative squares is defined by $k_-(T) = \dim(E_T(-\infty,0))$, where E_T is the spectral resolution of T. Suppose that $q \geq 0$, by Theorem 1.38 we obtain

$$k_-\left(\mathbf{C}_{G,D}\right) = k_-(GD^* - DM(0)D^*).$$

We calculate the Weyl function of $\mathbf{C}$ in terms of the Weyl function of $\mathbf{T}_i$.

Let $\lambda \in \cap_i^n \rho(\mathbf{T}_{i,0})$. By the Remark 1.65, $\mathbf{T}_i$ has deficiency indices $(1,1)$ for $i=0$ and $i=n$, and $\mathbf{T}_i$ has deficiency indices $(2,2)$ for $i=1,\dots,n-1$. Given that q is regular for all a_i, by Theorem 1.56 all solutions of (1.17) on (a_i,a_{i+1}) and its derivatives can be extended to the closed interval $[a_i,a_{i+1}]$ for $i=1,\dots,n-1$. It is well known [Tes14, Theorem 9.1] that there exist solutions $S_i(x,\lambda)$ and $C_i(x,\lambda)$ of the differential equation (1.17) on (a_i,a_{i+1})

$$S_i(a_i,\lambda)=0; \quad S_i'(a_i,\lambda)=1; \quad C_i(a_i,\lambda)=1; \quad C_i'(a_i,\lambda)=0, \tag{2.15}$$

and $S_i(\cdot,\lambda), C_i(\cdot,\lambda) \in L^2(a_i,a_{i+1})$ for $i=1,\dots n-1$. Note that $S_i(\cdot,\lambda)$ and $C_i(\cdot,\lambda)$ are linearly independent on (a_i,a_{i+1}), so $\{S_i(\cdot,\lambda), C_i(\cdot,\lambda)\}$ is a base for $\operatorname{Ker}(\mathbf{T}_i^*-\lambda)$. Is well known from [HS81] that given the solutions $S_0(x,\lambda)$ and $C_0(x,\lambda)$ on (∞,a_1) such that

$$S_0(a_1,\lambda)=0; \quad S_0'(a_1,\lambda)=1; \quad C_0(a_1,\lambda)=1; \quad C_0'(a_1,\lambda)=0, \tag{2.16}$$

there exists a unique complex number $m_0(\lambda)$ known as the Weyl-Titchmarsh function (that can be ∞ in the eigenvalues of $\mathbf{T}_{0,0}$) such that

$$u_0(x,\lambda) = C_0(x,\lambda) + m_0(\lambda)S_0(x,\lambda) \in L^2(-\infty,a_1).$$

In the same way there exist solutions $S_n(x,\lambda)$ and $C_n(x,\lambda)$ on (a_n,∞) such that (2.15) holds and a respective Weyl-Titchmarsh function $m_n(\lambda)$ such that

$$u_n(x,\lambda) = C_n(x,\lambda) + m_n(\lambda)S_n(x,\lambda) \in L^2(a_n,\infty).$$

Notice that $\{u_0(\cdot,\lambda)\}$ and $\{u_n(\cdot,\lambda)\}$ are bases for $\operatorname{Ker}(\mathbf{T}_0^*-\lambda)$ and $\operatorname{Ker}(\mathbf{T}_n^*-\lambda)$ respectively. Let f be a solution of $(\mathbf{C}^*-\lambda)\,f=0$, then $f|_{(a_i,a_{i+1})}$ is solution of $(\mathbf{T}_i^*-\lambda)f=0$ for $i=0,\dots,n$. Therefore

$$f = y_1u_0(\cdot,\lambda) + \sum_{i=1}^{n-1} y_{2i}S_i(\cdot,\lambda) + y_{2i+1}C_i(\cdot,\lambda) + y_{2n}u_n(\cdot,\lambda). \tag{2.17}$$

The equation (2.17) implies that

$$\begin{aligned} \operatorname{Ker}(\mathbf{C}_n^*-\lambda) &= \oplus_{i=0}^n \operatorname{Ker}(\mathbf{T}_i^*-\lambda) && (2.18)\\ &= \operatorname{Span}\{u_0(\cdot,\lambda)\} \oplus \cdots \oplus \operatorname{Span}\{u_n(\cdot,\lambda)\}. && (2.19) \end{aligned}$$

Let us denote by $M(\lambda)$ the Weyl function for $\mathbf{C}^*$ associated with the boundary triplet $(\mathbb{C}^{2n},\Gamma_0,\Gamma_1)$ defined by (2.10) and (2.11) and let $M_i(\lambda)$ be the Weyl function for each $\mathbf{T}_i$ associated with the boundary triplet $(\mathcal{K}, \Gamma_0^i, \Gamma_1^i)$ defined by (2.14). The equations (2.13) and (2.18) suggest that $M(\lambda)$ is of the form

$$M(\lambda) = \oplus_{i=0}^n M_i(\lambda).$$

We know that solutions u_i of $(\mathbf{T}_i^* - \lambda)u_i = 0$ for $i = 1, \dots, n-1$ are of the form

$$u_i(x, \lambda) = y_{2i} S_i(x, \lambda) + y_{2i+1} C_i(x, \lambda).$$

Now, using the boundary values of S_i and C_i, we obtain

$$u_i(x) = (u(a_{i+1}-) - u(a_i+)C_i(a_{i+1}, \lambda))\, S_i(a_{i+1}, \lambda)^{-1} S_i(x, \lambda) + u(a_i+)C_i(x, \lambda). \tag{2.20}$$

The equation $M_i(\lambda)\Gamma_0^i u_i = \Gamma_1^i u_i$ means that

$$M_i(\lambda) \begin{pmatrix} u_i(a_i+) \\ -u_i(a_{i+1}-) \end{pmatrix} = \begin{pmatrix} u_i'(a_i+) \\ u_i'(a_{i+1}-) \end{pmatrix}, \quad \text{for } u_i \in \operatorname{Ker}(T_i^* - \lambda).$$

Note that $S_i(a_{i+1}, \lambda) \neq 0$, if so, $\Gamma_0^i S_i(\cdot, \lambda) = 0$ and $\lambda \notin \rho(\mathbf{T}_{i,0})$. Inserting the values $u_i'(a_i)$ and $u_i'(a_{i+1})$ obtained from (2.20) a simple computation shows that

$$M_i(\lambda) = -\frac{1}{S_i(a_{i+1}, \lambda)} \begin{pmatrix} C_i(a_{i+1}, \lambda) & 1 \\ 1 & S_i'(a_{i+1}, \lambda) \end{pmatrix}. \tag{2.21}$$

For the case $i = n$ we know that if $f \in \ker(\mathbf{T}_0^* - \lambda)$ then it is of the form

$$f(x) = f(a_n+)\left(C_n(x, \lambda) + m_n(\lambda) S_n(x, \lambda)\right),$$

where $m_n(\lambda)$ is the Weyl-Titchmarsh function associated to $\mathbf{T}_n^*$. So, the equation $M_n(\lambda)\Gamma_0^n u_n = \Gamma_1^n u_n$ means that

$$M_n(\lambda) f(a_n+) = f'(a_n+)$$

which implies that $M_n(\lambda) = m_n(\lambda)$. Analogously we obtain that $M_0(\lambda) = -m_0(\lambda)$ where $m_0(\lambda)$ is the Weyl-Titchmarsh function associated to $\mathbf{T}_0^*$.

