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On spectrum of a dissipatively perturbed Schrödinger operator on the real semi-axis

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I am prepared to go anywhere, provided it be forward.

David Livingstone, *explorer*

Abstract

In this work, we consider self-adjoint Schrödinger operators in one dimension, with potentials which are either compactly supported or periodic. These operators are perturbed by a compactly supported dissipative term of the form $i\gamma\,\chi_{[0,R]}$, where γ and R are non-negative real parameters. Of particular interest is the limit of the (both Neumann and Dirichlet) spectrum as R tends to infinity. The Titchmarsh-Weyl M-functions are computed in all these cases, in order to find isolated eigenvalues of the perturbed (non-self-adjoint) operators. Some counter-intuitive results are obtained which show that any limit points of the spectrum off the lines $\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) = \gamma\}$ and $\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) = 0\}$ are either non-existent (in the case of compactly supported background potentials) or else countable, with no finite accumulation (periodic case). According to some numerical experiments, it is also conjected that this set is in general empty, similarly to the free case (null potential). It is finally shown that the limit points, if they exist, can be characterized in terms of the eigenvalues of a certain $\mathcal{PT}$-symmetric Schrödinger operator on the whole real line.

Sommario

In questo lavoro, consideriamo operatori di Schrödinger auto-aggiunti in una dimensione, con potenziali a supporto compatto o periodici. Questi operatori sono perturbati mediante un termine dissipativo ed a supporto compatto della forma $i\gamma\,\chi_{[0,R]}$, dove γ e R sono parametri reali non negativi. Particolarmente interessante è il limite dello spettro (Neumann e Dirichlet) per R che tende all'infinito. Nei casi di studio, è stata calcolata la funzione di Titchmarsh-Weyl (M-function), che permette di individuare gli autovalori isolati dell'operatore perturbato (non auto-aggiunto). Sono stati ottenuti alcuni risultati contro-intuitivi che mostrano come eventuali punti limite dello spettro al di fuori delle rette $\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) = \gamma\}$ e $\{\lambda \in \mathbb{C} : \mathrm{Im}(\lambda) = 0\}$ non esistono (nel caso di potenzali di fondo a supporto compatto) oppure costituiscono un insieme al più numerabile, privo di punti di accumulazione (caso periodico). Sulla base di alcuni esperimenti numerici e dell'analogia con il caso libero, si congettura che tale insieme sia in generale vuoto. Si è inoltre dimostrato che tali punti limite, se esistono, possono essere caratterizzati in termini di un certo operatore di Schrödinger $\mathcal{PT}$-simmetrico definito sull'intero asse reale.

Contents

Introduction

This work is devoted to the study of the spectrum of Schrödinger operators, defined on the real semi-axis, of the form

$$\mathrm{H}_{R,\gamma} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\gamma\chi_{[0,R]}(x)$$

where γ and R are non-negative real numbers. These operators are non-self-adjoint perturbations of self-adjoint (i.e. physical) Schrödinger operators

$$\mathrm{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)\ ;$$

in particular we consider background potentials q which are either compactly supported or periodic functions, for which the background spectrum is real and has a well-known structure.

However, the perturbation of H into $\mathrm{H}_{R,\gamma}$, defined by the dissipative multiplication operator $i\gamma\chi_{[0,R]}(x)$, is compact relative to H, thus the essential spectrum of the operators $\mathrm{H}_{R,\gamma}$ remains unchanged for all γ and R; therefore, finding the spectrum of $\mathrm{H}_{R,\gamma}$ is only a matter of calculating the isolated eigenvalues of the operator. To do this, a very useful tool is the Titchmarsh-Weyl M-function associated with the operator $\mathrm{H}_{R,\gamma}$, which has the property that its poles are precisely the eigenvalues of $\mathrm{H}_{R,\gamma}$.

Our interest in the study of this family of operators and specially in

$$\lim_{R\to\infty} \sigma(\mathrm{H}_{R,\gamma})$$

(for fixed γ) comes from the context of spectral pollution, i.e. appearance of spurious eigenvalues of the unperturbed operator H while trying to calculate numerically its spectrum by using variational methods (based on discretization) or by truncating the solution on finite subintervals of the real semi-axis. Several studies have been done, which present methods of different natures to detect and prevent spectral pollution (see [1, 5, 12, 19, 20]).

In this thesis, we are following Marletta's approach in [21] and [22] (the latter with Scheichl), where it is proposed changing the self-adjoint and polluted problem by replacing the potential q with

$$q(x) + i\,s(x) \ ,$$

being s a compactly supported "cut-off" function which takes constantly value 1 inside a ball of large radius (e.g. $s(x) = \chi_{[0,R]}(x)$). In this way, genuine eigenvalues are shifted up into the complex plane and can be easily identified from the spectrum of $\mathrm{H}_{R,\gamma}$, while spurious eigenvalues generally stay close to the real axis.
Let us now give a brief description of the content of the thesis.

In the beginning of Chapter 1, the main problem of this work is presented and formalized; in particular, invariance of the essential spectrum under relatively compact perturbation is derived. Chapter 1 also provides the notions and results which are necessary to the study of the problem and to the sequel of the thesis: Section 1.2 contains some preliminary information on basic functional analysis, spectral theory and complex analysis; Section 1.3 is meant to be an introduction to abstract Titchmarsh-Weyl M-functions, essentially based on the content of [7]; in Section 1.4 the classical limit-point, limit-circle theory for Sturm-Liouville operators, also known as Weyl alternative, and the more recent Sims classification are presented; Section 1.5 treats, in more detail than this introduction, the problem of spectral pollution which motivates our study of the family of operators $\mathrm{H}_{R,\gamma}$, and gives the flavour of some of the strategies adopted to deal with this problem.

In Chapter 2, both in the free and in the compactly supported case the Neumann-to-Dirichlet Titchmarsh-Weyl function associated with $\mathrm{H}_{R,\gamma}$ is computed. It is shown that the spectrum of $\mathrm{H}_{R,\gamma}$, qualitatively, has to lie in the strip

$$\{z \in \mathbb{C} \,:\, \mathrm{Re}(z) > -\|q\|_\infty, \quad 0 < \mathrm{Im}(z) < \gamma\}$$

and that in both cases the following theorem holds true (see Theorems 2.1 and 2.2):

Theorem. *Let q be a compactly supported function. For every compact set $K \subset \{z \in \mathbb{C} : 0 < \mathrm{Im}(z) < \gamma\}$, there exists $\bar{R} = \bar{R}_K$ such that for every $R \geq \bar{R}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}_{R,\gamma}$ are such that*

$$\sigma\left(\mathrm{H}_{R,\gamma}\right) \cap K = \emptyset \ .$$

This is somewhat a counter-intuitive fact, because, by continuity of the Titchmarsh-Weyl function with respect to the real parameter R, one would expect that for increasing R more and more spectral points move off the (real) spectrum of H into the complex upper half-plane and reach the spectrum of the limiting operator $\mathrm{H} + i\gamma\mathbb{I}$ on the line $\mathrm{Im}(\gamma)$, filling up the strip with eigenvalues of the perturbed operator $\mathrm{H}_{R,\gamma}$. But this does not happen in these two cases.

The aim of the final Chapter 3 is to formulate an extension to the case when q is a periodic function. In the beginning, the main results of classical Floquet theory for periodic Schrödinger operators (see [14]) are presented: in particular, Floquet theorem, which is an explicit description for a linear basis of solutions of the spectral equation, and two theorems about the structure of the spectrum (Theorems 3.3 and 3.4), become very useful in the calculation of the Titchmarsh-Weyl function, which is the main issue of Section 3.2.
It is shown that there is at most a discrete set D, with no accumulation point, in which there can possibly be accumulation points of eigenvalues of $\mathrm{H}_{nL,\gamma}$, where n is a (large) natural number and L is a period of q. The theorem which has been stated for null and compactly supported background potentials has to be modified as follows (Theorem 3.5):

Theorem. *Let q be a periodic function with period L; let D be as above. For every compact set*

$$K \subset \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma,\, z \notin D\} \ ,$$

there exists $\bar{N} = \bar{N}_K$ such that for every $n \geq \bar{N}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}^{per}_{nL,\gamma}$ are such that

$$\sigma\left(\mathrm{H}^{per}_{nL,\gamma}\right) \cap K = \emptyset \ .$$

However, we believe in and formulate some equivalent conjectures, based on numerical experiments contained in Section 3.3, which essentially say that the set D is empty, like in the free case.
With the additional assumption that $q(x)$ can be coherently extended as an even function for negative x, the points of D, if there be any, can be characterized in terms of the eigenvalues of a certain $\mathcal{PT}$-symmetric Schrödinger operator on the whole real line. This is the object of Theorem 3.6 in Section 3.4:

Theorem. *Let q be a periodic even function with period L, defined on $\mathbb{R}$. The set D is empty if, and only if, the Schrödinger operator*

$$\mathrm{H}^{per}_{\tilde{Q}_\gamma} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tilde{Q}_\gamma(x) \ ,$$

where

$$\tilde{Q}_\gamma(x) := \begin{cases} q(x) - i\frac{\gamma}{2} & , if \quad x > 0 \\ q(x) + i\frac{\gamma}{2} & , if \quad x < 0 \end{cases} \quad ,$$

has no eigenvalues.

Chapter 1

Preliminaries

1.1 Definition and formalization of the problem

In this work, we shall consider one-dimensional Schrödinger operators of the form

$$\mathrm{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) \tag{1.1}$$

on the Hilbert space $\mathrm{L}^2([0,+\infty[)$, having domain

$$\mathcal{D}\,(\mathrm{H}) = \left\{ u \in \mathrm{L}^2\,([0,+\infty[) \;:\; -u'' + q\,u \in \mathrm{L}^2([0,+\infty[),\, u'(0) = 0 \right\} \ , \tag{1.2}$$

that is, for any $u \in \mathcal{D}(\mathrm{H})$, $x \in [0,+\infty[$, H acts as follows:

$$\mathrm{H}\,u(x) = -u''(x) + q(x)\,u(x) \ .$$

In order to get self-adjointness of the operator H, the function q, which is often referred to as *potential* because of its physical meaning, has to be a real-valued measurable function, of class L^1 on some interval $[0,\varepsilon]$ and locally integrable on $]0,+\infty[$. The choice of the domain made above in (1.2) is actually the best one, in the sense that the most general hypothesis on q are made (see [2] and [13] for a wide explanation). We will not prove the self-adjointness of H; however, in Section 1.2 we will present a sufficient criterion for self-adjointness of Schrödinger operators (Sears Theorem).

In the thesis, we shall study Schrödinger operators having potentials which are either compactly supported or periodic; we will also assume for the sake of simplicity that $q \in \mathrm{L}^\infty([0,+\infty[$, so that our choice of the domain is less general than the one made in (1.2): indeed, in this case, to get self-adjointness it is enough that

$$\begin{aligned} \mathcal{D}\,(\mathrm{H}) &= \left\{ u \in \mathrm{L}^2\,([0,+\infty[) \;:\; -u'' \in \mathrm{L}^2([0,+\infty[),\, u'(0) = 0 \right\} \\ &= \left\{ u \in H^2\,([0,+\infty[) \;:\; u'(0) = 0 \right\} \ . \end{aligned} \tag{1.3}$$

This weaker assumption, however, does not change the meaning of the ideas that will be developed in the sequel.

Self-adjoint operators always have real spectrum (Theorem 1.7); in particular the spectra of compactly supported and periodic potentials can be thoroughly characterized (this will be done respectively in Chapters 2 and 3). For reasons that will be clear from Section 1.5, we will consider and study dissipative perturbations of these potentials that are defined as follows:

$$\mathrm{H}_{R,\gamma} := \mathrm{H} + i\gamma\chi_R(x) \ , \tag{1.4}$$

having the same domain of H, where χ_R denotes the characteristic function of the interval $[0, R]$, γ and R are non-negative parameters. In other terms, if $u \in \mathcal{D}(\mathrm{H}_{R,\gamma}) = \mathcal{D}(\mathrm{H})$,

$$\mathrm{H}_{R,\gamma}\, u(x) = -u''(x) + (q(x) + i\gamma\chi_R(x))\ u(x) \ .$$

In this work, we are interested in the following question: for fixed positive γ, how does the spectrum of $\mathrm{H}_{R,\gamma}$ evolve as R tends to infinity?

First of all, we know that the operator $\mathrm{H}_{R,\gamma}$ converges to $\mathrm{H} + i\gamma\mathbb{I}$ strongly, that is

$$\mathrm{H}_{R,\gamma} f \xrightarrow{\mathrm{L}^2} \mathrm{H}f + i\gamma f$$

for every $f \in \mathcal{D}(\mathrm{H}) = \mathcal{D}(\mathrm{H}_{R,\gamma})$. But it also comes straightforward that the operatorial norm

$$\|\mathrm{H}_{R,\gamma} - \mathrm{H}\| = \gamma > 0$$

for every R. This class of operators is not self-adjoint, since it is not even symmetric: indeed, for u, $v \in \mathcal{D}(\mathrm{H}_{R,\gamma})$

$$\begin{aligned}
(\mathrm{H}_{R,\gamma} u, v)_{\mathrm{L}^2} &= \int_{[0,+\infty[} [-u''(x) + (q(x) + i\gamma\chi_R(x))\ u(x)]\,\bar{v}(x)\,\mathrm{d}x \\
&= -u'\bar{v}\big|_0^{+\infty} + \int_{[0,+\infty[} [u'\bar{v}' + (q + i\gamma\chi_R)\,u\bar{v}]\,\mathrm{d}x \\
&= \int_{[0,+\infty[} u(x)\,[\bar{v}''(x) + (q(x) + i\gamma\chi_R(x))\,\bar{v}(x)]\ \mathrm{d}x \\
&= (u, \mathrm{H}_{R,-\gamma} v)_{\mathrm{L}^2} \neq (u, \mathrm{H}_{R,\gamma} v)_{\mathrm{L}^2} \ .
\end{aligned}$$

So, non-self-adjointness make us lose the information that the spectrum is real. Also, we are not able to apply some of the well-known results of convergence for spectrum of self-adjoint operators. To explain the last statement, let us first introduce the following definition of resolvent convergence and then we will formulate some theorems (all taken from [24]).

Definition 1.1. *Let* $\{T_n\}_{n\in\mathbb{N}}$ *and* T *be self-adjoint operators. Then* T_n *is said to converge to* A *(as* $n \to \infty$*) in the* norm resolvent sense *if* $R_\lambda(T_n) \to R_\lambda(T)$ *in norm for all* λ *with* $\operatorname{Im}\lambda \neq 0$. T_n *is said to converge to* T *in the* strong resolvent sense *if* $R_\lambda(T_n)\varphi \to R_\lambda(T)\varphi$ *for all* λ *such that* $\operatorname{Im}\lambda \neq 0$ *and admissible* φ.

The following theorem gives a characterization of norm resolvent and strong resolvent convergence.

Theorem 1.1. *Let* T_n *and* T *be self-adjoint operators.*

- *If* $T_n \to T$ *in the norm resolvent sense, then* $\|T_n - T\| \to 0$.
- *If* $T_n \to T$ *in the strong resolvent sense, then* $T_n\varphi \to T\varphi$ *for all admissible* φ.

Theorem 1.2. *Let* $\mu \in \mathbb{C}$, T_n *and* T *be self-adjoint operators and suppose that* $T_n \to T$ *in the norm resolvent sense. If* $\mu \notin \sigma(T)$*, then* $\mu \notin \sigma(T_n)$ *for* n *sufficiently large and*

$$\|R_\mu(T_n) \to R_\mu(T)\| \to 0 \ .$$

Theorem 1.3. *Let* T_n *and* T *be self-adjoint operators and suppose that* $T_n \to T$ *in the strong resolvent sense. If* $a, b \in \mathbb{R}$, $a < b$*, and* $]a,b[\cap\sigma(T_n) = \emptyset$ *for all* n*, then* $]a,b[\cap\sigma(T) = \emptyset$. *In other terms, if* $\lambda \in \sigma(T)$*, then there exists a sequence* $\{\lambda_n\}_n$, $\lambda_n \in \sigma(T_n)$ *such that* $\lambda_n \to \lambda$.

Theorem 1.3 tells us that that, under strong resolvent convergence, the spectrum of the limiting operator T cannot suddenly expand (*spectral inclusion*). If T_n converges to T in norm resolvent sense, Theorem 1.2 says that the spectrum of T cannot suddenly contract, i.e. if $\lambda \in \sigma(T_n)$ for all sufficiently large n, then $\lambda \in \sigma(T)$ (*spectral exactness*). Unfortunately, it is clear that this is not our case because both the operators considered

$$T_n = \mathrm{H}_{R_n,\gamma} \ ,$$

where R_n is a sequence of real numbers tending to infinity, and the limiting operator

$$T = \mathrm{H} + i\gamma\mathbb{I}$$

are not self-adjoint. It is important to note that the principle of noncontraction of the spectrum in the norm resolvent limit is still valid even when T_n and T are not self-adjoint, while the principle of nonexpansion of the spectrum under strong resolvent convergence is not always true. In our case, in particular, the multiplication operator $i\gamma\chi_R$ is a relatively compact perturbation, therefore the essential spectra[1] of $\mathrm{H}_{R,\gamma}$ and H are such that

$$\sigma_{ess}(\mathrm{H}_{R,\gamma}) = \sigma_{ess}(\mathrm{H})$$

for all R. Also, in our cases of study (compactly supported and periodic background potential), the essential spectrum of the operator H is non-trivial and in the periodic case the spectrum is purely essential (band-gaps structure, see Section 3.1).
In addition to this, we know, since $i\gamma$ is a constant complex number, that the spectrum of the limiting operator $\mathrm{H} + i\gamma\mathbb{I}$ is simply a "vertical shift" in the complex plane of the unperturbed spectrum, i.e.

$$\sigma(\mathrm{H} + i\gamma\mathbb{I}) = i\gamma + \sigma(\mathrm{H}) \ .$$

So, in order to characterize the spectrum of $\mathrm{H}_{R,\gamma}$ as $R \to \infty$, it remains to find, if they exist, isolated eigenvalues of the operator $\mathrm{H}_{R,\gamma}$, for large R, in the strip [2] $\{z \in \mathbb{C} : 0 \leq \mathrm{Im}(z) \leq \gamma\}$. This shall be done in Chapters 2 and 3; a useful tool will be the Titchmarsh-Weyl M-function, which is presented in Section 1.3.

The following Sections 1.2-1.4 are devoted to the justification and study of the notions and facts that we have used and that we use in the development of the work.

1.2 Preliminary notions and results

1.2.1 Classical notions and results of spectral theory

In this section, the classical concepts of resolvent, spectrum and numerical range for linear operators will be presented. Also some important results of spectral theory, which are used in the sequel of the thesis, will be shown. Good references can be [2], [11] and [24]. Before starting, let us introduce some notation for this section.

Notation. The symbol $\mathcal{H}$ will always denote a Hilbert space, so we will not define it every time. Unless differently stated, the symbol T will denote a linear operator $T : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}$ having dense domain $\mathcal{D}(T) \subset \mathcal{H}$ (which sometimes will be implicit in the definition of T).

[1] The definition of essential spectrum will be given in Section 1.2.2

[2] The spectrum of $\mathrm{H}_{R,\gamma}$ is necessarily contained in the strip $\{z \in \mathbb{C} : 0 \leq \mathrm{Im}(z) \leq \gamma\}$. Basically, this comes from estimates on the numerical range and will be proved in Section 2.1.3.