Remark 2.5. By [Tes14, Theorem 9.1], $S_i(\cdot, \lambda)$ and $C_i(\cdot, \lambda)$ are holomorphic with respect to λ and by Theorem 1.38 we know that $M_i(0) := \mathrm{S} - \mathrm{R} - \lim_{\lambda \uparrow 0} M_i(\lambda)$ exist. We know that the inverse as operation is continuous in the matrix norm, therefore

$$M_i(0) = \lim_{\lambda \uparrow 0} M_i(\lambda),$$

and (2.21) joint with the fact that the Wroskian is constant in all solution interval [BD01, Abel's theorem 3.3.2] we obtain:

$$M_i(0) = -\frac{1}{S_i(a_{i+1}, 0-)} \begin{pmatrix} C_i(a_{i+1}, 0-) & 1 \\ 1 & S_i'(a_{i+1}, 0-) \end{pmatrix} := -\frac{1}{s_i} \begin{pmatrix} c_i & 1 \\ 1 & s_i' \end{pmatrix} \tag{2.22}$$

For $i = 0$ and $i = n$, we obtain that the individual limits $m_n(0) := \lim_{\lambda \uparrow 0} m_n(\lambda)$ and $m_0(0) := \lim_{\lambda \uparrow 0} m_0(\lambda)$ exist.

Now we present a result similar to [GO10, Theorem 3.1].

Theorem 2.6. *Let $\mathbf{C}_\alpha$ be defined as in* (2.7) *and the Jacobi matrix*

$$Y = \begin{pmatrix} \gamma_1 & -s_1^{-1} & 0 & \dots & 0 & 0 \\ -s_1^{-1} & \gamma_2 & -s_2^{-1} & \dots & 0 & 0 \\ 0 & -s_2^{-1} & \gamma_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \gamma_{n-1} & -s_{n-1}^{-1} \\ 0 & 0 & 0 & \dots & -s_{n-1}^{-1} & \gamma_n \end{pmatrix},$$

where

$$\gamma_1 = \alpha_1 + m_0(0) + \frac{c_1}{s_1}, \tag{2.23}$$

$$\gamma_n = \alpha_n - m_n(0) + \frac{s'_{n-1}}{s_{n-1}}, \tag{2.24}$$

$$\gamma_i = \alpha_i + \frac{c_i}{s_i} + \frac{s'_{i-1}}{s_{i-1}}, \qquad \text{for } i = 2, \dots, n-1. \tag{2.25}$$

Then $k_-(\mathbf{C}_\alpha) = k_-(Y)$. In particular, $\mathbf{C}_\alpha$ can have at most n negative eigenvalues.

Proof. Recall that $\mathbf{C}_\alpha = \mathbf{C}_{G,D}$ with G and D defined by (2.12), and by (2.22)

$$M(0) = \oplus_{i=0}^{n} M_i(0) = \begin{pmatrix} -m_0(0) & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & -\frac{c_1}{s_1} & -s_1^{-1} & \dots & 0 & 0 & 0 \\ 0 & -s_1^{-1} & -\frac{s'_1}{s_1} & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -\frac{c_{n-1}}{s_{n-1}} & -s_{n-1}^{-1} & 0 \\ 0 & 0 & 0 & \dots & -s_{n-1}^{-1} & -\frac{s'_{n-1}}{s_{n-1}} & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & m_n(0) \end{pmatrix} \in \mathbb{M}(2n \times 2n).$$

Now by simple calculations we obtain that

$$GD^* - DM(0)D^* = \begin{pmatrix} \gamma_1 & 0 & -s_1^{-1} \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 \dots & 0 & 0 & 0 & 0 \\ -s_1^{-1} & 0 & \gamma_2 \dots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots \dots & \vdots & \vdots & \vdots & \\ 0 & 0 & 0 \dots & \gamma_{n-1} & 0 & -s_{n-1}^{-1} & 0 \\ 0 & 0 & 0 \dots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 \dots & -s_{n-1}^{-1} & 0 & \gamma_n & 0 \\ 0 & 0 & 0 \dots & 0 & 0 & 0 & 0 \end{pmatrix} \in \mathbb{M}(2n \times 2n).$$

With respect to the decomposition $\mathbb{C}^{2n} = H_1 \oplus H_2$, where $H_1 = \operatorname{Span}\{e_{2i-1}\}_{k=1}^{n}$ and $H_2 = \operatorname{Span}\{e_{2i}\}_{k=1}^{n}$, the operator $GD^* - DM(0)D^*$ admits the representation $GD^* - DM(0)D^* =$

$Y \oplus 0_{H_2}$, moreover

$$GD^* - DM(0)D^* = \begin{pmatrix} Y & 0 \\ 0 & 0 \end{pmatrix}.$$

Hence λ is an eigenvalue different from 0 of $GD^* - DM(0)D^*$ if and only if it is an eigenvalue of Y different from 0. So $k_-(GD^* - DM(0)D^*) = k_-(S)$, and applying the Theorem 1.38, the proof is complete. QED

In the same way, note that $\mathbf{C}_\beta = \mathbf{C}_{G',D'}$ with

$$D' = \begin{pmatrix} -1 & 1 & \cdots & 0 & 0 \\ 0 & \beta_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & -1 & 1 \\ 0 & 0 & \cdots & 0 & \beta_n \end{pmatrix}, \quad G' = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 1 & 1 \end{pmatrix}.$$

and and after few calculations we obtain that $R = G'D'^* - D'M(0)D'^* \in \mathbb{M}(2n \times 2n)$ is of the form

$$R = \begin{pmatrix} m_0(0) + \frac{c_1}{s_1} & \beta_1 \frac{c_1}{s_1} & -s_1^{-1} & \cdots & 0 & 0 & 0 & \\ \beta_1 \frac{c_1}{s_1} & \beta_1 + \beta_1^2 \frac{c_1}{s_1} & -\beta_1 s_1^{-1} & \cdots & 0 & 0 & 0 & \\ -s_1^{-1} & -\beta_1 s_1^{-1} & \frac{s_1'}{s_1} + \frac{c_2}{s_2} & \cdots & 0 & 0 & 0 & \\ 0 & 0 & \beta_2 \frac{c_2}{s_2} & \cdots & 0 & 0 & 0 & \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta_{n-1} \frac{c_{n-1}}{s_{n-1}} & -s_{n-1}^{-1} & 0 & \\ 0 & 0 & 0 & \cdots & \beta_{n-1} + \beta_{n-1}^2 \frac{c_{n-1}}{s_{n-1}} & -\beta_{n-1} s_{n-1}^{-1} & 0 & \\ 0 & 0 & 0 & \cdots & -\beta_{n-1} s_{n-1}^{-1} & \frac{s_{n-1}'}{s_{n-1}} - & -\beta_n m_n(0) & \\ 0 & 0 & 0 & \cdots & 0 & -\beta_n m_n(0) & \beta_n - \beta_n^2 m_n(0) & \end{pmatrix}.$$

By Theorem 1.38 $k_-(\mathbf{C}_\beta) = k_-(R)$. We want to obtain a sufficient condition for $k_-(\mathbf{C}_\alpha) \geq m$, as well as for the equality $k_-(\mathbf{C}_\alpha) = m$, with arbitrary natural $m \leq n$ by using the following Gerschgorin Theorem (see [LT85, Theorem 7.2.1]).