Let us recall some definitions in the context of Hilbert spaces, keeping well in mind that almost all of them can be given in more general frameworks (Banach spaces):

Definition 1.2. *Given a linear operator T, its* kernel, *denoted by* $\ker(T)$ *is the set*

$$\ker(T) := \{\varphi \in \mathcal{D}(T) \,:\, T\varphi = 0_{\mathcal{H}}\} \ ;$$

the set

$$\mathrm{Ran}(T) := \{\psi \in \mathcal{H} \,:\, \exists \varphi \in \mathcal{D}(T) \text{ s.t. } T\varphi = \psi\}$$

is called range *of the operator T.*

Definition 1.3 (Bounded operator)**.** *T is said to be a* bounded operator *if there exists $C > 0$ such that*

$$\|T\varphi\|_{\mathcal{H}} \leq C \, \|\varphi\|_{\mathcal{H}} \ . \tag{1.5}$$

for all $\varphi \in \mathcal{D}(T)$. The family of all bounded operators on the Hilbert space $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$.

Definition 1.4 (Closed operator)**.** *T is said to be a* closed operator *if, for any sequence $\{\varphi_n\}_{n\in\mathbb{N}} \subset \mathcal{D}(T)$ such that $\varphi_n \to \varphi$ and $T\varphi_n \to \psi$ in $\mathcal{H}$, necessarily $\varphi \in \mathcal{D}(T)$ and $\psi = T\varphi$. An operator is* closable *if it has a closed extension, i.e. there exists $T_1 : \mathcal{D}(T_1) \subset \mathcal{H} \to \mathcal{H}$ such that $\mathcal{D}(T) \subset \mathcal{D}(T_1)$ and $T_1|_{\mathcal{D}(T)} = T$. The minimal extension of T is called* closure *of T and denoted by $\overline{T}$.*

Definition 1.5 (Resolvent)**.** *Let T be a closed operator. The* resolvent set *is the set*

$$\rho(T) := \left\{z \in \mathbb{C} \,:\, (T - z\mathbb{I})^{-1} \in \mathcal{B}(\mathcal{H})\right\} \ .$$

The operator $R_\lambda(T) := (T - z\mathbb{I})^{-1}$ is called resolvent operator *or simply* resolvent*.*

The resolvent set and the resolvent operator have the following properties:

Theorem 1.4. *Let T be a closed operator in $\mathcal{H}$; let $z_0 \in \rho(T)$. Then:*

- $B\left(z_0, \frac{1}{\|R_{z_0}(T)\|}\right) \subset \rho(T)$*;*
- *$\rho(T)$ is an open set in $\mathbb{C}$;*
- *the map $R_{(\cdot)}(T) : \rho(T) \to \mathcal{B}(\mathcal{H})$, $\lambda \mapsto R_\lambda(T)$ is analytic.*

Proof. The proof is based on the Neumann series expansion for the resolvent operator:

$$R_z(T) = \sum_{n=0}^{+\infty} (z - z_0)^n R_{z_0}(T)^{n+1} ,$$

which holds for $z \in \mathbb{C}$ such that $|z - z_0| < \frac{1}{\|R_{z_0}(T)\|}$. See [24] for a detailed explanation. □

Let us define now the spectrum of a closed operator:

Definition 1.6. *The* spectrum $\sigma(T)$ *of* T *is the complementary of* $\rho(T)$ *in the complex plane:*

$$\sigma(T) := \mathbb{C} \setminus \rho(T) .$$

It has the following properties:

Theorem 1.5. *Let* T *be a closed operator in* $\mathcal{H}$*. Then:*

- *its spectrum* $\sigma(T)$ *is closed in* $\mathbb{C}$*;*
- *for all* $z \in \rho(T)$ *the estimate*

$$\|R_z(T)\| \geq \frac{1}{\operatorname{dist}(z, \sigma(T))} \tag{1.6}$$

  holds.

There are several ways of expressing and classifying the spectrum of a linear operator. The most widely used classification divides the spectrum in three parts:

(i) *point spectrum*, denoted by $\sigma_{\mathrm{pp}}(T)$, which is the set of $\lambda \in \mathbb{C}$ such that $T - \lambda\mathbb{I}$ is not injective (the analogue of the eigenvalues of the finite dimensional theory);

(ii) *continuous spectrum*, denoted by $\sigma_c(T)$, which is the set of λ such that $T - \lambda\mathbb{I}$ is invertible, but the inverse is not continuous;

(iii) *residual spectrum*, denoted by $\sigma_r(T)$, which is what remains:

$$\sigma_r(T) := \sigma(T) \setminus (\sigma_{\mathrm{pp}}(T) \cup \sigma_c(T)) .$$

In Section 1.2.2, we will introduce another characterization of the spectrum, based on the theory of compact operators. Some other important properties of the spectrum arise when T is also self-adjoint. Let us first recall the definition.

Definition 1.7. *The operator* $T^* : \mathcal{D}(T^*) \subset \mathcal{H} \to \mathcal{H}$ *defined by*

$$(T^*\varphi, \psi)_\mathcal{H} = (\varphi, T\psi)_\mathcal{H}$$

where

$$\mathcal{D}(T^*) = \{\psi \in \mathcal{H} \,:\, \exists C > 0 \,:\, |(T\varphi, \psi)| \leq C\|\varphi\| \;\forall\, \varphi \in \mathcal{D}(T)\}$$

is called adjoint *of* T. T *is called* symmetric *if* T^* *is an extension of* T, *i.e. for every* φ, $\psi \in \mathcal{D}(T)$

$$(T\varphi, \psi)_\mathcal{H} = (\varphi, T\psi)_\mathcal{H} \ .$$

The operator T *is said to be* self-adjoint *if* $\mathcal{D}(T) = \mathcal{D}(T^*)$ *and* $T = T^*$. T *is said to be* essentially self-adjoint *if* T *is closable and* $\overline{T} = T^*$.

Remark 1.2.1. It can be shown that every self-adjoint operator is in particular closed. The converse statement is false.

There are several criteria for checking self-adjointness and essential self-adjointness. For example:

Theorem 1.6. *Let* T *be a symmetric operator acting on* $\mathcal{H}$. *Then,* T *is self-adjoint if, and only if, the range of the two operators* $T \pm i\mathbb{I}$ *is precisely the whole Hilbert space* $\mathcal{H}$.

From this it follows that:

Theorem 1.7. *Let* T *be a symmetric operator acting on* $\mathcal{H}$. *Then,* T *is self-adjoint if, and only if, its spectrum is real.*

Also, it is known that:

Theorem 1.8. *Let* T *be a self-adjoint operator on* $\mathcal{H}$. *Then, the residual spectrum* $\sigma_r(T)$ *is empty.*

As we are talking about Schrödinger operators, it is worth mentioning a sufficient condition for (essential) self-adjointness.

Theorem 1.9 (Sears)**.** *Let us consider the Schrödinger operator* H *defined by*

$$\mathrm{H}\, u(x) = -u''(x) + q(x)\, u(x)$$

on $\mathcal{D}(\mathrm{H})$ *defined in (1.3), where* q *is a real-valued, measurable and locally bounded function of* $x \in [0, +\infty[$. *Let* q *also satisfy*

$$q(x) \geq -V(x), \;\; x \in [0, +\infty[\ ,$$

where V is a positive even continuous function, which is non-decreasing and satisfies

$$\int_0^{+\infty} \frac{1}{\sqrt{V(2x)}}\, \mathrm{d}x = +\infty \ .$$

Then H *is essentially self-adjoint.*

Proof. A detailed proof can be found in [4, Chap. 2]. □

A very useful tool to determine the spectrum of closed operators are Weyl (or singular) sequences.

Definition 1.8. *Let T be a closed operator; let $\lambda \in \mathbb{C}$. A* Weyl *(or* singular*)* sequence *associated with λ is a sequence $(u_n)_{n\in\mathbb{N}} \subset \mathcal{D}(T)$ such that*

- $\|u_n\|_{\mathcal{H}} = 1$ *for every n;*
- $\|(T - \lambda\mathbb{I})u_n\|_{\mathcal{H}} \longrightarrow 0$ *as $n \to \infty$.*

Proposition 1.1 (Weyl's criterion)**.** *Let $\lambda \in \mathbb{C}$, T be a closed linear operator.*

(i) If there exists a Weyl sequence associated with λ, then $\lambda \in \sigma(T)$.

(ii) If $\lambda \in \sigma(T) \cap \overline{\rho(T)}$, then there exists a Weyl sequence associated to λ.

Proof of (i). Suppose that such a sequence exists. If λ were in the resolvent set $\rho(T)$, then

$$1 = \|u_n\|_{\mathcal{H}} = \|R(\lambda, T)(T - \lambda\mathbb{I})u_n\|_{\mathcal{H}} \leq \|R(\lambda, T)\| \cdot \|(T - \lambda\mathbb{I})u_n\|_{\mathcal{H}} \longrightarrow 0$$

as $n \to \infty$, which is a contradiction. □

Proof of (ii). By hypothesis $\lambda \in \overline{\rho(T)}$. Thus, there exists a sequence $\{\lambda_n\} \subset \rho(T)$ such that $\lambda_n \to \lambda$. Since λ is also in $\sigma(T)$, $\operatorname{dist}(\lambda_n, \sigma(T)) \leq |\lambda_n - \lambda|$. Then, the estimate (1.6)

$$\|R_{\lambda_n}(T)\| \geq \frac{1}{\operatorname{dist}(\lambda_n, \sigma(T))}$$

shows that $\|R_{\lambda_n}(T)\| \to \infty$. By definition of operatorial norm, there exists a sequence $\varphi_n \in \mathcal{H}$, $\varphi_n \neq 0$ such that

$$\frac{\|R_{\lambda_n}(T)\varphi_n\|_{\mathcal{H}}}{\|\varphi_n\|_{\mathcal{H}}} \geq \frac{\|R_{\lambda_n}(T)\|}{2} \longrightarrow \infty \qquad (1.7)$$

as $n \to \infty$. Let $\psi_n := R_{\lambda_n}(T)\varphi_n$; we may suppose, without loss of generality, that $\|\psi_n\|_{\mathcal{H}} = 1$. So, (1.7) tells that $\|\varphi_n\|_{\mathcal{H}} \to 0$. By definition of ψ_n, we have that $(A - \lambda_n)\psi_n = \varphi_n$; then

$$\|(A-\lambda)\psi_n\|_{\mathcal{H}} = \|\phi_n + (\lambda_n - \lambda)\psi_n\|_{\mathcal{H}} \leq \|\varphi_n\|_{\mathcal{H}} + |\lambda_n - \lambda| \overset{n\to\infty}{\longrightarrow} 0 \ ,$$

which proves that $\{\psi_n\}$ is a Weyl sequence for λ. $\square$

Using Proposition 1.1, part (ii), a further result about the spectrum of self-adjoint operators can be proven.

Proposition 1.2. *Let $\alpha \in \mathbb{R}$, $\mathcal{H}$ be a Hilbert space, $T : \mathcal{D}(T) \subset \mathcal{H} \longrightarrow \mathcal{H}$ a self-adjoint linear operator such that for every $\varphi \in \mathcal{D}(T)$*

$$(T\varphi, \varphi)_{\mathcal{H}} \geq \alpha \|\varphi\|^2_{\mathcal{H}} \ . \tag{1.8}$$

Then the spectrum of T is contained in $[\alpha, +\infty[$.

Proof. We can suppose $\alpha = 0$. Indeed, if $\alpha \neq 0$, we can replace T by the operator $T - \alpha$.

First, the spectrum has to be real, because T is self-adjoint. It just remains to prove that every $\lambda < 0$ belongs to the resolvent set $\rho(T)$, that is the resolvent operator $R_\lambda(T)$ is defined and continuous for every λ.
Let $\lambda < 0$, $\varphi \in \mathcal{D}(T)$. Since T is a symmetric operator, by (1.8), we have that:

$$\begin{aligned} \|(T-\lambda\mathbb{I})\varphi\|^2_{\mathcal{H}} &= \|T\varphi\|^2_{\mathcal{H}} + \lambda^2 \|\varphi\|^2_{\mathcal{H}} - \lambda(T\varphi,\varphi)_{\mathcal{H}} - \lambda(\varphi, T\varphi)_{\mathcal{H}} \\ &= \|T\varphi\|^2_{\mathcal{H}} + \lambda^2 \|\varphi\|^2_{\mathcal{H}} - 2\lambda(T\varphi,\varphi)_{\mathcal{H}} \\ &\geq \lambda^2 \|\varphi\|^2_{\mathcal{H}} \ , \end{aligned}$$

that is

$$\|(T-\lambda\mathbb{I})\varphi\|_{\mathcal{H}} \geq |\lambda| \ \|\varphi\|_{\mathcal{H}}$$

If $(\varphi_n)_{n\in\mathbb{N}} \subset \mathcal{D}(T)$ is a sequence such that $\|\varphi_n\|_{\mathcal{H}} = 1$ for every n, then

$$\|(T-\lambda\mathbb{I})\varphi_n\|_{\mathcal{H}} \geq |\lambda| > 0 \ ;$$

thus it is impossible that $\|(T-\lambda\mathbb{I})\varphi_n\|_{\mathcal{H}} \longrightarrow 0$. This means, according to Proposition 1.1, part (ii), that $\lambda \in \rho(T)$. $\square$

Finally, we introduce the notion of numerical range, which will also be important to determine approximately the spectrum of the class of operators $\mathrm{H}_{R,\gamma}$.

Definition 1.9. *Let T be a densely defined closed operator on $\mathcal{H}$. The* numerical range *of T is the set*

$$\mathrm{Num}(T) := \{(T\varphi, \varphi)_{\mathcal{H}} \,:\, \varphi \in \mathcal{D}(T) \text{ and } \|\varphi\|_{\mathcal{H}} = 1\} \ .$$

The numerical range of an operator is closely related to its spectrum.

Theorem 1.10. *Let T be a densely defined closed operator on a Hilbert space $\mathcal{H}$. Suppose that $\mathbb{C} \setminus \mathrm{Num}(T)$ is connected and contains at least one point not in $\sigma(A)$; then*

$$\sigma(T) \subset \overline{\mathrm{Num}(T)} \ .$$

Moreover, for all $z \in \mathbb{C}$, $\varphi \in \mathcal{D}(T)$

$$\|(T - z\mathbb{I})\varphi\|_{\mathcal{H}} \geq \mathrm{dist}\left(z, \overline{\mathrm{Num}(T)}\right) \|\varphi\|_{\mathcal{H}} \ . \tag{1.9}$$

1.2.2 Invariance of the essential spectrum under relatively compact perturbations

There are really many definitions one can give about the essential spectrum of a closed operator T (see Definition 1.14). The easiest way to think about it - in the self-adjoint case - is as the set of non-isolated points of the spectrum of T (Theorem 1.15). However, our aim here is to show that the essential spectrum of a self-adjoint operator is invariant under relatively compact perturbations. This is the case for example when $T = \mathrm{H}$ and the relatively compact perturbation is given by the multiplication operator $i\gamma\chi_R(x)$.

Following [15], we shall explain the concept of essential spectrum and then state the announced result about invariance of the essential spectrum. First, we define what a compact operator is. Again, unless differently stated, we will assume that $\mathcal{H}$ is a Hilbert space and T is a linear operator T defined on $\mathcal{H}$, having some dense domain $\mathcal{D}(T)$. Note that the definition could be given in the more general framework of Banach spaces.

Definition 1.10 (Compact operator)**.** *A linear operator T is said to be* compact *(or* completely continuous*) if, for any bounded subset $B \in \mathcal{D}(T)$, the closure $\overline{T(B)}$ of $T(B)$ is compact. Equivalently, T is compact if, and only if, for every bounded sequence $\{\varphi_n\} \subset \mathcal{D}(T)$, $\{T\varphi_n\}$ contains a convergent subsequence.*

We denote by $\mathcal{K}(\mathcal{H})$ the family of all compact operators on the Hilbert space $\mathcal{H}$ (when possible, not declaring what is the domain); also, we set $\mathrm{nul}(T) := \dim(\ker(T))$: $\mathrm{nul}(T)$ is called the *nullity* of T.

Theorem 1.11. *Every compact operator is bounded; also if T_1 and T_2 are bounded operators on $\mathcal{H}$, then $T_1 T_2 \in \mathcal{K}(\mathcal{H})$ if at least one between T_1 and T_2 is compact.*

Theorem 1.12. *Suppose that the identity map on $\mathcal{H}$ is a compact operator. Then* $\dim(\mathcal{H}) < \infty$.

The spectrum of compact operators has peculiar properties.

Theorem 1.13. *Let $T \in \mathcal{K}(\mathcal{H})$; let $\lambda \in \mathbb{C} \setminus \{0\}$. Then:*

(i) if $\mathrm{Ran}(T - \lambda\mathbb{I}) = \mathcal{H}$, *then $T - \lambda\mathbb{I}$ is injective and $(T - \lambda\mathbb{I})^{-1} \in \mathcal{B}(\mathcal{H})$;*

(ii) $\mathrm{Ran}(T - \lambda\mathbb{I})$ *is closed;*

(iii) if $T - \lambda\mathbb{I}$ is injective, then $(T - \lambda\mathbb{I})^{-1} \in \mathcal{B}(\mathcal{H})$;

(iv) $\mathrm{nul}(T - \lambda\mathbb{I}) < \infty$.

In particular, Theorem 1.13 says that, if $\lambda \neq 0$, either λ belongs to the resolvent set $\rho(T)$, in which case $\mathrm{Ran}(T - \lambda\mathbb{I}) = \mathcal{H}$, or λ is in the point spectrum $\sigma_{pp}(T)$, in which case $\mathrm{Ran}(T - \lambda\mathbb{I})$ is a proper closed subset of $\mathcal{H}$. Also, it is worth remarking that, if $\dim(\mathcal{H}) = \infty$, then $0 \in \sigma(T)$ for all $T \in \mathcal{K}(\mathcal{H})$. *Indeed*, suppose that $0 \in \rho(T)$ for some compact T; then $T^{-1} \in \mathcal{B}(\mathcal{H})$ and so $T T^{-1} = \mathbb{I}$ is compact (Theorem 1.11). Then, Theorem 1.12 gives the desired contradiction.
Before introducing the various definitions of essential spectrum, let us give the notion of Fredholm (bounded) operator.

Definition 1.11. *Let T be a bounded operator on $\mathcal{H}$. T is said to be a* Fredholm *operator if* $\mathrm{Ran}(T)$ *is closed,* $\mathrm{nul}(T) < \infty$ *and*

$$\mathrm{def}(T) := \mathrm{codim}(\mathrm{Ran}(T)) < \infty \ ;$$

$\mathrm{def}(T)$ *is called the* deficiency *of T. The* index $\mathrm{ind}(T)$ *of T is defined by*

$$\mathrm{ind}(T) := \mathrm{nul}(T) - \mathrm{def}(T) \ .$$

Remark 1.2.2. It can be shown, using Theorem 1.13 and other properties of compact operators (see [15, Theorem 1.15]), that if T is a compact operator, then $T - \lambda\mathbb{I}$ is a Fredholm map of index 0 (for $\lambda \neq 0$).

The definition can be coherently extended to closed operators.

Definition 1.12. *Let T be a closed operator. T is called a* semi-Fredholm operator *if* $\mathrm{Ran}(T)$ *is closed and at least one of* $\mathrm{nul}(T)$ *and* $\mathrm{def}(T)$ *is finite; it is said to be* Fredholm *if* $\mathrm{Ran}(T)$ *is closed and both* $\mathrm{nul}(T)$ *and* $\mathrm{def}(T)$ *are finite.*

Definition 1.13. *The set of all semi-Fredholm maps $T \in \mathcal{B}(\mathcal{H})$ having* $\mathrm{nul}(T) < \infty$ *(*$\mathrm{def}(T) < \infty$*) will be denoted by $\mathcal{F}_+(\mathcal{H})$ ($\mathcal{F}_-(\mathcal{H})$). The set of all (bounded) Fredholm operators will be denoted by $\mathcal{F}(\mathcal{H})$.*

Remark 1.2.3. Definition 1.13, however, works also for closed operators. Indeed, if T is closed, then $T \in \mathcal{B}(X(T), \mathcal{H})$, where $X(T)$ denotes the space $\mathcal{D}(T)$ equipped with the graph norm; $\ker(T)$ and $\mathrm{Ran}(T)$ are then unchanged by this new view of the operator T.

The class of semi-Fredholm operators is invariant under compact perturbations. This will be crucial in proving our result about invariance of the spectrum.

Theorem 1.14. *Let $T \in \mathcal{F}_\pm(\mathcal{H})$ and $S \in \mathcal{K}(\mathcal{H})$. Then $S + T \in \mathcal{F}_\pm(\mathcal{H})$ and* $\mathrm{ind}(S + T) = \mathrm{ind}(T)$*.*

We are now ready to give some of the many definitions of essential spectrum which can be found in the literature (we follow the definition contained in [15]):

Definition 1.14 (Essential spectrum)**.** *Let T be a closed, densely defined linear operator on $\mathcal{H}$. Let*

$$\Phi_\pm(T) = \{\lambda \in \mathbb{C} \,:\, T - \lambda\mathbb{I} \in \mathcal{F}_\pm(\mathcal{H})\} \,.$$

The various essential spectra [3] *are defined to be the sets*

$$\sigma_{ess,\,j}(T) := \mathbb{C} \setminus \Delta_j(T) \ ,$$

$j = 1, \ldots, 5$, where

$$\begin{aligned}
\Delta_1(T) &= \Phi_+(T) \cup \Phi_-(T)\,, \\
\Delta_2(T) &= \Phi_+(T)\,, \\
\Delta_3(T) &= \{\lambda \in \mathbb{C} \,:\, T - \lambda\mathbb{I} \in \mathcal{F}(\mathcal{H})\} = \Phi_+(T) \cap \Phi_-(T)\,, \\
\Delta_4(T) &= \{\lambda \in \mathbb{C} \,:\, \lambda \in \Delta_3(T) \text{ and } \mathrm{ind}(T - \lambda\mathbb{I}) = 0\}\,, \\
\Delta_5(T) &= \text{union of all components of } \Delta_1(\mathrm{T}) \text{ which intersect } \rho(T)\,.
\end{aligned}$$

[3] A different notion of essential spectrum is given in [13]: the essential spectrum of T is the set of complex numbers λ such that the range of $T - \lambda\mathbb{I}$ is not closed in $\mathcal{H}$. Reed and Simon, in [24], give yet another definition for self-adjoint operators: let $P_\Omega(T)$ denote the spectral projection of a self-adjoint operator T on a Borel set of $\mathbb{R}$, Ω; λ belongs to the essential spectrum of T if the closure $\mathrm{Ran}P_{]\lambda-\varepsilon,\lambda+\varepsilon[}(T)$ is infinite dimensional for all $\varepsilon > 0$.

The sets $\sigma_{d,j} := \sigma(T) \setminus \sigma_{ess,j}(T)$, $j = 1, \ldots, 5$, *are called* discrete spectra *for a reason that will be clear later (Theorem 1.15). The* essential spectral radius *is defined by*

$$\sigma_{ess,j}(T) := \sup\{|\lambda| \,:\, \lambda \in \sigma_{ess,j}(T)\}$$

for all $j = 1, \ldots, 5$.

Maybe, the most common definition of essential spectrum is $\sigma_{ess,3}$, i.e. the set of λ such that $T - \lambda\mathbb{I}$ is not a Fredholm operator. Also, for some of the definitions, the essential spectrum can be characterized by Weyl sequences; for example

Proposition 1.3. *Let* T *be a closed operator. Then* $\lambda \in \sigma_{ess,2}(T)$ *if, and only if, there exists a Weyl sequence for* T *corresponding to* λ.

However, when T is self-adjoint, all the definitions given above are equivalent[4] and, in that case, the discrete spectrum can be characterized as follows.

Theorem 1.15. *Let* T *be a self-adjoint operator defined on* $\mathcal{H}$. *Then* $\lambda \in \sigma_d(T)$ *if, and only if, it is an isolated eigenvalue of finite multiplicity.*

Now, let us introduce the notion of relative compactness.

Definition 1.15. *Let* S, T *be densely defined, closed operators on* $\mathcal{H}$. *The operator* S *is said to be* T-compact *(or* compact relative to T*) if*

- $\mathcal{D}(T) \subset \mathcal{D}(S)$, *and*
- *for every sequence* $\{\varphi_n\} \subset \mathcal{D}(T)$ *such that* $\{\varphi_n\}$ *is bounded in the* T*-graph norm,* $\{S\varphi_n\}$ *contains a convergent subsequence in* $\mathcal{H}$.

Equivalently, S is T-compact if, and only if, $S \in \mathcal{K}(X(T), \mathcal{H})$.

Remark 1.2.4. The multiplication operator defined by

$$S = i\gamma\chi_R(x)$$

is H-compact. Indeed, let $\{u_n\} \subset \mathcal{D}(\mathrm{H})$ be a a bounded sequence in the graph norm $\|\cdot\|_{\mathrm{H}}$, i.e. there exists $C > 0$ such that

$$\|u_n\|_{\mathrm{H}} = \|u_n\|_2 + \|\mathrm{H}u_n\|_2 < C\ .$$

Then, since L^2 is a reflexive space, there is a subsequence $\{u_{n_k}\}$ which converges weakly in $X(T)$ to some u, in particular it converges weakly in $\mathcal{H}$. It clearly follows that, in particular, $S\,u_n = i\gamma\,u_n \longrightarrow S\,u = i\gamma\,u$ strongly in L^2. Also, $\mathcal{D}(S) = \mathrm{L}^2([0, +\infty[) \supset \mathcal{D}(\mathrm{H})$.

[4]See [15, IX.Theorem 1.6]

Finally, we are able to show the announced stability theorem under relatively compact perturbations.

Theorem 1.16. *Let S, T be densely defined, closed operators on $\mathcal{H}$; let S be T-compact. Then*

$$\sigma_{ess,j}(T) = \sigma_{ess,j}(T+S)$$

for $j = 1, \ldots, 4$. If T is self-adjoint

$$\sigma_{ess}(T) = \sigma_{ess}(T+S)$$

This finally explains why we have said that the essential spectrum of the perturbed operators $\mathrm{H}_{R,\gamma}$ is the same of H.

1.2.3 Some theorems of complex analysis

We will cite here only few well-known results of (one-variable) complex analysis, since we will use them in the following chapters.

Theorem 1.17 (Montel)**.** *Let $\{f_n\}_{n\in\mathbb{N}}$, f be analytic functions of one variable, having as common domain the open set $\Omega \subset \mathbb{C}$. Suppose $f_n \longrightarrow f$ pointwise on a compact set K and suppose that the family $\{f_n\}$ is uniformly bounded on an open set containing K. Then $f_n \longrightarrow f$ uniformly on K.*

Theorem 1.18 (Identity principle)**.** *Let Ω be a connected open set in $\mathbb{C}$; let $f : \Omega \to \mathbb{C}$ be an analytic function. For $c \in \Omega$, the following are equivalent:*

- *c is an accumulation point of the zero-set of f, $Z(f)$;*
- *c is contained in the topological interior of $Z(f)$;*
- *$f^{(n)}(c) = 0$ for all $n \in \mathbb{N}$, $n \geq 0$.*

Moreover, if Ω is also connected, f is identically 0 on Ω if, and only if, $Z(f)$ has at least one accumulation point.

Theorem 1.19 (Argument principle)**.** *Let f be analytic on an open connected set Ω except for a finite set P of polar singularities, and with a finite set of zeros Z. If Γ is a loop in $\Omega \setminus (P \cup Z)$, nullhomologus in Ω, then*

$$\frac{1}{2\pi i}\int_\Gamma \frac{f'(z)}{f(z)}\mathrm{d}z = \sum_{c\in Z\cup P} \mathrm{ind}_\Gamma(c)\,\mathrm{mult}(f,c) \ ,$$

where $\mathrm{ind}_\Gamma(c)$ is the winding number of Γ around c and $\mathrm{mult}(f,c)$ denotes both the order of c as a pole of f and the multiplicity of c as a zero for f.

Theorem 1.20 (Schwarz reflection principle)**.** *If f is an analytic function of one complex variable, defined on the upper half-plane and real-valued on the real axis, then*

$$f(\bar{z}) = \overline{f(z)}$$

defines an analytic extension of f on the whole $\mathbb{C}$.

1.2.4 Mollifiers and functions of "cap-shaped" type

In this section we will introduce the concepts of mollifier and "cap-shaped" function, which we will use in Section 2.1.1 to construct a Weyl singular sequence associated with the continuous spectrum of the free (unperturbed) Schrödinger operator. The discussion here is based on [9].

Definition 1.16 (Kernel of mollification)**.** *A function $\omega : \mathbb{R}^n \to \mathbb{R}$ is said to be a kernel of mollification if*

$$\omega \in \mathcal{C}_0^\infty(\mathbb{R}^n),\ \operatorname{supp}\omega \subset \overline{B(0,1)} \text{ and } \int_{\mathbb{R}^n} \omega \,\mathrm{d}x = 1\ .$$

For $\delta > 0$ and $x \in \mathbb{R}^n$ we set $\omega_\delta(x) := \frac{1}{\delta^n}\, \omega\left(\frac{x}{\delta^n}\right)$.

Remark 1.2.5. Clearly, by definition, $\omega_\delta \in \mathcal{C}_0^\infty(\mathbb{R}^n)$, $\operatorname{supp}\omega_\delta \subset \overline{B(0,\delta)}$ and $\int_{\mathbb{R}^n} \omega_\delta \,\mathrm{d}x = 1$.

Example 1.2.1. Kernels of mollification do exist. For example, the function

$$\omega(x) := \begin{cases} c \cdot e^{\frac{1}{|x|^2-1}} & ,\text{ if} \quad |x| < 1 \\ 0 & ,\text{ if} \quad |x| \geq 1 \end{cases} ,$$

where

$$c = \left(\int_{B(0,1)} e^{\frac{1}{|x|^2-1}} \,\mathrm{d}x \right)^{-1} ,$$

is a kernel of mollification.

Definition 1.17 (Mollifier with step δ)**.** *Let $\Omega \subset \mathbb{R}^n$ be a measurable set and $\delta > 0$. For a function f defined on Ω and such that, for each bounded set B, $f \in \mathrm{L}^1(\Omega \cap B)$, the* mollifier *with step δ is the operator A_δ defined by*

$$\left(A_\delta f\right)(x) = \frac{1}{\delta^n} \int_\Omega \omega\left(\frac{x-y}{\delta}\right) f(y) \,\mathrm{d}y$$

for almost all x in $\mathbb{R}^n$

Remark 1.2.6. Note that[5]

$$(A_\delta f)(x) = \frac{1}{\delta^n}\int_\Omega \omega\left(\frac{x-y}{\delta}\right) f^\circ(y)\,\mathrm{d}y = \int_{\mathbb{R}^n} \omega_\delta(x-y) f^\circ(y)\,\mathrm{d}y = (\omega_\delta * f^\circ)(x)\,.$$

Moreover, it can be shown that for each admissible f, $\forall\ \alpha \in \mathbb{N}^n$

$$D^\alpha A_\delta f = (D^\alpha \omega_\delta) * f^\circ\ ,$$

thus $A_\delta f \in \mathcal{C}^\infty(\mathbb{R}^n)$, and

$$\operatorname{supp} A_\delta f \subset \overline{(\operatorname{supp} f)^\delta}\ ,$$

where for a set G, $G^\delta := \bigcup_{x\in G} B(x,\delta)$ is the so-called *δ-neighbourhood* of G.

Definition 1.18 ("Cap-shaped" type function). *A function η is said to be of* "cap-shaped" *type if*

- $\eta \in \mathcal{C}^\infty(\mathbb{R}^n)$*;*
- $\operatorname{supp}\eta \subset \Omega^\delta$*;*
- $0 \le \eta \le 1$ *and* $\eta \equiv 1$ *on* Ω*.*

"Cap-shaped" type functions can be constructed with the help of non-negative kernels of mollification (they exist, see Example 1.2.1) for example by

$$\eta = A_{\frac{\delta}{4}} \chi_{\Omega^{\frac{\delta}{2}}}\ .$$

Indeed, η is of the class $\mathcal{C}^\infty(\mathbb{R}^n)$, $0 \le \eta \le 1$ (because we have chosen a non-negative kernel), $\eta \equiv 1$ on Ω and

$$\operatorname{supp}\eta \subset \overline{\left(\operatorname{supp}\chi_{\Omega^{\frac{\delta}{2}}}\right)^{\frac{\delta}{4}}} = \overline{\left(\Omega^{\frac{\delta}{2}}\right)^{\frac{\delta}{4}}} \subset \Omega^\delta\ .$$

1.3 Boundary triplets and Titchmarsh-Weyl M-functions: basic concepts and notation

The content of this section is essentially founded on the article [7]. We would like to introduce here a very useful tool, the Titchmarsh-Weyl function, which will allow us to find the isolated eigenvalues of the family of perturbed non-selfadjoint Schrödinger operators $\mathrm{H}_{R,\gamma}$, which is the object of this thesis. We will cite here some results and the basic ideas developed in the article.
Let us start with a definition, which is crucial in our context as we are talking about non self-adjoint operators:

[5] Here f° denotes the extension of f by zero outside Ω.

Definition 1.19. *Let A and $\tilde{A}$ be densely defined, closed operators on a Hilbert space $\mathcal{H}$. The operators A and $\tilde{A}$ are said to be an* adjoint pair *if $A^* \supseteq \tilde{A}$ and $\tilde{A}^* \supseteq A$.*

Throughout, we will assume that:

(i) the operators A and $\tilde{A}$ are an adjoint pair;

(ii) the linear space $\mathcal{D}(\tilde{A}^*)$ is equipped with the graph norm, so that, since $\tilde{A}^*$ is closed, it is a Hilbert space.

Proposition 1.4. *For each adjoint pair of closed densely defined operators A and $\tilde{A}$ on $\mathcal{H}$, there exist "boundary spaces" $\mathcal{K}_1$, $\mathcal{K}_2$ and "boundary operators"*

$$\begin{aligned} \Gamma_1 : \mathcal{D}(\tilde{A}^*) &\longrightarrow \mathcal{K}_1, \qquad & \Gamma_2 : \mathcal{D}(\tilde{A}^*) &\longrightarrow \mathcal{K}_2, \\ \tilde{\Gamma}_1 : \mathcal{D}(A^*) &\longrightarrow \mathcal{K}_2, \qquad & \tilde{\Gamma}_2 : \mathcal{D}(A^*) &\longrightarrow \mathcal{K}_1 \end{aligned}$$

such that for $u \in \mathcal{D}(\tilde{A}^*)$ and $v \in \mathcal{D}(A^*)$ there is an abstract Green formula

$$(\tilde{A}^* u, v)_{\mathcal{H}} - (u, A^* v)_{\mathcal{H}} = (\Gamma_1 u, \tilde{\Gamma}_2 v)_{\mathcal{K}_1} - (\Gamma_2 u, \tilde{\Gamma}_1 v)_{\mathcal{K}_2} \ . \tag{1.10}$$

The boundary operators Γ_1, Γ_2, $\tilde{\Gamma}_1$, $\tilde{\Gamma}_2$ are bounded with respect to the graph norm and surjective. Moreover, we have

$$\mathcal{D}(A) = \mathcal{D}(\tilde{A}^*) \cap \ker \Gamma_1 \cap \ker \Gamma_2 \quad \text{and} \quad \mathcal{D}(\tilde{A}) = \mathcal{D}(A^*) \cap \ker \tilde{\Gamma}_1 \cap \ker \tilde{\Gamma}_2 \ . \tag{1.11}$$

The collection $\left\{\mathcal{K}_1 \oplus \mathcal{K}_2,\ (\Gamma_1, \Gamma_2),\ (\tilde{\Gamma}_1, \tilde{\Gamma}_2)\right\}$ is called a boundary triplet *for the adjoint pair A, $\tilde{A}$.*

Proof. See [7] for detailed references. □

We will consider the following extensions of A and $\tilde{A}$.

Definition 1.20. *Let $B \in \mathcal{L}(\mathcal{K}_2, \mathcal{K}_1)$, $\tilde{B} \in \mathcal{L}(\mathcal{K}_1, \mathcal{K}_2)$ and define*

$$A_B := \tilde{A}^*\Big|_{\ker(\Gamma_1 - B\Gamma_2)} \quad \text{and} \quad \tilde{A}_{\tilde{B}} := A^*|_{\ker(\tilde{\Gamma}_1 - \tilde{B}\tilde{\Gamma}_2)} \ .$$

Remark 1.3.1. A_B is actually an extension of A because

$$\mathcal{D}(A_B) = \mathcal{D}(\tilde{A}^*) \cap \ker(\Gamma_1 - B\Gamma_2)$$

and, according to (1.11),

$$\mathcal{D}(A) = \mathcal{D}(\tilde{A}^*) \cap \ker \Gamma_1 \cap \ker \Gamma_2 \subset \mathcal{D}(\tilde{A}^*) \cap \ker(\Gamma_1 - B\Gamma_2) \ .$$

Definition 1.21. *Let us assume that* $\rho(A_B) \neq \emptyset$. *For* $\lambda \in \rho(A_B)$, *the* (Titchmarsh-Weyl) M-function *is the mapping*

$$M_B(\lambda) : \mathrm{Ran}(\Gamma_1 - B\Gamma_2) \longrightarrow \mathcal{K}_2$$

defined by

$$M_B(\lambda)(\Gamma_1 - B\Gamma_2)u = \Gamma_2 u \quad \forall u \in \ker(\tilde{A}^* - \lambda) \ ;$$

for $\lambda \in \rho(\tilde{A}_{\tilde{B}})$, *we define*

$$\tilde{M}_{\tilde{B}}(\lambda) : \mathrm{Ran}(\tilde{\Gamma}_1 - \tilde{B}\tilde{\Gamma}_2) \longrightarrow \mathcal{K}_1, \ \tilde{M}_{\tilde{B}}(\lambda)(\tilde{\Gamma}_1 - \tilde{B}\tilde{\Gamma}_2)v = \tilde{\Gamma}_2 v \quad \forall v \in \ker(A^* - \lambda)$$

Remark 1.3.2. Since the function $M_B(\lambda)$ is a linear mapping, when this is possible without ambiguity, we will refer to the term $M_B(\lambda)$ also as the Titchmarsh-Weyl *coefficient*, keeping in mind that the coefficient is still a **function** of λ.

Reading Definition 1.21 with some imagination, we can view $M_B(\lambda)$ as the function which maps a "generalized" Robin boundary condition $(\Gamma_1 - B\Gamma_2)u$ into a "generalized" Neumann or Dirichlet condition $\Gamma_2 u$. We will see this more clearly in the following examples.