Theorem 2.7. *All eigenvalues of a complex matrix $A = (a_{ij})_{i,j=1}^n$ are contained in the union of the Gershgorin disks*

$$G_i = \left\{ z \in \mathbb{C} : \; |z - a_{ii}| \leq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \right\}, \qquad i = 1, \ldots, n.$$

Theorem 2.8. *Let $K = \{k_i\}_{i=1}^m$ be a subset of $\{1, \ldots, n\}$ such that $|K| = m \leq n$. Assume that*

$$\alpha_{k_i} < -\left(\frac{c_{k_i}}{s_{k_i}} + \frac{s_{k_i-1}'}{s_{k_i-1}} \right) - s_{k_i}^{-1} - s_{k_i-1}^{-1}, \qquad k_i \in K, \; k_i \neq 1, \tag{2.26}$$

if $1 = k_1$ *then*

$$\alpha_1 < -\left(m_0(0) + \frac{c_1}{s_1}\right) - s_1^{-1}, \tag{2.27}$$

or $n = k_m$, *then*

$$\alpha_n < -\left(-m_n(0) + \frac{s'_{n-1}}{s_{n-1}}\right) - s_{n-1}^{-1}. \tag{2.28}$$

Then $k_-(\mathbf{C}_\alpha) \geq m$.

Proof. First assume that $K = \{1, \dots, m\}$. Denote by Y_m the submatrix in the upper left corner of the matrix Y defined as in Theorem 2.6. According to the minimax principle (see [Gla66]),

$$k_-(Y_m) \leq k_-(Y) = k_-(\mathbf{C}_\alpha).$$

Applying Theorem 2.7 to Y_m and using the equations (2.26) and (2.27), we obtain $k_-(Y_m) = m$. Further, setting $\alpha_k = 0$ for $k \in \{1, \dots, m\}$, we obtain a non-negative self-adjoint operator $\widehat{\mathbf{C}}_\alpha$. It is clear that $\mathbf{C}_\alpha$ is an $m-$dimensional perturbation of the operator $\widehat{\mathbf{C}}_\alpha$. Thus, from the minimax principle it follows that $k_-(\mathbf{C}_\alpha) \leq m$ and the theorem has been proved for all submatrices in the upper left corner.

Let K be an arbitrary set consisting of m natural numbers. This case can be reduced to the previous one. Namely, there exists a unitary transformation U such that

$$\widehat{Y} = U^* Y U, \quad U : s_{k_i k_i} \to \widehat{s_{ii}}, \quad \sum_{j \neq k_i} |s_{k_i j}| = \sum_{j \neq i} |\widehat{s_{k_i j}}|, \quad k_i \in K.$$

Applying the previous reasoning to the matrix $\widehat{Y}$, we complete the proof. QED

Finally we give an algorithm for the calculation of negative squares of $\mathbf{C}_\alpha$. We introduce the Sylvester criterion [Mal92, Lemma 4].

Proposition 2.9. *Let $T(H \to H)$ be a self-adjoint operator which admits the block-matrix representation*

$$T = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$

with respect to the orthogonal decomposition $H = H_1 \oplus H_2$, where $T_{11} \in C(H_1)$, $T_{12} = T_{21}^* \in C(H_2, H_1)$ and $T \in C(H_2)$. If $0 \in \rho(T_{11})$, then

$$k_-(T) = k_-(T_{11}) + k_-(T_{22} - T_{21} T_{11}^{-1} T_{12}). \tag{2.29}$$

Define the sequence $\{\zeta_k\}_{k=1}^n$ by

$$\zeta_1 := \gamma_1 \tag{2.30}$$

$$\text{if } \zeta_k \neq 0, \text{ then} \quad \zeta_{k+1} := \gamma_{k+1} - s_k^{-2} \zeta_k^{-1}, \ k \leq n-1, \tag{2.31}$$

$$\text{if } \zeta_k = 0, \text{ then} \quad \begin{cases} \zeta_{k+1} := \infty, \ k \leq n-1, \\ \zeta_{k+2} := \gamma_{k+2}, \ k \leq n-2. \end{cases} \tag{2.32}$$

The Sylvester criterion establishes the connection between the sequence $\{\zeta_k\}_{k=1}^\infty$ and $k_-(S)$.

Theorem 2.10. *Let $\boldsymbol{C}_\alpha$ be defined as in* (2.7) *and* $\zeta := \{\zeta_k\}_{k=1}^n$ *the sequence given by the equations* (2.30) *to* (2.32). *Then*

$$k_-(\boldsymbol{C}_\alpha) = k_-(\zeta) + N_\infty(\zeta),$$

where $k_-(\zeta)$ and $N_\infty(\zeta)$ are the number of negative and infinite elements respectively, in the sequence ζ.

Proof. We divide the proof in two cases

- Supose that $\zeta_1 \neq 0$. Then we can take the orthogonal descomposition of $\mathbb{C}^n = \mathbb{C} \oplus \mathbb{C}^{n-1}$ and

$$Y = \begin{pmatrix} \zeta_1 I_{\mathbb{C}} & T_{12} \\ T_{21} & T_{22} \end{pmatrix},$$

where

$$T_{12} = \begin{pmatrix} -s_1^{-1} & 0 & \cdots & 0 \end{pmatrix}; \quad T_{21} = \begin{pmatrix} -s_1^{-1} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

and

$$T_{22} = \begin{pmatrix} \gamma_2 & -s_2^{-1} & \dots & 0 & 0 \\ -s_2^{-1} & \gamma_3 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & \gamma_{n-1} & -s_{n-1}^{-1} \\ 0 & 0 & \dots & -s_{n-1}^{-1} & \gamma_n \end{pmatrix} \in \mathbb{M}(n-1 \times n-1).$$

Note that

$$\left[T_{21} \begin{pmatrix} x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} \right] y = -s_1^{-1} x_1 y = \begin{pmatrix} x_1 \\ \vdots \\ x_{n-1} \end{pmatrix} \cdot [T_{12}(y)],$$

for all $(x_1, \dots, x_{n-1}) \in \mathbb{C}^{n-1}$ and $y \in \mathbb{C}$. Then $T_{21} = T_{12}^*$. Applying the Proposition 2.29 we obtain

$$k_-(Y) = k_-(\zeta_1) + k_-(s_2)$$

where

$$s_2 = \begin{pmatrix} \zeta_2 & -s_2^{-1} & \dots & 0 & 0 \\ -s_2^{-1} & \gamma_3 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & \gamma_{n-1} & -s_{n-1}^{-1} \\ 0 & 0 & \dots & -s_{n-1}^{-1} & \gamma_n \end{pmatrix} \in \mathbb{M}(n-1 \times n-1).$$

Now if $\zeta_2 \neq 0$ then we can apply the above argument for the matrix Y_2. Thus, if $\zeta_k \neq 0$ for all $k \leq n$ then $N_\infty(\zeta) = 0$ and we obtain $k_-(Y) = k_-(\zeta)$.

- Assume that $\zeta_1 = 0$, then $\zeta_2 = \infty$ and $\zeta_3 = \gamma_3$. So we can take the orthogonal decomposition of $\mathbb{C}^n = \mathbb{C}^2 \oplus \mathbb{C}^{n-2}$ and

$$Y = \begin{pmatrix} T_{11} & T_{12} \\ T_{21} & Y_3 \end{pmatrix},$$

where

$$T_{11} = \begin{pmatrix} 0 & -s_1^{-1} \\ -s_1^{-1} & \gamma_2 \end{pmatrix}, \; T_{21} = \begin{pmatrix} 0 & -s_2^{-1} \\ \vdots & \vdots \\ 0 & 0 \end{pmatrix} \in \mathbb{M}(n-2 \times 2),$$

$$T_{12} = \begin{pmatrix} 0 & \cdots & 0 \\ -s_2^{-1} & \cdots & 0 \end{pmatrix} \in \mathbb{M}(2 \times n-2),$$

and

$$Y_3 = \begin{pmatrix} \gamma_3 & -s_3^{-1} & \dots & 0 & 0 \\ -s_3^{-1} & \gamma_4 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & \gamma_{n-1} & -s_{n-1}^{-1} \\ 0 & 0 & \dots & -s_{n-1}^{-1} & \gamma_n \end{pmatrix} \in \mathbb{M}(n-1 \times n-1).$$

Note that $\det(T_{11}) = -s_1^2 \neq 0$, therefore we can apply the Proposition 2.29 again, and given that the eigenvalues of T_{11} are

$$\lambda_1 = \frac{\gamma_2 + \sqrt{\gamma_2^2 + 4s_1^2}}{2} > 0, \quad \lambda_2 = \frac{\gamma_2 - \sqrt{\gamma_2^2 + 4s_1^2}}{2} < 0$$

we obtain $k_-(Y) = N_\infty\{\zeta_1, \zeta_2\} + k_-(Y_3)$. Proceeding as above we obtain de result.

QED

Remark 2.11. By [Tes14, Theorem 9.1] there exist solutions $U(\cdot, \lambda), W(\cdot, \lambda)$ of (1.17) such that

$$U(0, \lambda) = 0, \quad U'(0, \lambda) = 1, \quad W(0, \lambda) = 1, \quad W'(0, \lambda) = 0$$

on $\mathbb{R}$. So, U and W are solutions linearly independent on $\mathbb{R}$ with Wronskian equal to 1. In addition they are solutions in $L^2(a_i, a_{i+1})$ for $i = 1, \dots, n-1$. Then, the solutions S_i and C_i of (1.17) described by (2.16) can be written in terms of U and W. Taking account that $U(x, \lambda) \neq 0$, for $x \neq 0$ and $\lambda \in \rho(\Gamma_0)$ we obtain

$$S_i(x, z) = W(a_i, \lambda)U(x, \lambda) - U(a_i, \lambda)W(x, \lambda) \tag{2.33}$$

$$C_i(x, z) = U'(a_i, \lambda)W(x, \lambda) - W'(a_i, \lambda)U(x, \lambda). \tag{2.34}$$

2.2.1 Negative squares of the harmonic oscillator

For the harmonic oscillator it is well known (see for instance [BD01, Chapter 5]) that the solutions described in Remark 2.11 are

$$W(x, 0) = 1 + \sum_{i=1}^{\infty} \frac{x^{4i}}{\prod_{k=1}^{i} 4k(4k-1)}; \; U(x, 0) = x\left(1 + \sum_{i=1}^{\infty} \frac{x^{4i}}{\prod_{k=1}^{i} 4k(4k+1)}\right). \tag{2.35}$$

Note that W and U are even and odd respectively, and by [BD01, Theorem 5.3.1] both are defined in all $\mathbb{R}$.

Due to the following inequalities

$$\frac{1}{3^2 2n(2n-1)} < \frac{1}{4n(4n-1)} < \frac{1}{2^2 2n(2n-1)}, \qquad \text{for } n \in \mathbb{N},$$
$$\frac{1}{2^2 2n(2n+1)} < \frac{1}{4n(4n+1)} < \frac{1}{4n(2n+1)}, \qquad \text{for } n \in \mathbb{N}$$

by the parity of the functions we obtain

$$\cosh\left(\frac{x^2}{3}\right) < W(x,0) < \cosh\left(\frac{x^2}{2}\right) \qquad \text{for } x \in \mathbb{R},$$
$$\sinh\left(\frac{x^2}{2}\right) < U(x,0) < \sinh\left(\frac{x^2}{\sqrt{2}}\right), \qquad \text{for } x \in \mathbb{R}^+,$$
$$-\sinh\left(\frac{x^2}{2}\right) > U(x,0) > -\sinh\left(\frac{x^2}{\sqrt{2}}\right), \qquad \text{for } x \in \mathbb{R}^-$$

Now, recall that in [SW16, Lemma 6] it is shown that

$$V(x,-\omega^2) := W(x,-\omega^2)\int_x^\infty W(t,-\omega^2)^{-2}\,\mathrm{d}t,$$

is a solution of (1.17) with $\lambda = -\omega^2$ in $L^2(a_n,\infty)$, and we obtain that

$$m_n(-\omega^2) = \frac{V'(a_n,-\omega^2)}{V(a_n,-\omega^2)} = \frac{W'(a_n,-\omega^2)}{W(a_n,-\omega^2)} - \frac{\left(\int_{a_n}^\infty W(t,-\omega^2)^{-2}\,\mathrm{d}t\right)^{-1}}{W^2(a_n,-\omega^2)}.$$

In the same way $V(-x,-\omega^2)$ is a solution of (1.17) in $L^2(-\infty,a_1)$ and

$$m_0(-\omega^2) = -\frac{V'(-a_1,-\omega^2)}{V(-a_1,-\omega^2)} = \frac{W'(a_1,-\omega^2)}{W(a_1,-\omega^2)} + \frac{\left(\int_{-\infty}^{a_1} W(t,-\omega^2)^{-2}\,\mathrm{d}t\right)^{-1}}{W^2(a_1,-\omega^2)}.$$

Remark 2.12. Denote $W(a_{i+1},0) := W_i$, $U(a_{i+1},0) := U_i$ for all $i = 0,\dots,n$ and let $\phi(t) := \left(\int_x^\infty W(t,0)^{-2}\,\mathrm{d}t\right)^{-1}$. Now we will consider the next two cases

(a) Consider $\mathbf{C}_\alpha$ and $\mathbf{C}_\beta$ with only one interaction in a point a_1 with potential x^2. we have that the Weyl function is given by

$$M(0) = \begin{pmatrix} -m_0(0) & 0 \\ 0 & m_n(0) \end{pmatrix}$$

then:

- For $\mathbf{C}_\alpha$ we obtain

$$GD^* - DM(0)D^* = \begin{pmatrix} \alpha + \frac{\phi(a_1)+\phi(-a_1)}{W^2(a_1,0)} & 0 \\ 0 & 0 \end{pmatrix},$$

so, $\mathbf{C}_\alpha$ has a negative eigenvalue if and only if

$$\alpha < -\frac{\phi(a_1)+\phi(-a_1)}{W^2(a_1,0)} < 0.$$

Note that for the case $a_1 = 0$ we obtain that

$$\frac{\phi(a_1)+\phi(-a_1)}{W^2(a_1,0)} = 2\phi(0),$$

so, taking $\alpha = 2\cot(\theta)$ we obtain the same result as in [SW16, Lemma 11].