Example 1.3.1. Let the Hilbert space be $\mathcal{H} = \mathrm{L}^2([0,1])$; let V be a complex-valued locally integrable function defined on $[0,1]$. Consider the Schrödinger operator A defined by $Au := -u'' + Vu$ with domain

$$\mathcal{D}(A) = \left\{ u \in H^2([0,1]) \ : \ u(0) = 0 = u(1), u'(0) = 0 = u'(1) \right\} \ ;$$

let also $\tilde{A}$ be the operator

$$\tilde{A}u = -u'' + \bar{V}u$$

with same domain $\mathcal{D}(\tilde{A}) = \mathcal{D}(A)$. With this setting we have that

$$A^*u = -u'' + \bar{V}u \quad \text{and} \quad \tilde{A}^*u = -u'' + Vu \ ,$$

with respective domains $\mathcal{D}(A^*) = \mathcal{D}(\tilde{A}^*) = H^2([0,1])$. In this way A and $\tilde{A}$ form an adjoint pair. We do not need Proposition 1.4 to prove the existence of an abstract Green formula like (1.10), because we can find it explicitly. Indeed, if $u \in \mathcal{D}(\tilde{A}^*)$ and $v \in \mathcal{D}(A^*)$

$$\begin{aligned}
(\tilde{A}^*u, v)_{\mathcal{H}} - (u, A^*v)_{\mathcal{H}} &= \int_0^1 \left[(-u'' + Vu)\,\bar{v} - u\,\overline{(-v'' - \bar{V}v)} \right] \mathrm{d}x \\
&= \left[-u'(x)\bar{v}(x) + u(x)\bar{v}' \right]_{x=0}^{x=1} \\
&= \left(-u'(1)\overline{v(1)} + u'(0)\overline{v(0)} \right) \\
&\quad - \left(-u(1)\overline{v'(1)} + u(0)\overline{v'(0)} \right) \\
&= (\Gamma_1 u, \Gamma_2 v)_{\mathbb{C}^2} - (\Gamma_2 u, \Gamma_1 v)_{\mathbb{C}^2} \ ,
\end{aligned}$$

choosing

$$\Gamma_1 = \tilde{\Gamma}_1 : U \mapsto \begin{pmatrix} -U'(1) \\ +U'(0) \end{pmatrix}, \quad \Gamma_2 = \tilde{\Gamma}_2 : U \mapsto \begin{pmatrix} U(1) \\ U(0) \end{pmatrix}$$

as "boundary operators" in the "boundary space" $\mathbb{C}^2$. In this case, $B \in \mathcal{L}(\mathbb{C}^2)$ can be represented as a two-by-two matrix.

Therefore, if u is a solution in $\mathrm{L}^2([0,1]$ of the spectral equation

$$-u'' + V\,u = \lambda\,u$$

satisfying the boundary condition(s)

$$(\Gamma_1 - B\Gamma_2)u = \begin{pmatrix} -u'(1) \\ +u'(0) \end{pmatrix} - B \begin{pmatrix} u(1) \\ u(0) \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \mathbb{C}^2 ,$$

the Titchmarsh-Weyl function $M_B(\lambda)$ is the mapping

$$(\Gamma_1 - B\Gamma_2)u \in \mathbb{C}^2 \mapsto \Gamma_2 u \in \mathbb{C}^2 ,$$

which, as announced, looks like a "generalized" Robin-to-Dirichlet mapping on $\mathbb{C}^2$ (Neumann-to-Dirichlet if B is the null matrix).

Example 1.3.2. In this second model, let $\mathcal{H} = \mathrm{L}^2([0,b])$, with $b > 0$. Let A and $\tilde{A}$ as above but with domains

$$\mathcal{D}(A) = \mathcal{D}(\tilde{A}) = \big\{ u \in H^2([0,b]) \;:\; u(0) = 0 = u(b),\, u'(0) = 0 \big\} \;;$$

the respective adjoint operators have here domains

$$\mathcal{D}(A^*) = \mathcal{D}(\tilde{A}^*) = \big\{ u \in H^2([0,b]) \;:\; u(b) = 0 \big\} \;.$$

We have that

$$\begin{aligned} (\tilde{A}^* u, v)_{\mathcal{H}} - (u, A^* v)_{\mathcal{H}} &= \int_0^b \Big[(-u'' + Vu)\,\bar{v} - u\,\overline{(-v'' - Vv)} \Big] \,\mathrm{d}x \\ &= [-u'(x)\bar{v}(x) + u(x)\bar{v}']_{x=0}^{x=b} \\ &= \Big(u'(0)\overline{v(0)} - u(0)\overline{v'(0)} \Big) \\ &= (\Gamma_1 u, \Gamma_2 v)_{\mathbb{C}} - (\Gamma_2 u, \Gamma_1 v)_{\mathbb{C}} \;, \end{aligned}$$

where

$$\Gamma_1 = \tilde{\Gamma}_1 : U \mapsto U'(0),\; \Gamma_2 = \tilde{\Gamma}_2 : U \mapsto U(0) \;.$$

Here B is simply a complex number. Thus, the Titchmarsh-Weyl is precisely a Robin-to-Dirichlet map.

Remark 1.3.3. For our problem on $\mathrm{L}^2([0,+\infty[)$ we will use yet another model; it will be presented in full details through Section 2.1.

In order to prove the results which follow, we require an abstract unique continuation hypothesis, which is satisfied under fairly general conditions (again, see [7] for references), for example for Schrödinger operators.

Definition 1.22. *We say that the operator $\tilde{A}^* - \lambda$ satisfies the* unique continuation hypothesis *if*

$$\ker(\tilde{A}^* - \lambda) \cap \ker \Gamma_1 \cap \ker \Gamma_2 = \{0\} \ ;$$

similarly $A^* - \lambda$ satisfies the unique continuation hypothesis if

$$\ker(A^* - \lambda) \cap \ker \tilde{\Gamma}_1 \cap \ker \tilde{\Gamma}_2 = \{0\} \ .$$

Lemma 1.1. *Assume that the unique continuation hypothesis holds for $A^* - \bar{\lambda}$. Then, the range of $\tilde{A}^*$ is dense in $\mathcal{H}$.*

Theorem 1.21. *Let $\mu \in \mathbb{C}$ be an isolated eigenvalue of a finite algebraic multiplicity of the operator A_B. Assume that the unique continuation hypothesis holds for $\tilde{A}^* - \mu$ and $A^* - \bar{\mu}$. Then μ is a pole of finite multiplicity of $M_B(\cdot)$ and the order of the pole of $R(\cdot, A_B)$ at μ is the same as the order of the pole of $M_B(\cdot)$ at μ.*

Under slightly stronger hypotheses, it can be shown that the isolated eigenvalues of A_B correspond exactly to the isolated poles of the M-function.

Theorem 1.22. *Let $\mu \in \mathbb{C}$. Assume that $\rho(A_B) \neq \emptyset$ and that there exist operators B, $C \in \mathcal{L}(\mathcal{K}_2, \mathcal{K}_1)$ such that $\mu \in \rho(A_C) \cap \rho(A_{B-C})$. Then, μ is an isolated eigenvalue of finite algebraic multiplicity of the operator A_B if and only if μ is a pole of finite multiplicity of $M_B(\cdot)$; moreover, the order of the pole of $R(\cdot, A_B)$ at μ is the same as the order of the pole of $M_B(\cdot)$ at μ.*

We will not prove these two theorems, as the proof requires a lot of notation and intermediate results. For details, again, see the article [7]. However, a very basic proof can be found for the following proposition, which gives a useful relation between M-functions associated with different boundary conditions.

Proposition 1.5. *Let B, $C \in \mathcal{L}(\mathcal{K}_2, \mathcal{K}_1)$. For $\lambda \in \rho(A_B) \cap \rho(A_{B+C})$, we have that*

$$M_{B+C}(\lambda)(\mathbb{I} - C M_B(\lambda)) = M_B(\lambda) \ .$$

Proof. For $u \in \ker(\tilde{A}^* - \lambda)$

$$\begin{aligned} M_{B+C}(\lambda)(\mathbb{I} - CM_B(\lambda))(\Gamma_1 - B\Gamma_2)u &= M_{B+C}(\lambda)\,[(\Gamma_1 - B\Gamma_2)u - C(\Gamma_2 u)] \\ &= M_{B+C}(\lambda)\,[(\Gamma_1 - (B+C)\Gamma_2)u] \\ &= \Gamma_2 u \ . \end{aligned}$$

□

Corollary 1.1. *Let $B \in \mathcal{L}(\mathcal{K}_2, \mathcal{K}_1)$, $\lambda \in \rho(A_0) \cap \rho(A_B)$. Then*

$$M_B(\lambda)(\mathbb{I} - BM_0(\lambda)) = M_0(\lambda) \ .$$

Remark 1.3.4. When $(\Gamma_1 - B\Gamma_2)u = 0$ represents a (complex) Robin boundary condition, $\Gamma_1 u = 0$ a Neumann condition and consequently $(\Gamma_2)u = 0$ a Dirichlet condition, like in Example 1.3.2, the poles of $R(\cdot, A_B)$, that is the poles of the "Robin-to-Dirichlet" M-function defined in Definition 1.21, are usually referred to as *Robin eigenvalues*; if $B = 0$, which will be our case, we will call them *Neumann eigenvalues*.
Moreover, it can be easily seen, using the identity in Proposition 1.5 and adapting the statement of Theorem 1.22, that the *Dirichlet eigenvalues* are precisely the zeros of the M-function.

1.4 Limit-point case, limit-circle case and Sims classification for Sturm-Liouville operators

In this section, we will present the classical Weyl limit-point, limit-circle classification for Sturm-Liouville and its most famous extension, the Sims classification. In particular, the concept of Titchmarsh-Weyl function introduced in Section 1.3 arises from both these theories.

1.4.1 Limit-point and limit-circle alternative

Let L be the self-adjoint differential operator defined on a real interval $[a, b[$, with $-\infty \leq a < b \leq +\infty$, by

$$L\,u := -\,(-pu')' + q(x)u(x) \ , \tag{1.12}$$

where it is assumed that p, p',q are real and continuous functions[6], $p > 0$. If $[x_1, x_2]$ is an interval over which L is defined and f and g are any two

[6]To get self-adjointness, it suffices for q to be integrable over every finite subinterval of $[a, b]$ and p absolutely continuous.

functions such that Lf, Lg make sense, then the following Green's formula holds true:

$$\int_{x_1}^{x_2} \left(\bar{g}\, Lf - f\, \overline{Lg}\right)\, \mathrm{d}x = [f\, g](x_2) - [f\, g](x_1)\ , \tag{1.13}$$

where

$$[f\, g](x) := p(x)\left(f(x)\bar{g}'(x) - f'(x)\bar{g}(x)\right)$$

is the so-called *modified Wronskian.*

Remark 1.4.1. This family of operators is usually referred to as the family of *Sturm-Lioville* operators. Clearly, it is a generalization of the class of (physical) Schrödinger operators, since for a Schrödinger operator $p \equiv 1$.

In what follows, we shall deal only with the interval $[0, +\infty[$. The case $[R, +\infty[$ is very similar, while the case $]-\infty, +\infty[$ requires more work. Let us start with the Weyl limit-point, limit-circle classification.

Definition 1.23 (Limit-point and Limit-circle cases)**.** *If, for a particular complex number λ_0, every solution u of the differential equation (often called* spectral equation*)*

$$Lu = \lambda_0 u \tag{1.14}$$

is in $\mathrm{L}^2([0, +\infty[)$*, then L is said to be of the* limit-circle type *at infinity; otherwise L is said to be of* limit-point type *at infinity.*

Remark 1.4.2. The definition of limit-circle depends only on the operator L and not on the particular λ_0 chosen. Indeed, it can be shown that, if every solution of $Lu = \lambda_0 u$ is of class $\mathrm{L}^2([0, +\infty[)$ for λ_0, then, for any complex number λ, every solution of $\mathrm{H}u = \lambda u$ is in $\mathrm{L}^2([R, +\infty[)$.

Clearly, according to Definition 1.23, in the limit-point case at most one non-trivial solution of the spectral equation $Lu = \lambda u$ is of class $\mathrm{L}^2([0, +\infty[)$. Actually, there is exactly one solution (up to constant multiples) of $Lu = \lambda u$ which is in $\mathrm{L}^2([0, +\infty[)$ for any $\lambda \in \mathbb{C}$ such that $\mathrm{Im}(\lambda) \neq 0$, as shown by the following:

Theorem 1.23. *Let $\lambda \in \mathbb{C}$ such that* $\mathrm{Im}(\lambda) \neq 0$*; let ϕ_λ, ψ_λ be two linearly independent solutions of (1.14) satisfying*

$$\begin{pmatrix} \phi_\lambda(0) \\ p(0)\phi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} \sin\alpha \\ -\cos\alpha \end{pmatrix}, \qquad \begin{pmatrix} \psi_\lambda(0) \\ p(0)\psi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}\ ,$$

where $0 \leq \alpha < \pi$*; let* $m \in \mathbb{C}$*,* $\theta_\lambda := \phi_\lambda + m\psi_\lambda$*; let* b *be a real number,* $0 < b < +\infty$*. Then* θ_λ *satisfies the real boundary condition*

$$\cos\beta\, u(b) + \sin\beta\, u'(b) = 0 \tag{1.15}$$

for some $0 \leq \beta < \pi$*, if and only if* m *lies on a circle* C_b *in the complex plane whose equation is*

$$[\theta_\lambda\, \theta_\lambda]\,(b) = 0\ .$$

As $b \longrightarrow +\infty$*, either* C_b *tends to* m_∞*, a limit point, or* $C_b \longrightarrow C_\infty$*, a limit circle. In the first case exactly one non-trivial solution is in* $\mathrm{L}^2([0, +\infty[)$*; all solutions of* $\mathrm{L}u = \lambda u$ *are in* $\mathrm{L}^2([0, +\infty[)$ *in the latter case.*
Moreover, in the limit-circle case, a point is on the limit circle $C_\infty(\lambda)$ *if, and only if,*

$$\lim_{b \to +\infty} [\theta_\lambda\, \theta_\lambda]\,(b) = 0$$

Proof. According to the theory of complex linear systems, $\phi_\lambda(x) = \phi(x, \lambda)$, ψ_λ, ϕ'_λ and ψ_λ and are analytic functions of the complex spectral parameter λ and continuous in both the variables (x, λ). Moreover, the (classical) Wronksian of the two solutions $[\phi_\lambda\, \psi_\lambda](x) = 1$ for all $x \in [0, +\infty[$.

Every other solution θ_λ of $\mathrm{L}u = \lambda u$ is, up to constant multiples, of the form

$$\theta_\lambda = \phi_\lambda + m\psi_\lambda$$

for some m depending on λ. In order to satisfy the boundary condition (1.15) at b, clearly m must be

$$m = -\frac{\cot\beta\, \phi_\lambda(b) + p(b)\phi'_\lambda(b)}{\cot\beta\psi_\lambda(b) + p(b)\psi'_\lambda(b)} \tag{1.16}$$

Since ϕ_λ, ψ_λ, ϕ'_λ and ψ_λ are analytic and real-valued when λ is real, it follows that $m = m(\lambda, b, \beta)$ is a meromorphic function of the variable λ and real for real λ. Putting $z = \cot\beta$ and holding (λ, b) fixed, (1.16) can be written as

$$m = -\frac{A\,z + B}{C\,z + D}$$

with A, B, C, D fixed while z varies over the real line as $0 \leq \beta < \pi$. From well-known properties of Möbius transformations, the real axis of the z-plane is mapped into a circle C_b in the m-plane. Thus, θ_λ satisfies (1.15) if, and only if, m lies on C_b. Moreover, the circle can be explicitly found. Indeed, clearly

$$z = -\frac{B + D\,m}{A + C\,m}$$

and the condition of reality of z, $\mathrm{Im}(z) = 0$, becomes

$$(\bar{A} + \bar{C}\,\bar{m})(B + D\,m) - (A + C\,m)(\bar{B} + \bar{D}\bar{m}) = 0 \ ,$$

that is

$$(\bar{C}D - C\bar{D})|m|^2 + (\bar{A}D - \bar{B}C)m - (A\bar{D} - B\bar{C})\bar{m} + (\bar{A}B - A\bar{B}) = 0 \ . \quad (1.17)$$

This is an equation for a circle C_b of center

$$\tilde{m}_b = \frac{A\bar{D} - B\bar{C}}{\bar{C}D - C\bar{D}}$$

and radius

$$r_b = \frac{|AD - BC|}{|\bar{C}D - C\bar{D}|} \ .$$

By definition of A, B, C, D, it is readily seen that (1.17) can be written as

$$\left[\theta_\lambda\, \theta_\lambda\right](b) = 0 \ . \quad (1.18)$$

and that

$$\begin{aligned} A\bar{D} - B\bar{C} &= \left[\phi_\lambda\, \psi_\lambda\right](b) \\ \bar{C}D - C\bar{D} &= -\left[\psi_\lambda\, \psi_\lambda\right](b) \\ AD - BC &= \left[\phi_\lambda\, \bar{\psi_\lambda}\right](b) = 1 \ . \end{aligned}$$

So

$$\tilde{m}_b = -\frac{\left[\phi_\lambda\, \psi_\lambda\right](b)}{\left[\psi_\lambda\, \psi_\lambda\right](b)} \text{ and } r_b = \frac{1}{\left[\psi_\lambda\, \psi_\lambda\right](b)} \ .$$

The interior of C_b in the m-plane is given by

$$\frac{\left[\theta_\lambda\, \theta_\lambda\right](b)}{\left[\psi_\lambda\, \psi_\lambda\right](b)} < 0 \ . \quad (1.19)$$

By Green's formula (1.13),

$$\left[\theta_\lambda\, \theta_\lambda\right](b) = 2i\mathrm{Im}(\lambda) \int_0^b |\theta_\lambda|^2 \, \mathrm{d}x + \left[\theta_\lambda\, \theta_\lambda\right](0)$$

and

$$\left[\psi_\lambda\, \psi_\lambda\right](b) = 2i\mathrm{Im}(\lambda) \int_0^b |\psi_\lambda|^2 \, \mathrm{d}x \ .$$

Since $[\theta_\lambda\,\theta_\lambda]\,(0) = -2i\mathrm{Im}(\lambda)$, the equation for the interior of C_b (1.19) becomes for $\mathrm{Im}(\lambda) > 0$

$$\int_0^b |\theta_\lambda|^2\,\mathrm{d}x < \frac{\mathrm{Im}(m)}{\mathrm{Im}(\lambda)}\ ;$$

the radius r_b is given for λ in the upper half-plane by

$$r_b = \left(2i\mathrm{Im}(\lambda)\int_0^b |\psi_\lambda|^2\,\mathrm{d}x\right)^{-1}\ . \tag{1.20}$$

Now, let $0 < a < b < \infty$. Then if m is inside or on C_b

$$\int_0^a |\theta_\lambda|^2\,\mathrm{d}x < \int_0^b |\theta_\lambda|^2\,\mathrm{d}x \leq \frac{\mathrm{Im}(m)}{\mathrm{Im}(\lambda)}\ ,$$

which means that C_b is contained in the interior of C_a. Therefore, if $\mathrm{Im}(\lambda)$, as $b \to \infty$ the circles C_b have to converge either to a circle C_∞ or to a point m_∞. If the C_b converges to a circle, then its radius r_∞ is positive, thus by (1.20) $\psi_\lambda \in \mathrm{L}^2([0, +\infty[)$. If $\hat{m}_\infty$ is any point of C_∞, then m_∞ is inside any C_b, hence

$$\int_0^b |\phi_\lambda + \hat{m}_\infty\psi_\lambda|^2\,\mathrm{d}x < \frac{\mathrm{Im}(\hat{m}_\infty)}{\mathrm{Im}(\lambda)}\ ;$$

letting $b \to \infty$ one sees that $\phi_\lambda + \hat{m}_\infty\psi_\lambda$, that is any solution except ψ_λ is in $\mathrm{L}^2([0, +\infty[)$. The same argument holds if C_b reduces to the point m_∞, in which case - again by (1.20)- $\psi_\lambda \notin \mathrm{L}^2([0, +\infty[)$, so there is only one non-trivial solution (up to constant multiples) of class $\mathrm{L}^2([0, +\infty[)$. □

The classification is then consistent: the two cases are mutually exclusive. Sometimes, this is referred to as the *Weyl alternative*.
In particular, the periodic Schrödinger operator is in the limit-point case, as implied by the following criterion.