- For $\mathbf{C}_\beta$ we obtain that

$$G'D'^* - D'M(0)D'^* = \begin{pmatrix} \frac{\phi(a_1)+\phi(-a_1)}{W^2(a_1,0)} & -\left(\frac{W'(a_1,0)}{W(a_1,0)} - \frac{\phi(a_1)}{W^2(a_1,0)}\right)\beta \\ -\left(\frac{W'(a_1,0)}{W(a_1,0)} - \frac{\phi(a_1)}{W^2(a_1,0)}\right)\beta & \beta - \left(\frac{W'(a_1,0)}{W(a_1,0)} - \frac{\phi(a_1)}{W^2(a_1,0)}\right)\beta^2 \end{pmatrix}.$$

For the case $a_1 = 0$

$$\det(G'D'^* - D'M(0)D'^*) = \phi(0)\left(\beta^2 + \frac{2}{\phi(0)}\beta\right)$$

so, given that $\phi(0) > 0$, $G'D'^* - D'M(0)D'^*$ has a negative eigenvalue if and only if $\beta \in (-\frac{2}{\phi(0)}, 0)$ (see for instance [Str06, Chapter 6]).

(b) Consider $\mathbf{C}_\alpha$ with 2 or more interactions. By the Remark 2.11 and equations (2.26)-(2.28), we obtain that $\mathbf{C}_\alpha$ has n negative eigenvalues if

$$\alpha_i < -\frac{U'_{i-1}W_i - W'_{i-1}U_i + 1}{W_{i-1}U_i - U_{i-1}W_i} - \frac{W_{i-2}U'_{i-1} - U_{i-2}W'_{i-1} + 1}{W_{i-2}U_{i-1} - U_{i-2}W_{i-1}}, \quad i \neq n, 1,$$

$$\alpha_1 < -\frac{W'_0}{W_0} - \frac{\phi(a_1)}{W_0^2} - \frac{U'_0W_1 - W'_0U_1 + 1}{W_0U_1 - U_0W_1},$$

$$\alpha_n < \frac{W'_{n-1}}{W_{n-1}} - \frac{\phi(a_n)}{W_{n-1}^2} - \frac{W_{n-2}U'_{n-1} - U_{n-2}W'_{n-1} + 1}{W_{n-2}U_{n-1} - U_{n-2}W_{n-1}}.$$

2.2.2 Numerical experiments

Now we make two experiments, the first is about the number of eigenvalues of the matrix Y when the potential $q = 0$ (see [GO10, Theorem 3.2]). The second experiment is about the case of the harmonic oscillator with three point interactions and how the distance of the interactions can change the bounds (2.26)-(2.28). The objectives of the first experiment is to see the behavior of the eigenvalues when the strengths α_i are close to the bounds (2.26)-(2.28), and make a comparison of the algorithm given in the Theorem 2.10 and the direct calculation of the eigenvalues of Y in terms of the efficiency. For the first experiment we made two tables, the first table is obtained from direct calculation of eigenvalues of the matrix Y and the second is the results obtained using the Theorem 2.10. For the next test, we take as the distance between interaction as $d_i = 1$ and $\alpha_i = \alpha$ for all i. Therefore the bound given by (2.26) is -4.

α	n	Computational time	Max. eigenvalue
-3.9	5	0.030597	-0.28196
-3.9	10	0.031959	0.00211
-3.99	10	0.032795	-0.08788
-3.99	20	0.032584	-0.014623
-3.99	50	0.031883	0.006053
-3.999999	50	0.032344	-0.003945
-3.999999	100	0.0450589	-0.00098
-3.999999	1000	0.371749	-0.0000008
-3.999999	2000	0.672909	-1.467e-06
-3.999999	5000	2.22348	0.00000007
-4	5000	2.45348	-3.947e-07
-4.1	1000	0.298444	-0.1
-4.1	2000	0.672909	-0.1
-4.1	5000	2.22348	-0.1
-4.1	10000	N/A	N/A

Table 2.1: Results obtained by command LA.eigvalsh

α	n	Computational time	Max. value of ζ_k
-3.9	5	0.030718	-1.10444
-3.9	10	0.028454	0.53963
-3.99	10	0.032511	-1.08267
-3.99	20	0.032544	-0.96628
-3.99	50	0.032651	0.10777
-3.999999	50	0.040036	-1.020601
-3.999999	100	0.050386	-1.01011
-3.999999	1000	0.251176	-1.00064
-3.999999	2000	0.050751	-0.999954
-3.999999	5000	1.15776	9.80818
-4	5000	1.264367	-1.0002
-4	10000	3.051423	-1.0001
-4	50000	11.893887	-1.00002
-4	100000	22.908413	-1.00001
-4	1000000	63.43254	-1.000001
-4.1	1000	0.251494	-1.37015
-4.1	2000	0.508712	-1.37015
-4	5000	1.24437	-1.37015
-4	10000	3.043575	-1.37015
-4	50000	11.71224	-1.37015
-4	100000	22.35594	-1.37015
-4	1000000	64.44554	-1.37015

Table 2.2: Results obtained by the sequence ζ_k

Remark 2.13. For above results we can conclude:

- In the two tables we can observe that if we take values of α near of -4, the maximum eigenvalue of the matrix Y esclose to 0. Moreover if we take $\alpha > -4$ for some n we find at least one positive eigenvalue. So we can conclude that if $n \to \infty$ the bound condition (2.26) is also necessary.
- Using the Theorem 2.10 we note that the computational time has a linear growth with respect to the number of perturbations n and is less than the computational time of the direct calculus.

For the second experiment we will consider the potential $q(x) = x^2$ with interactions $a_1 = 0, a_2 = 1$ and a free point $a_3 > 1$. We know that $S_1(x, \lambda) = U(x, \lambda)$ and $C_1(x, \lambda) = W(x, \lambda)$. Using the same notation that in the Remark 2.12 we have that the associated matrix Y is

$$\begin{pmatrix} \alpha_1 + m_0(0) + \frac{W_1}{U_1} & -U_1^{-1} & 0 \\ -U_1^{-1} & \alpha_2 + \frac{c_2}{s_2} + \frac{s_1'}{s_1} & -s_2^{-1} \\ 0 & -s_2^{-1} & \alpha_3 - m_3(0) + \frac{s_2'}{s_2} \end{pmatrix}$$

By Theorem 2.8 and Remarks 2.12 we have to analyze the inequalities

$$\alpha_1 < -\frac{W_1'}{W_1} - \frac{\phi(0)}{W_1^2} - \frac{W_2}{U_2} = -\phi(0) - \frac{W_2}{U_2},$$

$$\alpha_2 < -\frac{U_2'W_3 - W_2'U_3 + 1}{W_2U_3 - U_2W_3} - \frac{U_2' + 1}{U_2},$$

$$\alpha_3 < -\frac{W_3'}{W_3} + \frac{\phi(a_3)}{W_3^2} - \frac{W_2U_3' - U_2W_3' + 1}{W_2U_3 - U_2W_3}.$$

Given that a_3 is the unique variable we have to see the behavior in $(1, \infty)$ of the functions

$$O(x) := \frac{U'(1,0)W(x,0) - W'(1,0)U(x,0)}{W(1,0)U(x,0) - U(1,0)W(x,0)},$$

$$N(x) := \frac{W(1,0)U(x,0) - U(1,0)W'(x,0)}{W(1,0)U(x,0) - U(1,0)W(x,0)},$$

$$\frac{V'(x,0)}{V(x,0)} = \frac{W'(x,0)}{W(x,0)} - \frac{\phi(x)}{W_3^2}$$

- The graphic of $O(x)$:

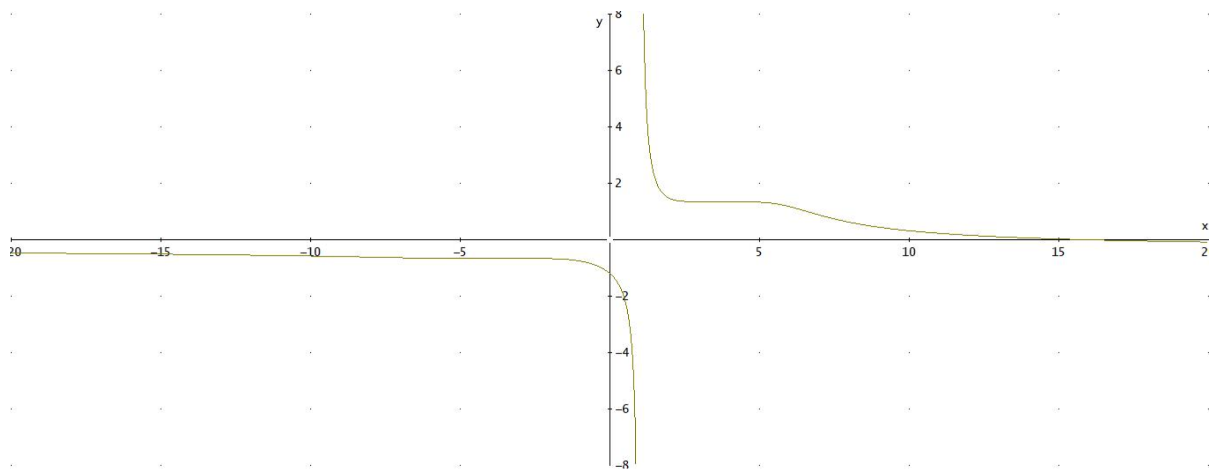


Figure 2.1: Function O

- The graphic of $N(x)$:

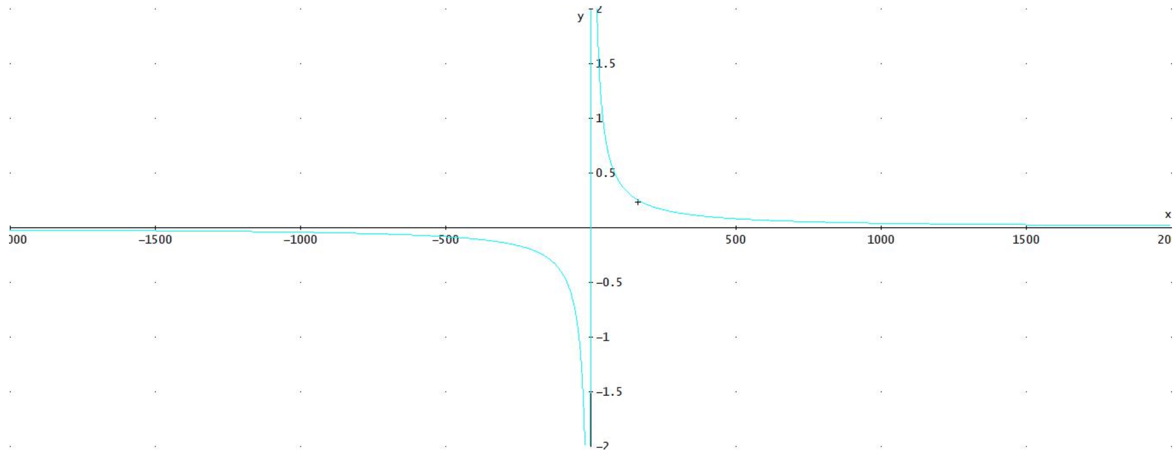


Figure 2.2: Function N

- The graphic of $\frac{W'(x,0)}{W(x,0)}$:

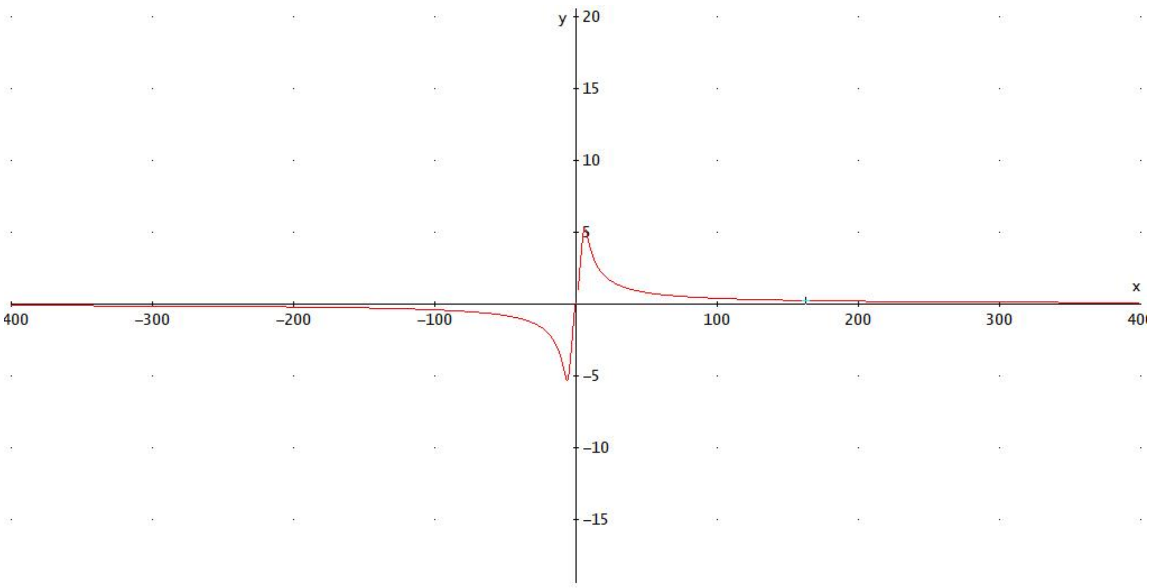


Figure 2.3: Function $\frac{W'(x,0)}{W(x,0)}$

For $\frac{\phi(x)}{W(x,0)}$ we used the next commands in DERIVE 6

```
W(x) :=1 + sum(x^(4n)/product(4k(4k − 1), k, 1, n), n, 1, 10)
Q(x) := 1/(int(W(d)^(−2), d, x, 10000)W(x)^2)
VECTOR(Q(x), x, 1, 500, 5)
```

This command generates a vector with values of the function $\frac{\phi(x)}{W^2(x,0)}$ until 500. The following table shows some of these values

$\frac{\phi(x)}{W^2(x,0)}$	x
1.663	1
10.745	6
7.103	11
4.92	16
3.759	21
3.037	26
2.547	31
2.194	36
1.926	41
1.717	46
1.548	51
0.173	456
0.171	461
0.169	166
0.167	471
0.165	476
0.164	481
0.162	486
0.160	491
0.159	496

Table 2.3: values of $\frac{\phi(x)}{W^2(x,0)}$

Remark 2.14. From the above results, we can conclude the following.

- If $a_2 = 1$ is fixed and $a_3 \to 1$, then α_2 and α_3 must tend to $-\infty$ in order guarantee existence of two negative eigenvalues.
- The Table 2.3 indicates that $\frac{\phi(x)}{W^2(x,0)} \to 0$ when $x \to \infty$. So, we obtain that $m_n(0) \to 0$ when $a_n \to \infty$ and by the parity of $W(x,0)$ we conclude that $m_0(0) \to 0$ when $a_1 \to -\infty$.
- For the case $n = 1$ we conclude that for any value of a_1, $\mathbf{C}_\alpha$ has a negative eigenvalue if $\alpha_1 < -\sup_{x\in\mathbb{R}} \frac{\phi(x)+\phi(-x)}{W^2(x,0)}$.