Theorem 1.24. *Let S be a positive differentiable (real) function and k_1, k_2 positive constants such that for large x*

$$q(x) \geq -k_1 S(x)\,,\ \int_0^{+\infty} (pS)^{\frac{1}{2}} = +\infty\,,$$
$$\left|p^{\frac{1}{2}}(x)S'(x)S^{-\frac{3}{2}}(x)\right| \leq k_2\ . \tag{1.21}$$

Then L is in the limit-point case at infinity.

Proof. Suppose that θ is a real solution of $L\,u = 0$ belonging to $\mathrm{L}^2([0,+\infty[)$. Then for some c

$$\int_c^x \frac{(p\theta')'\theta}{S}\,\mathrm{d}x' = \int_c^x \frac{q}{S}\theta^2\,\mathrm{d}x' \geq -k_1 \int_c^t \theta^2\,\mathrm{d}x' \ .$$

Integrating by parts, it comes straightforward that

$$-\frac{p\theta'\theta}{S} + \int_c^x \frac{p(\theta')^2}{S}\,\mathrm{d}x' - \int_c^x \frac{p\theta'\theta S'}{S^2}\,\mathrm{d}x' < k_3$$

for some constant k_3. Calling

$$I(x) = \int_c^x \frac{p(\theta')^2}{S}\,\mathrm{d}x' \ ,$$

by Cauchy-Schwarz inequality and hypothesis (1.21)

$$\left|\int_c^x \frac{p\theta'\theta S'}{S^2}\,\mathrm{d}x'\right|^2 \leq k_2^2\,I(x) \int_c^t \theta^2\,\mathrm{d}x' \ .$$

There exists a constant k_4 such that

$$-\frac{p\theta'\theta}{S} + I - k_4\,I^{\frac{1}{2}} < k_3 \ . \tag{1.22}$$

If $I(x) \longrightarrow +\infty$ as $x \to \infty$, then (1.22) would imply that for large x, θ and θ' have the same sign, which clearly contradicts the assumption $\theta \in \mathrm{L}^2([0,+\infty[)$. Thus I has to remain finite.

Now, suppose that there are two linearly independent (real) solutions of $L\,u = 0$ on $\mathrm{L}^2([0,+\infty[)$, say ψ and ψ (limit-circle case). For the sake of simplicity, assume that these solutions have Wronskian 1. It follows that

$$\phi\frac{p^{\frac{1}{2}}\psi'}{S^{\frac{1}{2}}} - \psi\frac{p^{\frac{1}{2}}\phi'}{S^{\frac{1}{2}}} = \frac{1}{(p\,S)^{\frac{1}{2}}} \ . \tag{1.23}$$

Again by Cauchy-Schwartz integral inequality, the left hand side of (1.23) is integrable over $[c,+\infty[$. This contradicts the hypothesis that $\int_0^{+\infty}(pS)^{\frac{1}{2}} = +\infty$. Thus the limit-circle case is ruled out. □

Indeed, in the periodic Schrödinger case, all the conditions above are satisfied, since q is clearly bounded from below (thus M is a constant function) and $p(x) \equiv 1$. Also, we can use weaker assumptions for the Schrödinger operators to be in the limit-point case.

Corollary 1.2. *If $p(x) = 1$ for any positive x and $q(x) \geq -kx^2$ for some positive constant k, then L is in the limit point case at infinity.*

In the limit-point case, if m is any point on the "circle" C_b, then m tends to the limit point m_∞ as $b \to \infty$, and this holds independent of the choice of β in the boundary condition (1.15). In particular, when $\beta = 0$, that is

$$u(b) = 0 \ ,$$

the limit point is given by

$$m_\infty(\lambda) = -\lim_{b \to +\infty} \frac{\phi_\lambda(b)}{\psi_\lambda(b)} \ . \tag{1.24}$$

The limit point computed above, viewed as a function of the complex variable λ has got interesting properties.

Theorem 1.25. *In the limit-point case, the limit point m_∞ is an analytic function of λ for $\mathrm{Im}\,\lambda > 0$ (and $\mathrm{Im}\,\lambda < 0$). Moreover, $\mathrm{Im}(m_\infty) > 0$ if $\mathrm{Im}\lambda > 0$ (i.e. m_∞ is a Nevanlinna function) and, if m_∞ has zeros or poles on the real axis, they are all simple.*

Sometimes the limit point m_∞ is called *Titchmarsh-Weyl coefficient*, like in Definition 1.21, which is however a more general (and abstract) extension because in that case the operator is not necessarily self-adjoint. The general Titchmarsh-Weyl theory for self-adjoint problems, which extends what we have done to complex valued p and q, may be developed either using mehods of complex analysis (like in Titchmarsh's original works, 1946) or using the theory of deficiency indices for symmetric operators on Hilbert spaces (see [13]).

1.4.2 The Sims classification

In 1957, A.R. Sims obtained an extension of the classical Weyl alternative for the (Schrödinger) differential equation

$$\mathrm{H}[u] = -u'' + q\,u = \lambda\,u\,,\ \lambda \in \mathbb{C}\ , \tag{1.25}$$

on an interval $[a, b[$, where q is complex valued and the end-points a, b are, respectively, regular and singular (for example if $a = 0$ and $b = +\infty$). Under the assumption that $\mathrm{Im}(q(x)) \leq 0$ for all $x \in [a, b[$, he proved that for λ in the upper (complex) half-plane, there exists at least one solution of (1.25) which is in the weighted space $\mathrm{L}^2\left([0, +\infty[; \mathrm{Im}(\lambda - q)\mathrm{d}x\right)$; such a solution also lies in $\mathrm{L}^2([0, +\infty[)$. There are three alternatives for λ such that $\mathrm{Im}(\lambda) > 0$:

(i) there is precisely one[7] solution of (1.25) in $\mathrm{L}^2([0,+\infty[;\mathrm{Im}(\lambda-q)\mathrm{d}x)$ and in $\mathrm{L}^2([0,+\infty[)$;

(ii) only one solution lies in the weighted space $\mathrm{L}^2([0,+\infty[;\mathrm{Im}(\lambda-q)\mathrm{d}x)$, but all are in $\mathrm{L}^2([0,+\infty[)$;

(iii) all solutions are in $\mathrm{L}^2([0,+\infty[;\mathrm{Im}(\lambda-q)\mathrm{d}x)$.

Similarly to the limit-point, limit-circle cases presented in the previous section, the classification is independent of λ: indeed, if all solutions are in $\mathrm{L}^2([0,+\infty[)$ or $\mathrm{L}^2([0,+\infty[;\mathrm{Im}(\lambda-q)\mathrm{d}x)$ for some λ in the upper half-plane, then it remains so for all $\lambda\in\mathbb{C}$.
In [8], the pioneering work of Sims has been extended to more general Sturm-Lioville operators:

$$M[u]=\frac{1}{w}\left(-(p\,u')'+q\,u\right)$$

on $[a,b[$, where

- p, q are complex valued;
- $p\neq 0$ almost everywhere on $[a,b[$;
- q, $1/p\in\mathrm{L}^1_{loc}([a,b[)$;
- $w>0$ and $w\in\mathrm{L}^1_{loc}([a,b[)$.

In this paper, also, an analogue of the Titchmarsh-Weyl M-function in the Sims case is constructed.

1.5 Motivation: spectral pollution

This section is meant to be an introduction to the problem of spectral pollution and an explanation of the reasons for our interest in the study of the spectrum of the operator

$$\mathrm{H}_{R,\gamma}=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+q(x)+i\gamma\chi_R(x)$$

and of the limit

$$\lim_{R\to\infty}\sigma(\mathrm{H}_{R,\gamma})\ .$$

Firstly, let us explain what spectral pollution is. This phenomenon may occur for example when one tries to calculate numerically the spectrum of a

[7] Up to constant multiples.

self-adjoint operator L on an infinite-dimensional (separable) Hilbert space $\mathcal{H}$, using a projection method on finite-dimensional subspaces. Let $\{\psi_j\}_{j=1}^{\infty}$ be an orthonormal basis of $\mathcal{H}$, where $\psi_j \in \mathcal{D}(L)$; let

$$\mathcal{M}_N := \operatorname{span}\{\psi_1, \dots, \psi_N\} \ .$$

Define for $N \in \mathbb{N}$ the $N \times N$ matrices

$$L_N := [(L\,\psi_i,\, \psi_j)_{\mathcal{H}}]_{i,\,j=1}^{N} \ , \tag{1.26}$$

which are the ortogonal projections of the operator L onto the subspace $\mathcal{M}_N$. Eigenvalues of L are so approximated by eigenvalues of the finite-dimensional matrices L_N. Ideally, one would like that

$$\lim_{N\to\infty} \sigma(L_N) = \sigma(L) \ .$$

This is not true, in general. However, with the help of some natural conditions on $\mathcal{M}_N$, the inclusion

$$\sigma(L) \subseteq \lim_{N\to\infty} \sigma(L_N)$$

can be guaranteed. Spectral pollution appears when

$$\lim_{N\to\infty} \sigma(L_N) \nsubseteq \sigma(L) \ ;$$

in other terms, in this context, $\lambda \notin \sigma(L)$ is said to be a *point of spectral pollution* if there exists a sequence of complex numbers $\{\lambda_N\}_{N\in\mathbb{N}}$ such that $\lambda_N \in \sigma(L_N)$ for all N and

$$\lambda_N \longrightarrow \lambda$$

as $N \to \infty$. Points of spectral pollution are also referred to as *spurious eigenvalues.*

Spectral pollution is typical when the essential spectrum of L has a disconnected band-gaps structure (e.g. periodic Schrödinger operators) and one wishes to compute eigenvalues in the gaps of the essential spectrum, due to the instrinsic nature of variational methods like the one presented above: what happens is that the spectral gaps fill up with eigenvalues of the discrete problem, which are so closely spaced that it is impossible to distinguish the spectral gaps from the spectral bands. Variational eigenvalues (i.e. below $\inf \sigma_{ess}(L)$), instead, are safe from spectral pollution, due to the min-max theorem.

In principle, one should think that there is no universal recipe to prevent or detect spurious eigenvalues using the projection method. Several methods have been proposed to deal with the problem: see [12], [19] and [5] for variants of the standard variational methods, [20] for a different approach founded on the choice of a special basis for the Hilbert space.

For differential operators on infinite domains or with singularities, spectral pollution can be also caused by domain truncation. An explicit example of this phenomenon has been given in [1].

Example 1.5.1. Let L be a self-adjoint Schrödinger operator

$$L := \mathrm{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)$$

defined on the Hilbert space $\mathrm{L}^2([0, +\infty[)$, with Dirichlet boundary condition 0. Suppose that $\sigma_{ess}(\mathrm{H})$ is disconnected and bounded below (for example when the potential q is periodic). It is proven therein that:

(i) if $\lambda < \inf \sigma_{ess}(\mathrm{H})$, then every non-trivial solution of the λ-spectral equation

$$-u'' + q\,u = \lambda\,u \tag{1.27}$$

has finitely many zeros in $]0, \infty[$;

(ii) if $\lambda > \inf \sigma_{ess}(\mathrm{H})$, then every non-trivial solution of (1.27) has infinitely many zeros in $]0, \infty[$.

Take a solution of (1.27) u satisfying $u(0; \lambda) = 0$ and $u'(0; \lambda) = 0$. Take λ in a spectral gap, that is $\lambda > \inf \sigma_{ess}(\mathrm{H})$ and $\lambda \notin \sigma(\mathrm{H})$. By (ii), there are infinitely many zeros of $u(\cdot\,; \lambda)$, say $\{Z_n\}_{n=1}^{\infty}$; of course, $Z_n \uparrow \infty$ as $n \to \infty$.

Consider now the regular problems

$$\begin{aligned} -v'' + q\,v &= \mu\,v \\ v(0) &= 0 \\ v(Z_n) &= 0 \end{aligned}$$

on $\mathrm{L}^2([0, Z_n])$ for $n \in \mathbb{N}$. So, λ is an eigenvalue of all these problems (with eigenfunction u), but λ is not eigenvalue of the limiting problem on $\mathrm{L}^2([0, +\infty[$ (having Dirichlet boundary condition at 0). A spurious eigenvalue for the operator H on $[0, \infty[$ has been then generated.

However, in this case, pollution can be always avoided by choosing appropriate λ-adapted boundary conditions on the boundary of the truncated domain.

In this thesis, we are considering yet another method, proposed by Marletta in [21] in the more general context of PDEs. Considering the computation of eigenvalues of self-adjoint Schrödinger operators

$$\mathrm{H} = -\Delta + q(x)$$

in infinite domains in $\mathbb{R}^d$, having band-gaps spectral structure, he proposes changing the problem by perturbing the potential as follows:

$$q(x) \longrightarrow q(x) + i\gamma\, s(x) \ ,$$

where s is a compactly supported function which takes the value 1 everywhere inside a ball of radius R, γ is a non-negative number. Compactness of $\operatorname{supp} s$ implies that the essential spectrum of the problem is unchanged. The eigenfunctions belonging to isolated eigenvalues in the spectral gaps are exponentially decaying and, if R is large, they will "see" the function $s(x)$ almost as if it took the value 1 everywhere: consequently, the corresponding genuine eigenvalues, say λ, which are perturbed into λ_γ, are approximately

$$\lambda \approx \mathrm{Re}(\lambda_\gamma) \approx \mathrm{Re}(\lambda + i\gamma) \ .$$

So, when R is sufficiently large, true isolated eigenvalues are lifted up into the upper half-plane; on the other hand, spurious eigenvalues stay close to the real axis, as shown in [22, Theorem 2]. Numerical results in [21] and error bounds in the more recent [22] say that the quality of this approach for many problems is really good and the error due to the perturbation is many orders of magnitude smaller than the error due to discretization, even without requiring that γ is small.

This explains why we are interested in the study of the family of one-dimensional Schrödinger operators

$$\mathrm{H}_{R,\gamma} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\gamma\, \chi_R(x)$$

and in the limit of $\sigma(\mathrm{H}_{R,\gamma})$ for large R, being here $s(x) = \chi_R(x)$. In particular, one would wish that there be no isolated eigenvalues of $\mathrm{H}_{R,\gamma}$ inside the strip $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, so that the perturbed versions λ_γ of the genuine eigenvalues can be easily identified.

Chapter 2

Solution of the problem for compactly supported background potentials

In this Section we study the spectrum of the operator

$$\mathrm{H}_{R,\gamma} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)$$

either when the potential q is identically zero (free case) and when q has compact support in $[0, +\infty[$. The main tool for calculating the spectrum (actually, the isolated eigenvalues of $\mathrm{H}_{R,\gamma}$, since the essential spectrum is known in both cases) is the Titchmarsh-Weyl function, already presented throughout Section 1.3.

2.1 A first example: the Titchmarsh-Weyl M-function of the free (perturbed) case

We will consider as a first example the self-adjoint Schrödinger operator

$$\mathrm{H}^{free} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} , \tag{2.1}$$

with domain

$$\mathcal{D}\left(\mathrm{H}^{free}\right) = \left\{ u \in \mathrm{L}^2([0, +\infty[) \,:\, -u'' \in \mathrm{L}^2([0, +\infty[),\, u'(0) = 0 \right\} , \tag{2.2}$$

in the Hilbert space $\mathrm{L}^2([0, +\infty[)$, and its perturbed version:

$$\mathrm{H}^{free}_{R,\gamma} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\gamma\, \chi_R(x) = \mathrm{H}^{free} + i\gamma\, \chi_R(x) ,$$

where R, γ are non-negative parameters and χ_R denotes the characteristic function of the interval $[0, R]$.

2.1.1 Spectrum of H^{free}

The spectrum of the operator H^{free} is simply the half-line $[0, +\infty[$. To prove this, let us recall Propositions 1.1 and 1.2.

Proposition (Weyl's criterion)**.** *Let* $\lambda \in \mathbb{C}$, $\mathcal{H}$ *be a Hilbert space,* $T : \mathcal{D}(T) \subset \mathcal{H} \longrightarrow \mathcal{H}$ *be a closed linear operator.*

(i) If there exists a Weyl sequence *associated to* λ*, that is* $(u_n)_{n\in\mathbb{N}} \subset \mathcal{D}(T)$ *such that*

- $\|u_n\|_{\mathcal{H}} = 1$ *for every* n*,*
- $\|(T - \lambda\mathbb{I})u_n\|_{\mathcal{H}} \longrightarrow 0$ *as* $n \to \infty$*,*

then $\lambda \in \sigma(T)$*.*

(ii) If $\lambda \in \sigma(T) \cap \overline{\rho(T)}$*, then there exists a Weyl sequence associated to* λ*.*

Proposition. *Let* $\alpha \in \mathbb{R}$, $\mathcal{H}$ *be a Hilbert space,* $T : \mathcal{D}(T) \subset \mathcal{H} \longrightarrow \mathcal{H}$ *a self-adjoint linear operator such that for every* $\varphi \in \mathcal{D}(T)$

$$(T\varphi, \varphi)_{\mathcal{H}} \geq \alpha \, \|\varphi\|^2_{\mathcal{H}} \ .$$

Then the spectrum of T *is contained in* $[\alpha, +\infty[$*.*

The operator $\mathrm{H}^{free} : \mathcal{D}\left(\mathrm{H}^{free}\right) \subset \mathrm{L}^2([0, +\infty[) \longrightarrow \mathrm{L}^2([0, +\infty[)$ is self-adjoint and such that

$$\left(\mathrm{H}^{free}u, u\right)_{\mathrm{L}^2} = -\int_0^{+\infty} u'' \, \bar{u} \, \mathrm{d}x = - \, u' \, \bar{u}\big|_0^{+\infty} + \int_0^{+\infty} u' \, \bar{u}' \, \mathrm{d}x \geq 0 \ .$$

Thus $\sigma(\mathrm{H}^{free})$ is contained in $[0, +\infty[$. Also, if $\lambda > 0$, the spectral equation

$$(\mathrm{H}^{free} - \lambda\mathbb{I})u = 0 \tag{2.3}$$

does not even have a (non trivial) solution in $\mathrm{L}^2([0, +\infty[)$, a fortiori neither in $\mathcal{D}\left(\mathrm{H}^{free}\right)$; thus the operator $(\mathrm{H}^{free} - \lambda\mathbb{I})$ is injective: this means that there cannot be point spectrum.

Our aim is now to construct a Weyl sequence for H^{free} associated with $\lambda > 0$. To this purpose, let $\eta \in \mathcal{C}_c^\infty\left([0, +\infty[\right)$ a function of "cap-shaped" type (see Section 1.2.4) such that $\eta = 1$ on $[0,1]$ and for every $n \in \mathbb{N}$, for every $x \in [0,+\infty[$ let

$$\eta_n(x) := \eta\left(\frac{x}{n}\right) .$$

It is well known that the spectral equation (2.3) for $\lambda > 0$ has the following general solution

$$u(x) = C_1\, e^{i\sqrt{\lambda}} + C_2\, e^{-i\sqrt{\lambda}} \; ; \tag{2.4}$$

if we want u to be in $\mathcal{D}(\mathrm{H}^{free})$, then, using the Neumann condition coming from (2.2), we get $C_1 - C_2 = 0$, that is $C_1 = C_2$. Clearly, the solution in (2.4) is not in $\mathrm{L}^2([0,+\infty[)$, unless $C_1 = 0$ (which corresponds to the trivial solution $u \equiv 0$); in any case, all non-trivial solutions are bounded on $[0,+\infty[$. Let us define $u_n := \eta_n u$. Since u and its derivatives are bounded and $\mathrm{supp}(\eta)$ is contained in some neighbourhood of $[0,1]$, then $\mathrm{supp}(\eta_n)$ is contained some neighbourhood of $[0,n]$ and u_n is in L^2 for every $n \in \mathbb{N}$; also

- $u_n' = \eta_n' u + \eta_n u' \;\; \in \mathrm{L}^2([0,\infty[)$,
- $u_n'' = \eta_n'' u + 2\eta_n' u' + \eta_n u'' \;\; \in \mathrm{L}^2([0,\infty[)$,

because, by the definition of η_n and an easy change of variables in the integrals, it holds that

$$\|\eta_n'\|_2^2 = \frac{1}{n}\,\|\eta'\|_2^2 , \quad \|\eta_n''\|_2^2 = \frac{1}{n^3}\,\|\eta''\|_2^2 \; .$$

Thus, $u_n \in \mathcal{D}\left(\mathrm{H}^{free}\right)$; we can also assume, without loss of generality, that every u_n is multiplied by some normalizing factor, i.e.

$$\|u_n\|_2 = 1 \;\; \forall\, n \in \mathbb{N} \; .$$

Now

$$\begin{aligned}
(\mathrm{H}^{free} - \lambda\mathbb{I})u_n &= -u_n'' - \lambda u_n \\
&= -\eta_n'' u - 2\eta_n' u' - \eta_n u'' - \lambda \eta_n u \\
&= -\eta_n'' u - 2\eta_n' u' + \eta_n(-u'' - \lambda u) \\
&= -\eta_n'' u - 2\eta_n' u'
\end{aligned}$$

and

$$\left\|(\mathrm{H}^{free} - \lambda\mathbb{I})u_n\right\|_2 \le \|\eta_n'' u\| + 2\,\|\eta_n' u'\|_2 \;\; ;$$

since

$$\begin{aligned}
\|\eta_n' u'\|_2^2 &= \int_0^{+\infty} |\eta_n' u'|^2 \le \|u'\|_\infty^2 \,\|\eta_n'\|^2 \le K \cdot \frac{1}{n}\,\|\eta'\|_2^2 , \\
\|\eta_n'' u\|_2^2 &= \int_0^{+\infty} |\eta_n'' u|^2 \le \|u\|_\infty^2 \,\|\eta_n''\|^2 \le K \cdot \frac{1}{n^3}\,\|\eta''\|_2^2 ,
\end{aligned}$$

it follows that

$$\left\|(\mathrm{H}^{free} - \lambda \mathbb{I}) u_n\right\|_2 \to 0 \tag{2.5}$$

as $n \to +\infty$.

Therefore, by Proposition 1.1, we can say that every positive λ is in the spectrum. Also 0 belongs to the spectrum, because the spectrum of any closed operator is a closed set (Theorem 1.5). This finally proves that the spectrum of H^{free} is exactly $[0, +\infty[$

2.1.2 Construction of the Titchmarsh-Weyl function

Let us fix γ and, for the moment, keep also R fixed. In order to compute the M-function we have to consider the spectral equation

$$\mathrm{H}^{free}_{R,\gamma}\, u(x) = \lambda\, u(x) \tag{2.6}$$

globally in $[0, +\infty[$.

Out of $[0, R]$, (2.6) becomes

$$-u''(x) = \lambda u(x) \ ,$$

which has general solution of the form

$$u(x) = c_1 e^{\sqrt{-\lambda}\, x} + c_2 e^{-\sqrt{-\lambda}\, x} \ .$$

To get a solution in $\mathcal{D}(\mathrm{H}^{free}) \subset \mathrm{L}^2\left([R, +\infty[\right)$, we need that $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ and $c_1 = 0$ or $c_2 = 0$ depending on the real part of the complex number $\sqrt{-\lambda}$. By our choice of the branch of the square root, we know that $\mathrm{Re}(\sqrt{-\lambda}) > 0$, so the general L^2-solution is of the form

$$u(x) = C e^{-\sqrt{-\lambda}\, x} \tag{2.7}$$

with C real constant.

We do not want trivial solutions, so we may assume that $C \neq 0$. Indeed, if $C = 0$, this forces (by existence and uniqueness theorem) the global solution of (2.6) to be identically null on $[0, +\infty[$. Therefore, note that

$$\frac{u'(x)}{u(x)} = -\sqrt{-\lambda}$$

for every $x \geq R$; in particular we will use the value of this constant ratio at $x = R$ as boundary condition for the solution to the spectral equation in $[0, R]$ (this will be a "matching" condition at $x = R$ for the global solution).

In $[0, R]$, equation (2.6) can be written as:

$$-u''(x) + i\gamma\, u(x) = \lambda u(x) \ . \tag{2.8}$$

It has the following general solution:

$$u(x) = \alpha e^{\sqrt{i\gamma-\lambda}\,x} + \beta e^{-\sqrt{i\gamma-\lambda}\,x} \ . \tag{2.9}$$

Our aim is to construct a global solution, but but so far we have just one boundary condition at $x = R$, which is

$$\frac{u'(R-)}{u(R-)} = -\sqrt{-\lambda} \tag{2.10}$$

Following the content of Section 1.3, we want to construct a suitable model for the Titchmarsh-Weyl function of our problem. Let us consider the Hilbert space $\mathcal{H} = \mathrm{L}^2\left([0, +\infty[\right)$, the operators

$$A := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\,\gamma\,\chi_R(x)$$

having domain

$$\mathcal{D}(A) = \left\{u \in H^2\left([0, +\infty[\right)\ :\ u(0) = u'(0) = 0\right\} \ ;$$

and

$$\tilde{A} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - i\,\gamma\,\chi_R(x)$$

on the domain $\mathcal{D}(\tilde{A}) = \mathcal{D}(A)$; the respective adjoint operators are

$$A^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - i\,\gamma\,\chi_R(x) \ , \quad \tilde{A}^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\,\gamma\,\chi_R(x)$$

with domains $\mathcal{D}(A^*) = \mathcal{D}(\tilde{A}^*) = H^2\left([0, +\infty[\right)$. In this way, the operators A and $\tilde{A}$ form an adjoint pair, that is $A^* \supseteq \tilde{A}$ and $\tilde{A}^* \supseteq A$. By suitable integrations by parts, we get the following abstract Green formula for $u \in \mathcal{D}(\tilde{A}^*)$ and $v \in \mathcal{D}(A^*)$:

$$\begin{aligned}
(\tilde{A}^*u, v)_{\mathcal{H}} - (u, A^*v)_{\mathcal{H}} &= \int_0^{+\infty} \left[(-u'' + i\gamma u\,\chi_R)\,\bar{v} - u\,\overline{(-v'' - i\gamma v\,\chi_R)}\right]\,\mathrm{d}x \\
&= \left[-u'\bar{v} + u\overline{v'}\right]\Big|_{x=0}^{+\infty} = \\
&= u'(0)\bar{v}(0) - u(0)\bar{v}'(0) = \\
&= (\Gamma_1 u, \Gamma_2 v)_{\mathbb{C}} - (\Gamma_2 u, \Gamma_1 v)_{\mathbb{C}} \ ,
\end{aligned}$$

where $\Gamma_1 u := u'(0)$ and $\Gamma_2 u := u(0)$.

The Titchmarsh-Weyl M_B-function, by definition, maps the "Robin" condition $(\Gamma_1 - B\Gamma_2)u$ to the Dirichlet $\Gamma_2 u$; we are interested in the knowledge of Dirichlet and Neumann poles, so suppose $B \equiv 0$ (*"Neumann-to-Dirichlet" mapping*). So, according to this assumption, the second boundary condition we need is given by a Neumann condition at the origin:

$$u'(0) = \Gamma_1 u = z \in \mathbb{C} \ . \tag{2.11}$$

Together with the condition (2.10), we have that

$$\begin{cases} \alpha\sqrt{i\gamma-\lambda} - \beta\sqrt{i\gamma-\lambda} = z \\ \dfrac{\alpha\sqrt{i\gamma-\lambda}\, e^{\sqrt{i\gamma-\lambda}\,R} - \beta\sqrt{i\gamma-\lambda}\, e^{-\sqrt{i\gamma-\lambda}\,R}}{\alpha e^{\sqrt{i\gamma-\lambda}\,R} + \beta e^{-\sqrt{i\gamma-\lambda}\,R}} = -\sqrt{-\lambda} \end{cases} ; \tag{2.12}$$

this gives, by Cramer's rule, the values of α and β:

$$\alpha = \frac{-z(\sqrt{i\gamma-\lambda} - \sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R}}{\sqrt{i\gamma-\lambda}\left[(\sqrt{i\gamma-\lambda} + \sqrt{-\lambda})e^{+\sqrt{i\gamma-\lambda}\,R} - (\sqrt{i\gamma-\lambda} - \sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R}\right]} ,$$

$$\beta = \frac{-z(\sqrt{i\gamma-\lambda} + \sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R}}{\sqrt{i\gamma-\lambda}\left[(\sqrt{i\gamma-\lambda} + \sqrt{-\lambda})e^{+\sqrt{i\gamma-\lambda}\,R} - (\sqrt{i\gamma-\lambda} - \sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R}\right]} .$$

So, we have completely determined the global solution of (2.6); all we need now is to recover its value at $x = 0$:

$$\Gamma_2 u = u(0) = \alpha + \beta \ ;$$

therefore the Titchmarsh-Weyl (Neumann-to-Dirichlet) function maps the complex number z to $\alpha + \beta$, that is the Titchmarsh-Weyl coefficient is

$$M_{ND}(\lambda) = \frac{-\left[(\sqrt{i\gamma-\lambda} + \sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R} + (\sqrt{i\gamma-\lambda} - \sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R}\right]}{\sqrt{i\gamma-\lambda}\left[(\sqrt{i\gamma-\lambda} + \sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R} - (\sqrt{i\gamma-\lambda} - \sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R}\right]} . \tag{2.13}$$

2.1.3 Asymptotic behaviour of the M-function for large R

First of all, we notice that, by estimates on the numerical range of $\mathrm{H}_{R,\gamma}^{free}$, the λ*'s* of interest necessarily have to be in the strip $\{z \,:\, 0 \le \mathrm{Im}(z) \le \gamma\}$.

Actually this holds not only for $\mathrm{H}_{R,\gamma}^{free}$, but in general for $\mathrm{H}_{R,\gamma}$. *Indeed*, for $u \in \mathcal{D}\left(\mathrm{H}_{R,\gamma}\right)$

$$\begin{aligned}
(\mathrm{H}_{R,\gamma} u,\, u)_{\mathrm{L}^2([0,+\infty[)} &= \int_0^{+\infty} [-u'' + (q + i\gamma\,\chi_R)\,u]\,\bar{u}\,\mathrm{d}x \\
&= -\int_0^{+\infty} u''\,\bar{u}\,\mathrm{d}x + \int_0^{+\infty} q\,u\,\bar{u}\,\mathrm{d}x + i\gamma \int_0^{R} u\,\bar{u}\,\mathrm{d}x \\
&= \int_0^{+\infty} u'\,\bar{u}'\,\mathrm{d}x + \int_0^{+\infty} q\,u\,\bar{u}\,\mathrm{d}x + i\gamma \int_0^{R} u\,\bar{u}\,\mathrm{d}x \\
&= \int_0^{+\infty} |u'|^2\,\mathrm{d}x + \int_0^{+\infty} q|u|^2\,\mathrm{d}x + i\gamma \int_0^{R} |u|^2\,\mathrm{d}x\ ;
\end{aligned}$$

taking $\|u\|_2 = 1$ as in the definition of the numerical range, this implies that

$$\mathrm{Im}\,(\mathrm{H}_{R,\gamma} u,\, u)_{\mathrm{L}^2([0,+\infty[)} \leq |i\gamma| \cdot \|u\|_2 \leq \gamma\ .$$

Also

$$\mathrm{Im}\,(\mathrm{H}_{R,\gamma} u,\, u) \geq 0\ ,$$

because $\gamma \geq 0$; thus the numerical range of $\mathrm{H}_{R,\gamma}^{free}$ has to be contained in the strip $\{z\,:\,0 \leq \mathrm{Im}(z) \leq \gamma\}$. We need now to recall Theorem 1.10:

Theorem. *Let T be a densely defined closed operator on a Hilbert space. Let $\Lambda := \left\{z \in \mathbb{C}\,:\,\mathrm{dist}\left(z, \overline{\mathrm{Num}(T)}\right) > 0\right\}$. Then, if $z \in \Lambda$, $\phi \in \mathcal{D}(T)$*

$$\|(z - T)\phi\| \geq \mathrm{dist}\left(z, \overline{\mathrm{Num}(T)}\right)\, \|\phi\|\ . \tag{2.14}$$

By inequality (2.14) applied to the operator $\mathrm{H}_{R,\gamma}$, it follows that if $\lambda \in \Lambda$, in particular if $\lambda \in \{z\,:\,\mathrm{Im}(z) < 0\}$ or $\lambda \in \{z\,:\,\mathrm{Im}(z) > \gamma\}$, then

- λ does not belong to the point spectrum $\sigma_{pp}(\mathrm{H}_{R,\gamma})$, because in such a case the operator $(\lambda - \mathrm{H}_{R,\gamma})$ would be injective, thus not in the point spectrum;

- λ is not in the continuous spectrum $\sigma_c(\mathrm{H}_{R,\gamma})$, because if $(\lambda - \mathrm{H}_{R,\gamma})$ were invertible, then $(\lambda - \mathrm{H}_{R,\gamma})^{-1}$ would have to be continuous and $\lambda \in \rho(\mathrm{H}_{R,\gamma})$, which is a contradiction.

This proves that the spectrum of $\mathrm{H}_{R,\gamma}$ has to be contained in the strip $\{z\,:\,0 \leq \mathrm{Im}(z) \leq \gamma\}$; in particular

$$\sigma(\mathrm{H}_{R,\gamma}^{free}) \subset \{z\,:\,0 \leq \mathrm{Im}(z) \leq \gamma\}$$

for all R.

In order to characterize the spectrum, we want is to investigate the asymptotic behaviour of the M-function as R tends to $+\infty$. Let us define a sequence $\{R_n\}_{n\in\mathbb{N}}$ of cut-off values such that $R_n \longrightarrow +\infty$.
If $\lambda = i\gamma$, the Titchmarsh-Weyl function is not even defined; if $\mathrm{Im}(\lambda) = \gamma$ and $\mathrm{Re}(\lambda) > 0$, then $\mathrm{Re}(\sqrt{i\gamma-\lambda}) = 0$ and $\mathrm{Im}(\sqrt{i\gamma-\lambda}) > 0$, which implies that $M_{ND}(R_n,\lambda)$ is oscillating and does not converge to anything as $n \longrightarrow +\infty$; in all the other possible cases, $\mathrm{Re}(\sqrt{i\gamma-\lambda})$ is stricltý positive, thus the asymptotic behaviour is clear. Indeed, the multiplicative coefficient of the Titchmarsh-Weyl function

$$\frac{-\left[(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R_n}+(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R_n}\right]}{\sqrt{i\gamma-\lambda}\left[(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R_n}-(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R_n}\right]}\,.$$

tends to

$$\left(-\frac{1}{\sqrt{i\gamma-\lambda}}\right)$$

as $n \longrightarrow +\infty$.

Moreover, by a suitable application of Montel's theorem, the convergence of the coefficient is uniform in any compact set which is contained in the strip $\{\lambda\in\mathbb{C} \,:\, 0<\mathrm{Im}(\lambda)<\gamma\}$.
Indeed, let $K \subset\subset \{\lambda\in\mathbb{C} \,:\, 0<\mathrm{Im}(\lambda)<\gamma\}$ and

$$c = \inf_{\lambda\in K}\mathrm{Re}(\sqrt{i\gamma-\lambda}) = \min_{\lambda\in K}\mathrm{Re}(\sqrt{i\gamma-\lambda}) > 0\ .$$

Consider the modulus of the denominator $\mathrm{den}_M(\lambda,R)$ of the M-function; we have that for $\lambda\in K$

$$\begin{aligned}
|\mathrm{den}_M(\lambda,R)| &= \Big|\ \sqrt{i\gamma-\lambda}\ e^{\sqrt{i\gamma-\lambda}\,R}\ \Big[(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}) \\
&\qquad -(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda})e^{-2\sqrt{i\gamma-\lambda}\,R}\Big]\ \Big| \\
&\geq \left|\sqrt{i\gamma-\lambda}\right|\ e^{\sqrt{i\gamma-\lambda}\,R}\ \Big[\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right| \\
&\qquad -\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|\,e^{-2R\left(\mathrm{Re}(\sqrt{i\gamma-\lambda})\right)}\Big] \\
&\geq c\,e^{c\,R}\left(\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|-\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|e^{-2Rc}\right) \\
&= c\,e^{c\,R}\left(\frac{|i\gamma|}{\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|}-\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|e^{-2Rc}\right) \\
&= c\,e^{c\,R}\left(\frac{\gamma}{\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|}-\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|e^{-2Rc}\right)\ .
\end{aligned}$$

Now, in order to ensure uniform positivity, choose R sufficiently large to get

$$\frac{\gamma}{\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|}-\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|e^{-2Rc}>k>0\ ,$$

where for some (positive) constant k. For example, this is guaranteed by taking

$$R>\frac{1}{2c}\log\left(\frac{\gamma}{\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|^{2}}\right)\geq\frac{1}{2c}\log\left(\frac{\gamma}{a^{2}}\right)\ ,$$

where

$$a=\sup_{\lambda\in K}\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|=\max_{\lambda\in K}\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|\ ,$$

since

$$\frac{\gamma}{\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|}-\left|\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right|e^{-2Rc}$$

is a continuous function of the variable λ (when $\gamma>0$).
In addition to this, the numerator of the coefficient of the Titchmarsh-Weyl function is a continuous function of the variable λ, hence the Titchmarsh-Weyl coefficient $M(\lambda)$ satisfies:

$$\left|\frac{\mathrm{num}_{M(\lambda)}}{\mathrm{den}_{M(\lambda)}}\right|<\frac{b\cdot e^{\left(\mathrm{Re}\sqrt{i\gamma-\lambda}\right)R}+a}{k'\cdot e^{\left(\mathrm{Re}\sqrt{i\gamma-\lambda}\right)R}}\leq\frac{b+a}{k'}\ ,$$

where

$$b=\max_{\lambda\in K}\left|\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right|\ .$$

the coefficient of the sequence of M-functions $\{M_{ND}(R_n,\cdot)\}_{n\in\mathbb{N}}$ is then uniformly bounded in the compact set K. By Montel's theorem, we deduce uniform convergence.