2.3 Classical distributional approach

In this sections we will give a summary of the approach in [CLMM14, Section 2.1] where their results are obtained using physical principles.

For a solution f of the Schrödinger equation with a time-independent potential $V(x)$ the function $j(x) = -i\left[\bar{f}(x)f'(x) - \bar{f}'(x)f(x)\right]$, is its *probability current.*

Recall that the one-dimensional time-independent Schrödinger equation for a non-relativistic particle moving under the influence of a potential $q \in L^1_{loc}(\mathbb{R})$, is given by

$$\left(-\frac{h}{2\mu}\frac{d^2}{dx^2} + q\right) f = Ef \tag{2.36}$$

where h is the Planck constant, μ is the reduced mass of the particle and E is a constant obtained of separations of variables of the time-dependent Schödinger equation. We want to define the equation (2.36) when $q = \Psi - q_2$, where q_2 is a fixed function in $L^1_{loc}(\mathbb{R})$ and Ψ is a singular distribution in a fixed $x_0 \in \mathbb{R}$. Without loss of generality we assume that $\frac{h}{\mu} = 1$. We introduce the distributional version of (2.36):

$$f''(x) + Ef(x) + q_2(x)f(x) = \Psi[f](x) \tag{2.37}$$

where the primes indicate the derivative in sense of distributions and $\Psi[f]$ is a distribution such that $\text{supp}(\Psi[f]) = \{x_0\}$. In addition we require that the probability current must be conserved everywhere. By Theorem 1.52 we know that

$$\Psi[f](x) = \sum_{n=0}^{r} \alpha_n[f]\delta^{(n)}(x - x_0),$$

where $\alpha_n[f]$ are constants that depend of the behavior of f around of x_0 (see [Zem87, Theorem 3.5-1]), that is $\alpha_n[f(x_0\pm), f'(x_0\pm)]$.

We are interested in $f \in L^2(\mathbb{R})$ only, so $r = 1$ is the maximum order allowed for $\Psi[f]$. If $r > 1$ then f'' must have order equal to r and hence f has order greater than or equal to 0, and by the Remark 1.51 f would necessarily be singular. Since Ψ has order 1, the functions f'', f', f must have order 1, 0 and -1 respectively. We have that

$$\Psi[f](x) = \alpha_0[f]\delta(x - x_0) + \alpha_1[f]\delta'(x - x_0). \tag{2.38}$$

Recall that the primitive $f^{(-1)}$ has order -2 and it is a function which is continuous at x_0. In the same way given that q_2 is regular its order is at most -1, therefore the order of $q_2 f$ has order at most -1, so the primitive $(q_2 f)^{(-1)}$ has order at most -2 and it is continuous at x_0. If we integrate on both sides of (2.37) we obtain

$$f'(x) + Ef^{(-1)}(x) + (fq_2)^{(-1)} = \alpha_0\theta(x - x_0) + \alpha_1\delta(x - x_0) + c_1. \tag{2.39}$$

In any interval which does not include the point x_0, both sides of (2.39) are equal to ordinary functions, in particular δ vanishes in this interval. Taking into account the continuity of $f^{(-1)}$ and $(q_2 f)^{(-1)}$ at x_0, we find

$$f'(x_0+) - f'(x_0-) = \alpha_0[f]. \tag{2.40}$$

If we integrate on both sides of (2.39) obtain

$$f(x_0+) - f(x_0-) = \alpha_1[f]. \tag{2.41}$$

The conservation of the probability current across x_0 is simply the continuity of $j(x)$, that is $j(x_0+) = j(x_0-)$. Note that by the polarization identity we can write

$$p_0 j(x) = \frac{1}{2}\left[\left|p_0 f'(x) + i f(x)\right|^2 - \left|i f(x) - p_0 f'(x)\right|^2\right],$$

for any $p_0 \in \mathbb{R}$. Now, if we define the vectors

$$V_1[f] := \begin{pmatrix} p_0 f'(x_0+) + i f(x_0+) \\ -p_0 f'(x_0-) + i f(x_0-) \end{pmatrix}; \quad V_2[f] := \begin{pmatrix} -p_0 f'(x_0+) + i f(x_0+) \\ p_0 f'(x_0-) + i f(x_0-) \end{pmatrix},$$

the conservation of probability current can be rewritten as $\|V_1[f]\| = \|V_2[f]\|$. This implies that there exists a unitary matrix U such that

$$V_2[f] = U V_1[f].$$

where

$$U = e^{i\theta}\begin{pmatrix} z & w \\ -\bar{w} & \bar{z} \end{pmatrix}, \quad \theta \in [0, \pi), \quad \|(z, w)\|^2 = 1.$$

By the equations (2.40)-(2.41)

$$K_1 V_1[f] - K_2 V_2[f] = \begin{pmatrix} f(x_0+) - f(x_0-) \\ f'(x_0+) - f'(x_0-) \end{pmatrix}, \tag{2.42}$$

with

$$K_1 = \frac{1}{2}\begin{pmatrix} -i & i \\ L^{-1} & L^{-1} \end{pmatrix}, \quad K_2 = \frac{1}{2}\begin{pmatrix} i & -i \\ L^{-1} & L^{-1} \end{pmatrix}.$$

Notice that

$$V_1[f] = \begin{pmatrix} i & p_0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} f(x_0+) \\ f'(x_0+) \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ -i & p_0 \end{pmatrix}\begin{pmatrix} f(x_0-) \\ f'(x_0-) \end{pmatrix}.$$

Then, after a few calculations we obtain

$$(K_1 - K_2 U)\, V_1[f] = M_+ \Phi(x_0+) - M_- \Phi(x_0-), \tag{2.43}$$

where

$$\Phi(x) := \begin{pmatrix} f(x) \\ f'(x) \end{pmatrix},$$

and

$$M_+ = \frac{1}{2}\begin{pmatrix} 1 + e^{i\theta}(z + \bar{w}) & -ip_0\left[1 + e^{i\theta}(z + \bar{w})\right] \\ ip_0\left[1 - e^{i\theta}(z - \bar{w})\right] & 1 - e^{i\theta}(z + \bar{w}) \end{pmatrix},$$
$$M_- = \frac{-1}{2}\begin{pmatrix} -1 - e^{i\theta}(z - \bar{w}) & -ip_0\left[1 + e^{i\theta}(z - \bar{w})\right] \\ ip_0\left[1 - e^{i\theta}(z + \bar{w})\right] & e^{i\theta}(z + \bar{w}) - 1 \end{pmatrix}.$$

Replacing (2.43) in (2.42) we obtain the equality

$$R_+\Phi(x_0+) = R_-\Phi(x_0-),$$

where $R_\pm = I - M_\pm$, with $\det(R_+) = -\bar{w}e^{i\theta}$ and $\det(R_+) = we^{i\theta}$. If $w \neq 0$ then $R_\pm$ are invertible and we can write

$$\Phi(x_0+) = A\Phi(x_0-), \tag{2.44}$$

with $A = R_+^{-1}R_-$. Note that $|\det(A)| = 1$ so,

$$A = e^{i\varphi}\begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

with $a, b, c, d \in \mathbb{R}$ such that $ad - bc = 1$. Then we obtain the equation

$$\Phi(x_0+) - \Phi(x_0-) = (A - I)\Phi(x_0-)$$

So we can obtain the explicit form of the distribution $s[f]$

$$\begin{aligned} \Psi[f](x) = &\left[ce^{i\varphi}f(x_0-) + \left(de^{i\varphi} - 1\right)f'(x_0-)\right]\delta(x - x_0) \\ &+ \left[\left(ae^{i\varphi} - 1\right)f(x_0-) + be^{i\varphi}f'(x_0-)\right]\delta'(x - x_0). \end{aligned} \tag{2.45}$$

In the same way we can invert A and obtain

$$\begin{aligned} \Psi[f](x) = &\left[ce^{-i\varphi}f(x_0+) - \left(ae^{i\varphi} - 1\right)f'(x_0+)\right]\delta(x - x_0) \\ &- \left[\left(de^{-i\varphi} - 1\right)f(x_0+) - be^{-i\varphi}f'(x_0+)\right]\delta'(x - x_0). \end{aligned} \tag{2.46}$$

Now suppose that $w = 0$. So we simply have the equations

$$\begin{aligned} \left(ze^{i\theta} - 1\right)f(x_0+) &= ip_0\left(ze^{i\theta} + 1\right)f'(x_0+) \\ \left(\bar{z}e^{i\theta} - 1\right)f(x_0-) &= -ip_0\left(\bar{z}e^{i\theta} + 1\right)f'(x_0-). \end{aligned}$$

Now we have two cases for the solution of the equations

(i) If $ze^{i\theta} + 1 = 0$ we obtain that $f(x_0+) = 0 = f(x_0-)$ with $f'(x_0+)$ and $f'(x_0-)$ arbitrary.
(ii) If $ze^{i\theta} + 1 \neq 0$ it follows that

$$f'(x_0\pm) = h_\pm f(x_x) \tag{2.47}$$

with

$$h_+ = \frac{ze^{i\theta} - 1}{ip_0(ze^{i\theta} + 1)} = \frac{2\mathrm{Im}(ze^{i\theta})}{p_0\|1 + ze^{i\theta}\|}, \quad h_- = \frac{1 - \bar{z}e^{i\theta}}{ip_0(\bar{z}e^{i\theta} + 1)} = -\frac{2\mathrm{Im}(\bar{z}e^{i\theta})}{p_0\|1 + \bar{z}e^{i\theta}\|}.$$

So $h_\pm \in \mathbb{R}$. We can obtain the explicit form of the interaction distribution

$$\Psi[f](x) = \left[h_+f(x_0+) - h_-f(x_0-)\right]\delta(x - x_0) + \left[h_+^{-1}f'(x_0+) - h_-^{-1}f'(x_0-)\right]\delta'(x - x_0)$$

Remark 2.15.
- In [ADK98, Theorem 1] it is shown that all self-adjoint extensions of **C** for only one interaction are given by the boundary condition

$$\begin{pmatrix} f(x_0+) \\ f'(x_0+) \end{pmatrix} = e^{i\varphi} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} f(x_0-) \\ f'(x_0-) \end{pmatrix},$$

  with $a, b, c, d \in \mathbb{R}$ such that $ad - bc = 1$, or

$$f'(x_0+) = h_+ f(x_0+), \qquad f'(x_0-) = h_+ f(x_0-).$$

  These are exactly the equations (2.44) and (2.47).
- If we take $\alpha_1 = 0$, then

$$f'(x_0+) - f'(x_0-) = \nu f(x_0), \text{with } \nu = h_+ - h_- \in \mathbb{R}$$

  . In the same way if we take $\alpha_1 = 0$, then

$$f(x_0+) - f(x_0-) = \nu f'(x_0), \text{with } \mu = h_+^{-1} - h_-^{-1} \in \mathbb{R}.$$

  The above equations coincide with the boundary conditions obtained in (2.8) and (2.9).

3 Appendix

3.1 Apendix A. Notation

Simbol	Page-Ref
s_T	12-(1.2)
T_0	13-(1.3)
T_1	13-(1.4)
T_B	13-(1.5)
T^V	13-(1.6)
$T_{C,D}$	14-(1.7)
$k_-(\cdot)$	16- 1.37
$\mathcal{U}$	19-(1.15)
$\mathbf{E}_i$	23-(2.1)
$\mathbf{E}$	23-(2.2)
$\mathbf{A}$	23-(2.3)
$\mathbf{T}$	23-(2.4)
$\mathbf{T}_i$	23-(2.3)
$\mathbf{B}$	24-(2.5)
$\mathbf{C}$	24-(2.6)
$\mathbf{B}_\alpha$	25-(2.7)
$\mathbf{C}_\alpha$	25-(2.8)
$\mathbf{C}_\beta$	25-(2.9)
Γ_0	26-(2.10)
Γ_1	26-(2.11)
G, D	28-(2.12)
Γ_0^i, Γ_1^i	28-(2.14)
$S_i(x,\lambda), C_i(x,\lambda)$	29-(2.15)
s_i, c_i, s_i'	30-(2.22)
$W(x,0), U(x,\lambda)$	35-(2.35)

Table 3.1: Table of symbols

3.2 Appendix B. Python codes

Listing 3.1: Python code for eigenvalues of matrix Y of dimension n

```
import time
import numpy as np
import math
from numpy import linalg as LA
L=2000 #Number of perturbations
z = np.zeros(L, int) # The distances vector d_{i}
x = np.zeros(L, float) # The S_{i} vectors
y = np.zeros(L, float) # The diagonal Vector C_{i+1}/S_{i+1} +S'_{i}/S_{i}
w = np.zeros(L, float) # Alpha values
for i in range(0, L):          #Here we give the distances d_{i}
            z[i] = 1
for i in range(0,L):
    w[i]=-3.999999
for i in range(0, L):
            x[i] = -1/z[i]
for i in range(1, L-1):
            y[i] = w[i]-x[i-1]-x[i]
y[0]=w[0]-x[0]
y[L-1]=w[L-1]-x[L-1]
a = np.zeros([L,L],float)
for i in range(0, L):          #Here we generate the matrix
    a[i][i] =y[i]
for i in range(0,L-1):
    a[i][i+1]=x[i]
    a[i+1][i]=x[i]
np.amax(LA.eigvalsh(a))                 #Compute the maximum of eigenvalues
time.clock()
```

Listing 3.2: Python code for sequence (2.30)-(2.32)

```
import time
import numpy as np
import math
from numpy import linalg as LA
L=1000000 #Number of perturbations
z = np.zeros(L, int) # The distances vector d_{i}
x = np.zeros(L, float) # The S_{i} vectors
y = np.zeros(L, float) # The diagonal Vector C_{i+1}/S_{i+1} +S'_{i}/S_{i}
w = np.zeros(L, float) # Alpha values
zeta = np.zeros(L,float)#sequence zeta_{i}
for i in range(0, L):          #Here we give the distances d_{i}
            z[i] = 1
for i in range(0,L):
    w[i]=-4.1
for i in range(0, L):
            x[i] = -1/z[i]
for i in range(1, L-1):
            y[i] = w[i]-x[i-1]-x[i]
y[0]=w[0]-x[0]
y[L-1]=w[L-1]-x[L-1]
zeta[0]=y[0]
for i in range(0,L-1): #Here we apply the algorithm
    if zeta[i]==0:
        zeta[i+1]=-10**100
    else:
        if zeta[i]==-10**100:
            zeta[i+1]=y[i+1]
        else:
            zeta[i+1]=y[i+1]-(x[i]**2)*(1/zeta[i])
np.amax(zeta)   #compute the maximum of the zeta sequence
time.clock()
```

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