The argument above also proves that the Neumann to Dirichlet function $M_{ND}(R,\lambda)$ has no poles for sufficiently large R, hence the operator $\mathrm{H}^{free}_{R,\gamma}$ has got no Neumann eigenvalues.

By a similar estimate, one can show that also the numerator is uniformly positive if the cut-off R is sufficiently large, that is $\mathrm{H}^{free}_{R,\gamma}$ has got no Dirichlet eigenvalues. We have thus proved the following:

Theorem 2.1. *For every compact set $K\subset\{z\in\mathbb{C}\,:\,0<\mathrm{Im}(z)<\gamma\}$, there exists $\bar{R}=\bar{R}_K$ such that for every $R\geq\bar{R}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}^{free}_{R,\gamma}$ are such that*

$$\sigma\left(\mathrm{H}^{free}_{R,\gamma}\right)\cap K=\emptyset\ .$$

2.2 Generalization to compactly supported potentials

With minor improvements, it is possible to extend the results of the previous section to Schrödinger operators with compactly supported background potentials.
Let $q \in \mathrm{L}^\infty([0,+\infty[)$ a real valued function with compact support, say $[0,b]$ (of course $b>0$). As we did in Section 2.1, we would like to construct a model for the Titchmarsh-Weyl function in this case, in order to find the isolated eigenvalues in the strip $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$ of the operator

$$\mathrm{H}^c_{R,\gamma} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (q(x) + i\gamma\,\chi_R(x))$$

with $\gamma \geq 0$ and $R > b$.
$\mathrm{H}^c_{R,\gamma}$ is a perturbation of the operator

$$\mathrm{H}^c := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x)$$

having domain

$$\mathcal{D}\left(\mathrm{H}^c\right) = \left\{u \in \mathrm{L}^2([0,+\infty[) \,:\, -u'' \in \mathrm{L}^2([0,+\infty[),\, u'(0) = 0\right\}.$$

Remark 2.2.1 (Spectrum of H^c)**.** We have already found, in Section 2.1.1, that the spectrum of the free operator is precisely $[0,+\infty[$.

Using similar methods, we can also say something about the spectrum of H^c. If for simplicity q is also continuous, since q is compactly supported, it is clear that $\forall\, x \in [0,+\infty[$

$$q(x) \geq \min q =: a$$

then, integrating by parts, we can see that the following estimate holds for $u \in \mathcal{D}\left(\mathrm{H}^c\right)$:

$$\begin{aligned}(\mathrm{H}^c u, u)_{\mathrm{L}^2} &= -\int_0^{+\infty} u''\,\bar{u}\,\mathrm{d}x + \int_0^{+\infty} q(x) u\,\bar{u}\,\mathrm{d}x \\ &= \int_0^{+\infty} q(x)\,|u|^2\,\mathrm{d}x + \int_0^{+\infty} |u'|^2\,\mathrm{d}x \geq a\,\|u\|_2^2\ .\end{aligned}$$

According to Proposition 1.2, we have found that

$$\sigma(\mathrm{H}^c) \subset [a,+\infty[\ . \tag{2.15}$$

If $a \geq 0$ there is no point spectrum and the spectrum is exactly $[a, +\infty[$ (repeating the argument of the free case, Section 2.1.1). Instead, if $a < 0$, for sure $[0, +\infty[$ is included in the spectrum; in $[a, 0[$ there may also be some point spectrum. However, the number of eigenvalues will always be finite: indeed, it is estimated by

$$\frac{1}{\pi}\int_0^{+\infty}\sqrt{q_-(x)}\mathrm{d}x\ ,$$

where q_- denotes the negative part of the potential. This estimate can be found, for instance, in [3, Chap. 10]; the justification is by the WKB theory.

2.2.1 Construction of the Titchmarsh-Weyl function related to $\mathrm{H}^c_{R,\gamma}$

Let the Hilbert space be, as before, $\mathcal{H} = \mathrm{L}^2([0, +\infty[)$. Let also:

$$A := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\,\gamma\,\chi_R(x)$$

and

$$\tilde{A} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) - i\,\gamma\,\chi_R(x)$$

with domains

$$\mathcal{D}(A) = \mathcal{D}(\tilde{A}) = \left\{u \in H^2\left([0, +\infty[\right)\ :\ u(0) = u'(0) = 0\right\}\ ;$$

in order to form two adjoint pairs, as required by [7], let us define the respective adjoint operators:

$$A^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) - i\,\gamma\,\chi_R(x) \quad \text{and} \quad \tilde{A}^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\,\gamma\,\chi_R(x)\ ,$$

both having domains $\mathcal{D}(A^*) = \mathcal{D}(\tilde{A}^*) = H^2\left([0, +\infty[\right)$.
Now, we would like to find an abstract Green formula, in order to identify the "boundary" operators and spaces prescribed by Proposition 1.4. If $u \in \mathcal{D}(\tilde{A}^*)$ and $v \in \mathcal{D}(A^*)$, by suitable integrations by parts, we have that:

$$\begin{aligned}
(\tilde{A}^*u, v)_{\mathrm{L}^2} - (u, A^*v)_{\mathrm{L}^2} &= \int_0^{+\infty}(-u'' + (q(x) + i\gamma\,\chi_R)\,u)\,\bar{v}\,\mathrm{d}x \\
&\quad - \int_0^{+\infty} u\,(\overline{-v'' + (q(x) - i\gamma\,\chi_R)\,v})\,\mathrm{d}x \\
&= \int_0^{+\infty}(-u''\bar{v} + u\bar{v}'')\,\mathrm{d}x \\
&= u'(0)\bar{v}(0) - u(0)\bar{v}'(0) = \\
&= (\Gamma_1 u, \Gamma_2 v)_{\mathbb{C}} - (\Gamma_2 u, \Gamma_1 v)_{\mathbb{C}}\ ,
\end{aligned}$$

where $\Gamma_1 u := u'(0)$ and $\Gamma_2 u := u(0)$.

We look for a global solution on $[0,+\infty[$ of the spectral equation

$$-u''(x) + (q(x) + i\gamma\, \chi_R(x))\, u = \lambda\, u \tag{2.16}$$

having initial boundary condition

$$\Gamma_1 u = z \in \mathbb{C}\ . \tag{2.17}$$

First, the solution of (2.16) in $[0, b[$ (where, of course, $\chi_R \equiv 1$) can be expressed as

$$u(x) = \alpha_1\, \phi(x; \lambda - i\gamma) + \alpha_2\, \psi(x; \lambda - i\gamma)\ :$$

here $\phi(\cdot; \lambda - i\gamma)$ and $\psi(\cdot; \lambda - i\gamma)$ are two linearly independent (non trivial) solutions of

$$-u'' + q(x)u = (\lambda - i\gamma)u \tag{2.18}$$

satisfying

$$\begin{pmatrix} \phi(0; \lambda - i\gamma) \\ \phi'(0; \lambda - i\gamma) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \psi(0; \lambda - i\gamma) \\ \psi'(0; \lambda - i\gamma) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We cannot be more explicit in this case; however in $]b, R]$, since $q \equiv 0$, we can writed the solution in the form:

$$\alpha_3\, g_+(x; \lambda - i\gamma) + \alpha_4\, g_-(x; \lambda - i\gamma)$$

where

$$g_\pm(x; \lambda - i\gamma) := e^{\pm\sqrt{i\gamma - \lambda}\, x}$$

are linearly independent solutions of

$$-u'' = (\lambda - i\gamma)u\ .$$

Finally, in $]R, +\infty[$, like in the free case, if $\lambda \in \mathbb{C} \setminus \mathbb{R}_+$ we can find an exponentially decaying solution:

$$u(x) = \alpha_5\, g_-(x; \lambda) = \alpha_5\, e^{-\sqrt{-\lambda}\, x}\ .$$

In order to find a global solution, in addition to the "Titchmarsh-Weyl boundary condition" (2.17), which can be rewritten as

$$\alpha_1\, \phi'(0; \lambda - i\gamma) + \alpha_2\, \psi'(0; \lambda - i\gamma) = z\ ,$$

we should impose other natural boundary conditions, that is

- continuity at $x = b$:

  $$\alpha_1\, \phi(b; \lambda - i\gamma) + \alpha_2, \psi(b; \lambda - i\gamma) = \alpha_3\, g_+(b; \lambda - i\gamma) + \alpha_4\, g_-(b; \lambda - i\gamma)\ ;$$

- derivability at $x = b$:

  $$\alpha_1\, \phi'(b; \lambda - i\gamma) + \alpha_2, \psi'(b; \lambda - i\gamma) = \alpha_3\, g'_+(b; \lambda - i\gamma) + \alpha_4\, g'_-(b; \lambda - i\gamma)\ ;$$

- "matching" condition in $x = R$:

  $$\frac{\alpha_3\, g'_+(R; \lambda - i\gamma) + \alpha_4\, g'_-(R; \lambda - i\gamma)}{\alpha_3\, g_+(R; \lambda - i\gamma) + \alpha_4\, g_-(R; \lambda - i\gamma)} = \frac{g'_-(R; \lambda)}{g_-(R; \lambda)}\ .$$

We want to determine exactly the global solution, that is the constants α_1, α_2, α_3 and α_4, which are solutions of the linear system with matrix:

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ \phi(b) & \psi(b) & -e^{\sqrt{i\gamma-\lambda}\,b} & -e^{-\sqrt{i\gamma-\lambda}\,b} \\ \phi'(b) & \psi'(b) & -\sqrt{i\gamma-\lambda}\, e^{\sqrt{i\gamma-\lambda}\,b} & +\sqrt{i\gamma-\lambda}\, e^{-\sqrt{i\gamma-\lambda}\,b} \\ 0 & 0 & (\sqrt{i\gamma-\lambda}+\sqrt{-\lambda})e^{\sqrt{i\gamma-\lambda}\,R} & -(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda})e^{-\sqrt{i\gamma-\lambda}\,R} \end{pmatrix}$$

and known term

$$\begin{pmatrix} z \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

Actually, to compute the Titchmarsh-Weyl function, it suffices to recover the value of α_1, because, if u is the global solution of (2.16), then

$$\Gamma_2 u = u(0) = \alpha_1\, \phi(0; \lambda - i\gamma) + \alpha_2\, \psi(0; \lambda - i\gamma) = \alpha_1$$

by construction of ϕ and ψ. By the Cramer's rule, the numerator of α_1, that is of the Titchmarsh-Weyl function, is

$$\begin{aligned} z\Big[\Big(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\Big)\Big(-\psi'(b)-\sqrt{i\gamma-\lambda}\,\psi(b)\Big)\Big]\, e^{+\sqrt{i\gamma-\lambda}\,(R-b)} \\ +\Big[\Big(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\Big)\Big(-\psi'(b)+\sqrt{i\gamma-\lambda}\,\psi(b)\Big)\Big]\, e^{-\sqrt{i\gamma-\lambda}\,(R-b)}\ , \end{aligned} \tag{2.19}$$

while the denominator $\mathrm{den}_M = \mathrm{den}_M(\lambda, R)$ is given by:

$$\begin{aligned} \mathrm{den}_M = \quad & \Big[\Big(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\Big)\Big(\phi'(b)+\sqrt{i\gamma-\lambda}\,\phi(b)\Big)\Big]\, e^{+\sqrt{i\gamma-\lambda}\,(R-b)} \\ & +\Big[\Big(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\Big)\Big(\phi'(b)-\sqrt{i\gamma-\lambda}\,\phi(b)\Big)\Big]\, e^{-\sqrt{i\gamma-\lambda}\,(R-b)}\ . \end{aligned} \tag{2.20}$$

Putting $b = 0$, we can clearly see that this is nothing but a generalization of the Titchmarsh-Weyl function which have already been computed in the free case (see formula (2.13)).

2.2.2 Asymptotic behaviour of the Titchmarsh - Weyl function

The asymptotic behaviour (as $R \longrightarrow +\infty$) of the Titchmarsh-Weyl is again leaded by the exponentially growing term

$$e^{+\sqrt{i\gamma-\lambda}\,(R-b)} \; .$$

To formulate a similar result to the free case (like in Theorem 2.1), we need that at least the multiplicative coefficients of the leading terms in expressions (2.19) and (2.20) are non-null, as stated by the following Lemma and Corollary.

Lemma 2.1. *Let* $\mu \in \mathbb{C}$ *such that* $\mathrm{Im}(\mu) < 0$*; let* $g(\cdot) = g(\cdot\,;\mu)$ *be a non-trivial solution of equation*

$$-g''(x) + q(x)\,g(x) = \mu\,g(x) \tag{2.21}$$

on $[0, b[$*. Then*

$$g'(b;\mu) + \sqrt{-\mu}\,g(b;\mu) \neq 0 \; .$$

Proof. Multiplying both sides of (2.21) by $\bar{g}(x)$ and integrating on $[0, b]$, we get:

$$-\int_0^b g''\,\bar{g}\,\mathrm{d}x + \int_0^b q\;|g|^2\;\mathrm{d}x = \mu\int_0^b |g|^2\;\mathrm{d}x \; .$$

An integration by parts on the first integral gives:

$$-g'(b)\bar{g}(b) + \int_0^b \left[|g'|^2 + (q-\mu)\;|g|^2\right]\;\mathrm{d}x = 0 \; . \tag{2.22}$$

Suppose

$$g'(b;\mu) + \sqrt{-\mu}\,g(b;\mu) = 0 \; ;$$

then (2.22) becomes

$$\sqrt{-\mu}\;|g(b)|^2 + \int_0^b \left[|g'|^2 + (q-\mu)\;|g|^2\right]\;\mathrm{d}x = 0 \; .$$

In particular, considering the imaginary part

$$\mathrm{Im}\left(\sqrt{-\mu}\right)\;|g(b)|^2 + \mathrm{Im}(-\mu)\int_0^b |g(x)|^2\;\mathrm{d}x = 0 \; .$$

Since $\mathrm{Im}(-\mu) > 0$, we clearly have that $\mathrm{Im}\left(\sqrt{-\mu}\right) > 0$, so

$$g(b) = 0 \quad \text{and} \quad \int_0^b |g(x)|^2 \,\mathrm{d}x = 0 \; .$$

This is a contradiction, because g is supposed to be a non-trivial solution to equation (2.21). □

Corollary 2.1. *If $\lambda \in \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, the functions $\phi(\cdot\,; \lambda - i\gamma)$ and $\psi(\cdot\,; \lambda - i\gamma)$ are such that*

- $\phi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\,\phi(b; \lambda - i\gamma) \neq 0$ *;*
- $\psi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\,\psi(b; \lambda - i\gamma) \neq 0$ *.*

Proof. By construction, $\phi(\cdot\,; \lambda - i\gamma)$ and $\psi(\cdot\,; \lambda - i\gamma)$ are **non-trivial** solutions of the equation

$$-u''(x) + q(x)\,u(x) = (\lambda - i\gamma)\,u(x)$$

on $[0, b]$; also, since $\lambda \in \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, then $\mathrm{Im}(\lambda - i\gamma) < 0$. Therefore the hypotheses of Lemma 2.1 are satisfied. □

Remark 2.2.2. The theory of complex linear differential systems tells us that the linearly independent solutions of (2.18) $\phi(\cdot\,; \lambda - i\gamma)$ and $\psi(\cdot\,; \lambda - i\gamma)$ are analytic functions of the variable λ (for details see [10, Chap. 1, Sec. 8]).

We also know that:

Lemma 2.2. *At least one between $\phi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\,\phi(b; \lambda - i\gamma)$ and $\psi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\,\psi(b; \lambda - i\gamma)$ is not zero.*

Proof. Suppose that

$$\begin{aligned} \phi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\,\phi(b; \lambda - i\gamma) &= 0 \; , \\ \psi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\,\psi(b; \lambda - i\gamma) &= 0 \; . \end{aligned} \tag{2.23}$$

We know that the Wronskian of the solutions ϕ and ψ

$$\hat{W}(\phi, \psi)(x) = \det \begin{pmatrix} \phi(x; \lambda - i\gamma) & \psi(x; \lambda - i\gamma) \\ \phi'(x; \lambda - i\gamma) & \psi'(x; \lambda - i\gamma) \end{pmatrix}$$

is constant and equal to $\hat{W}(\phi, \psi)(0)$, which is 1 by definition. In particular

$$\hat{W}(\phi, \psi)(b) = \phi(b)\,\psi'(b) - \psi(b)\,\phi'(b) = 1 \; ;$$

but, according to the assumptions (2.23)

$$\phi(b)\,\psi'(b) - \psi(b)\,\phi'(b) = \sqrt{i\gamma - \lambda}\,\phi(b)\,\psi(b) - \sqrt{i\gamma - \lambda}\,\phi(b)\,\psi(b) = 0 \; ,$$

which clearly is a contradiction. □

We are now ready to formulate the main theorem of this section:

Theorem 2.2. *For every compact set $K \subset \{z \in \mathbb{C} : 0 < \mathrm{Im}(z) < \gamma\}$, there exists $\bar{R} = \bar{R}_K$ such that for every $R \geq \bar{R}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}^c_{R,\gamma}$ are such that*

$$\sigma\left(\mathrm{H}^c_{R,\gamma}\right) \cap K = \emptyset \ .$$

Proof. Let $K \subset\subset \{\lambda \in \mathbb{C} : 0 < \mathrm{Im}(\lambda) < \gamma\}$ and

$$c := \inf_{\lambda \in K} \mathrm{Re}(\sqrt{i\gamma - \lambda}) = \min_{\lambda \in K} \mathrm{Re}(\sqrt{i\gamma - \lambda}) > 0 \ ;$$

let also

$$C_1 := \min_{\lambda \in K} \left| \phi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\, \phi(b; \lambda - i\gamma) \right|$$

and

$$C_2 := \max_{\lambda \in K} \left| \phi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\, \phi(b; \lambda - i\gamma) \right| \ .$$

Suppose $C_2 > 0$, otherwise $|\mathrm{den}_M| > 0$ for every positive R. Consider the modulus of denominator of the M-function

$$\begin{aligned}
|\mathrm{den}_M| \ &= \ \Big| \left(\sqrt{i\gamma - \lambda} + \sqrt{-\lambda}\right) \left(\phi'(b) + \sqrt{i\gamma - \lambda}\, \phi(b)\right) \ e^{+\sqrt{i\gamma-\lambda}\,(R-b)} \\
&\quad + \left(\sqrt{i\gamma - \lambda} - \sqrt{-\lambda}\right) \left(\phi'(b) - \sqrt{i\gamma - \lambda}\, \phi(b)\right) \ e^{-\sqrt{i\gamma-\lambda}\,(R-b)} \Big| \\
&\geq \ \left| \left(\sqrt{i\gamma - \lambda} + \sqrt{-\lambda}\right) \left(\phi'(b) + \sqrt{i\gamma - \lambda}\, \phi(b)\right) \ e^{+\sqrt{i\gamma-\lambda}\,(R-b)} \right| \\
&\quad - \left| \left(\sqrt{i\gamma - \lambda} - \sqrt{-\lambda}\right) \left(\phi'(b) - \sqrt{i\gamma - \lambda}\, \phi(b)\right) \ e^{-\sqrt{i\gamma-\lambda}\,(R-b)} \right| \\
&= \ e^{\sqrt{i\gamma-\lambda}\,(R-b)} \Big[\left| \sqrt{i\gamma - \lambda} + \sqrt{-\lambda} \right| \cdot \left| \phi'(b) + \sqrt{i\gamma - \lambda}\, \phi(b) \right| \\
&\quad - \left| \sqrt{i\gamma - \lambda} - \sqrt{-\lambda} \right| \cdot \left| \phi'(b) - \sqrt{i\gamma - \lambda}\, \phi(b) \right| \ e^{-2\sqrt{i\gamma-\lambda}\,(R-b)} \Big] \\
&\geq \ e^{(R-b)c} \left(\frac{|i\gamma| \cdot C_1}{\left|\sqrt{i\gamma - \lambda} - \sqrt{-\lambda}\right|} - C_2 \left| \sqrt{i\gamma - \lambda} - \sqrt{-\lambda} \right| \ e^{-2(R-b)c} \right) .
\end{aligned}$$

Now, we want $|\mathrm{den}_M|$ to be positive, so choose R large enough to get

$$\frac{\gamma \cdot C_1}{\left|\sqrt{i\gamma - \lambda} - \sqrt{-\lambda}\right|} - C_2 \left| \sqrt{i\gamma - \lambda} - \sqrt{-\lambda} \right| \ e^{-2(R-b)c} > k > 0 \ ;$$

for example take

$$R > b + \frac{1}{2c} \log\left(\frac{\gamma \cdot C_1}{C_2 \cdot C_3}\right) =: \bar{R}^{(1)}_K \ ,$$

where

$$C_3 = \max_{\lambda \in K} \left| \sqrt{i\gamma - \lambda} - \sqrt{-\lambda} \right|^2 .$$

This shows that, for large R, the Titchmarsh-Weyl function has got no poles, that is the operator $\mathrm{H}^c_{R,\gamma}$ has got no Neumann eigenvalues.

Similarly, if

$$R > b + \frac{1}{2c} \log \left(\frac{\gamma \cdot C_4}{C_5 \cdot C_3} \right) =: \bar{R}^{(2)}_K ,$$

where

$$C_4 := \min_{\lambda \in K} \left| -\psi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\, \psi(b; \lambda - i\gamma) \right|$$

and

$$C_5 := \max_{\lambda \in K} \left| -\psi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\, \psi(b; \lambda - i\gamma) \right| > 0 ,$$

the modulus of the numerator of the Titchmarsh-Weyl coefficient, denoted by num_M, is uniformly positive in K, that is the operator $\mathrm{H}^c_{R,\gamma}$ has got no Dirichlet eigenvalues.
Note that if C_5 were 0, this would be true for every admissible R.

Taking $\bar{R}_K := \max \left\{ \bar{R}^{(1)}_K , \bar{R}^{(2)}_K \right\}$, we can conclude. □

The spectrum of the operator $\mathrm{H}^c_{R,\gamma}$ has now been characterized.

Remark 2.2.3. Moreover, the estimates in the proof of the previous theorem and

$$\left| \frac{\mathrm{num}_M}{\mathrm{den}_M} \right| < \frac{C_6 \cdot e^{\mathrm{Re}\sqrt{i\gamma - \lambda}\,(R-b)} + C_5 \cdot e^{-\mathrm{Re}\sqrt{i\gamma-\lambda}\,(R-b)}}{k \cdot e^{\mathrm{Re}(\sqrt{i\gamma-\lambda})\,(R-b)}} \leq \frac{C_6 + C_5}{k}$$

for large R, where

$$C_6 := \max_{\lambda \in K} \left| \sqrt{i\gamma - \lambda} + \sqrt{-\lambda} \right| \cdot \left| -\psi'(b; \lambda - i\gamma) - \sqrt{i\gamma - \lambda}\, \psi(b; \lambda - i\gamma) \right| ,$$

together with Montel's theorem (Theorem 1.17), show that the coefficient of the M-function converges **uniformly** (as R tends to infinity) to

$$\frac{\psi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\, \psi(b; \lambda - i\gamma)}{\phi'(b; \lambda - i\gamma) + \sqrt{i\gamma - \lambda}\, \phi(b; \lambda - i\gamma)} \neq 0 .$$

To conclude the Section, we want now to find explicitly the Titchmarsh-Weyl function for a given potential.

Example. In this example, we want to solve explicitly the problem associated with the particular compactly supported potential

$$q(x) := \begin{cases} a & , \text{ if } \quad x < 1 \\ 0 & , \text{ if } \quad x \geq 1 \end{cases} ,$$

where a is a negative real number.

The functional setting is the same of Section 2.2.1.

In $[0,1]$ (the support of q), the spectral equation for complex λ can be written as

$$-u'' + (a + i\gamma)\, u = \lambda\, u \ .$$

It is known that there are two linearly independent solutions $\phi(\cdot\,;\lambda - i\gamma) := \cosh(\sqrt{a + i\gamma - \lambda}\,\cdot)$ and $\psi(\cdot\,;\lambda - i\gamma) := \frac{\sinh(\sqrt{a+i\gamma-\lambda}\,\cdot)}{\sqrt{a+i\gamma-\lambda}}$ such that the solution in $[0,1[$ can be written as

$$u(x) = \alpha_1\, \phi(x;\lambda - i\gamma) + \alpha_2\, \psi(x;\lambda - i\gamma) \ .$$

In $]1, R[$ the solution is of the form

$$\alpha_3 \cosh(\sqrt{i\gamma - \lambda}\,\cdot) + \alpha_4\, \frac{\sinh(\sqrt{i\gamma - \lambda}\,\cdot)}{\sqrt{i\gamma - \lambda}}$$

and in $]R, +\infty[$, since we want the global solution to be in $H^2([0, +\infty[)$, we may select the exponentially decaying solution at $+\infty$: that is, in $]R, +\infty[$ the solution of the spectral equation is

$$u(x) = \alpha_5\, e^{-\sqrt{-\lambda}\, x} \ .$$

The global solution should satisfy the following boundary conditions:

$$\begin{aligned} \alpha_1 \cosh(\sqrt{a + i\gamma - \lambda}) + \alpha_2\, \frac{\sinh(\sqrt{a + i\gamma - \lambda})}{\sqrt{a + i\gamma - \lambda}} &= \\ = \alpha_3 \cosh(\sqrt{i\gamma - \lambda}) + \alpha_4\, \frac{\sinh(\sqrt{i\gamma - \lambda})}{\sqrt{i\gamma - \lambda}} & \ , \end{aligned}$$

$$\begin{aligned} \alpha_1 \sqrt{a + i\gamma - \lambda}\, \sinh(\sqrt{a + i\gamma - \lambda}) + \alpha_2 \cosh(\sqrt{a + i\gamma - \lambda}) &= \\ = \alpha_3 \sqrt{i\gamma - \lambda}\, \sinh(\sqrt{i\gamma - \lambda}) + \alpha_4 \cosh(\sqrt{i\gamma - \lambda}) & \end{aligned}$$

and

$$\frac{\alpha_3 \sqrt{i\gamma - \lambda}\, \sinh(\sqrt{i\gamma - \lambda}\, R) + \alpha_4 \cosh(\sqrt{i\gamma - \lambda}\, R)}{\alpha_3 \cosh(\sqrt{i\gamma - \lambda}\, R) + \alpha_4\, \frac{\sinh(\sqrt{i\gamma - \lambda}\, R)}{\sqrt{i\gamma - \lambda}}} \quad = \quad -\sqrt{-\lambda} \ .$$

Also, at $x = 0$, the global solution must satisfy a general Neumann condition (by construction of the Titchmarsh-Weyl function):

$$\alpha_1 \sqrt{a + i\gamma - \lambda}\, \sinh(\sqrt{a + i\gamma - \lambda}\, R) + \alpha_2 \cosh(\sqrt{a + i\gamma - \lambda}\, R)\Big|_{x=0} = z \ ,$$

that is $\alpha_2 = z$. The coefficient α_j, $j = 1, \ldots, 4$, are solutions of the linear system with known term $(z, 0, 0, 0)^T$ and matrix

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ \cosh\left(\sqrt{a+i\gamma-\lambda}\right) & \frac{\sinh\left(\sqrt{a+i\gamma-\lambda}\right)}{\sqrt{a+i\gamma-\lambda}} & -\cosh\left(\sqrt{i\gamma-\lambda}\right) & -\frac{\sinh\left(\sqrt{i\gamma-\lambda}\right)}{\sqrt{i\gamma-\lambda}} \\ \sqrt{a+i\gamma-\lambda}\,\sinh\left(\sqrt{a+i\gamma-\lambda}\right) & \cosh\left(\sqrt{a+i\gamma-\lambda}\right) & -\sqrt{i\gamma-\lambda}\,\sinh\left(\sqrt{i\gamma-\lambda}\right) & -\cosh\left(\sqrt{i\gamma-\lambda}\right) \\ 0 & 0 & a(\lambda, R) & b(\lambda, R) \end{pmatrix}$$

where

$$\begin{aligned} a(\lambda, R) &:= \sqrt{i\gamma - \lambda}\, \sinh(\sqrt{i\gamma - \lambda}\, R) + \sqrt{-\lambda}\cosh(\sqrt{i\gamma - \lambda}\, R) \ , \\ b(\lambda, R) &:= \cosh(\sqrt{i\gamma - \lambda}\, R) + \frac{\sqrt{-\lambda}}{\sqrt{i\gamma - \lambda}} \sinh(\sqrt{i\gamma - \lambda}\, R) \ . \end{aligned}$$

The Neumann-to-Dirichlet M-function is the mapping

$$z \longmapsto u(0) = \alpha_1 \ ,$$

so by Cramer's rule the denominator of α_1, i.e. of the Titchmarsh-Weyl function is:

$$\begin{aligned} \mathrm{den}_M &= a(\lambda, R) \cdot \Big[-\cosh(\sqrt{i\gamma - \lambda}) \cosh(\sqrt{a + i\gamma - \lambda}) \\ &\quad + \sinh(\sqrt{i\gamma - \lambda}) \sinh(\sqrt{a + i\gamma - \lambda}) \Big] \\ &\quad + b(\lambda, R) \cdot \Big[\sqrt{i\gamma - \lambda}\, \sinh(\sqrt{i\gamma - \lambda}) \cosh(\sqrt{a + i\gamma - \lambda}) \\ &\quad - \sqrt{a + i\gamma - \lambda}\, \cosh(\sqrt{i\gamma - \lambda}) \sinh(\sqrt{a + i\gamma - \lambda}) \Big] \end{aligned}$$

and the numerator

$$\begin{aligned} \mathrm{num}_M &= z \left\{ \frac{\sinh\left(\sqrt{a + i\gamma - \lambda}\right)}{\sqrt{a + i\gamma - \lambda}} \left[a(\lambda, R) \cosh\left(\sqrt{i\gamma - \lambda}\right) \right.\right. \\ &\quad \left. - \sqrt{i\gamma - \lambda}\, b(\lambda, R) \sinh(\sqrt{i\gamma - \lambda}) \right] \\ &\quad + \cosh\left(\sqrt{a + i\gamma - \lambda}\right) \cdot \left[b(\lambda, R) \cosh\left(\sqrt{i\gamma - \lambda}\right) \right. \\ &\quad \left.\left. - a(\lambda, R) \frac{\sinh\left(\sqrt{i\gamma - \lambda}\right)}{\sqrt{i\gamma - \lambda}} \right] \right\} \end{aligned}$$

Using

$$\begin{aligned}
\cosh(\alpha \pm \beta) &= \cosh(\alpha)\cosh(\beta) \pm \sinh(\alpha)\sinh(\beta) \ , \\
\sinh(\alpha \pm \beta) &= \sinh(\alpha)\cosh(\beta) \pm \cosh(\alpha)\sinh(\beta) \ ,
\end{aligned}$$

it follows for example that

$$\begin{aligned}
\mathrm{num}_M &= z\left\{\frac{\sinh\left(\sqrt{a+i\gamma-\lambda}\right)}{\sqrt{a+i\gamma-\lambda}}\left[\sqrt{i\gamma-\lambda}\,\sinh\left(\sqrt{i\gamma-\lambda}\,(R-1)\right)\right.\right. \\
&\quad \left. +\sqrt{-\lambda}\,\cosh\left(\sqrt{i\gamma-\lambda}\,(R-1)\right)\right] \\
&\quad +\sinh\left(\sqrt{a+i\gamma-\lambda}\right)\left[\cosh\left(\sqrt{i\gamma-\lambda}\,(R-1)\right)\right. \\
&\quad \left.\left. +\frac{\sqrt{-\lambda}}{\sqrt{i\gamma-\lambda}}\sinh\left(\sqrt{i\gamma-\lambda}\,(R-1)\right)\right]\right\} \ .
\end{aligned}$$

Chapter 3

Solution of the problem for periodic background potentials

Theorems 2.1 and 2.2 in the previous chapter say that, given any compact set in the strip $\{z \in \mathbb{C} : 0 < \mathrm{Im}(z) < \gamma\}$, R can be chosen sufficiently large to ensure that the spectrum of $\mathrm{H}_{R,\gamma}$ (for free and compactly supported q) lies outside of the compact set. Also, uniform convergence of the Titchmarsh-Weyl function has been proven. Our object in this chapter is to extend the free case to the periodic case, using the fact that Floquet theory provides a good expression for exponentially decaying solutions of the spectral equation. Unfortunately, the results of Chapter 2 cannot be completely generalized, since the asymptotic behaviour of the Titchmarsh-Weyl function is unknown on a discrete, with no accumulation point and possibly countable, set of points D inside the strip. Some numerical experiments show that it is reasonable to think that this set is empty.
With the additional assumption that the potential q can be extended as an even function on the whole real axis, in Section 3.4 it is demonstrated that the set D can be characterized as the set of eigenvalues of a $\mathcal{PT}$-symmetric Schrödinger operator on $\mathbb{R}$.

3.1 Floquet theory for the unperturbed case

The main tool in the study of ordinary differential equations with periodic coefficients is the so-called *Floquet theory*. In this section, we shall consider the Floquet theory for periodic Schrödinger operators: it will give in Theorem 3.2 (Floquet theorem) an explicit description of the solutions of the spectral equation, in terms of basic properties of the dynamical system and of the period of the potential. This explicit form will be extensively used in the sequel of the chapter. We shall formulate here some of the known results about this classical case, without proof except for Theorem 3.1.

Let us fix $\lambda \in \mathbb{C}$ and consider the spectral equation associated to such a λ for a periodic Schrödinger operator, that is:

$$-u''(x) + (V(x) - \lambda)\, u(x) = 0, \ x \in [0, \infty[\tag{3.1}$$

on $\mathrm{L}^2(\mathbb{R})$, where V is a (general) complex-valued bounded and periodic function with period L.

Let ϕ_λ, ψ_λ be solutions of (3.1) such that

$$\begin{pmatrix} \phi_\lambda(0) \\ \phi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \psi_\lambda(0) \\ \psi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{3.2}$$

Let

$$M_\lambda := \begin{pmatrix} \phi_\lambda(L) & \psi_\lambda(L) \\ \phi'_\lambda(L) & \psi'_\lambda(L) \end{pmatrix} .$$

Call M_λ *monodromy* (or *Floquet*) *matrix*.

Remark 3.1.1. In the context of dynamical systems, M_λ is usually called fundamental or wronskian matrix. Note that $\det(M_\lambda) = 1$, because it is well known the Wronskian associated to the equation (3.1)

$$\hat{W}(\phi_\lambda, \psi_\lambda)(x) := \det \begin{pmatrix} \phi_\lambda(x) & \psi_\lambda(x) \\ \phi'_\lambda(x) & \psi'_\lambda(x) \end{pmatrix}$$

is constant, thus equal to 1 $(= \hat{W}(\phi_\lambda, \psi_\lambda)(0))$.

The following theorem shows an interesting property of some solutions of the equation (3.1), which will be crucial for Theorem 3.2.

Theorem 3.1. *Let $\lambda \in \mathbb{C}$. There exists a non-zero complex number $\rho = \rho_\lambda$ and a non-trivial solution u_λ of (3.1) such that for every $x \in [0, +\infty[$*

$$u_\lambda(x + L) = \rho\, u_\lambda(x) \tag{3.3}$$

and

$$u'_\lambda(x + L) = \rho\, u'_\lambda(x) \ .$$

Proof. ϕ_λ and ψ_λ be, as above, solutions of (3.1) satisfying (3.2). Since also $\phi_\lambda(x+L)$ and $\psi_\lambda(x+L)$ are solutions of (3.1), using the boundary conditions (3.2), we can write

$$\begin{aligned} \phi_\lambda(x + L) &= \phi_\lambda(L)\phi_\lambda(x) + \phi'_\lambda(L)\psi_\lambda(x) \\ \psi_\lambda(x + L) &= \psi_\lambda(L)\phi_\lambda(x) + \psi'_\lambda(L)\psi_\lambda(x). \end{aligned} \tag{3.4}$$

Since every solution $u_\lambda(x)$ of (3.1) can be written as $u_\lambda(x) = c_1\phi_\lambda(x) + c_2\psi_\lambda(x)$, it suffices to show that there exist a vector $(c_1, c_2)^t \in \mathbb{C}^2 \setminus \{0\}$ and a complex number $\rho = \rho_\lambda$ such that

$$\begin{pmatrix} \phi_{\lambda-i\gamma}(L) & \psi_{\lambda-i\gamma}(L) \\ \phi'_{\lambda-i\gamma}(L) & \psi'_{\lambda-i\gamma}(L) \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \rho \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} ,$$

because, by (3.4), this is equivalent to (3.3)

$$u_\lambda(x+L) = \rho\, u_\lambda(x) \ .$$

Therefore, now the question is whether the monodromy matrix M_λ has a non-zero eigenvector with the corresponding (non-zero) eigenvalue ρ. But this is clear, because $\det(M_\lambda) = 1$ and it is not possible for M_λ to have a null eigenvalue.

□

Let us give some important definitions.

Definition 3.1. *Let the symbol* Tr *denote the trace of a matrix One calls*

$$\Delta(\lambda) := \mathrm{Tr}\,[M_\lambda]$$

the Floquet discriminant *of equation (3.1). The solutions ρ_+ and ρ_- of the* characteristic equation

$$\rho^2 - \Delta(\lambda)\rho + 1 = 0$$

are called the Floquet multipliers *of equation (3.1). Note that they are the eigenvalues of M_λ: since* $\det M_\lambda = 1$, *they can be written in the form*

$$\rho_\pm = e^{\pm w(\lambda)L} .$$

We will also call $w(\lambda) \in \mathbb{C}$ the Floquet exponent *(or* quasi-momentum*) associated with the equation (3.1).*

As already announced in the beginning of this section, the key result of Floquet theory is the so-called Floquet theorem: it gives a description for a linear basis of solutions of the spectral equation (3.1).

Theorem 3.2 (Floquet)**.** *Let $\lambda \in \mathbb{C}$. The equation (3.1) has linearly independent solutions $u_\lambda^{(+)}$ and $u_\lambda^{(-)}$ such that either*

$$u_\lambda^{(+)}(x) = e^{+w(\lambda)x}\, p_+(x;\lambda) \quad \text{and} \quad u_\lambda^{(-)}(x) = e^{-w(\lambda)x}\, p_-(x;\lambda) \ , \qquad (3.5)$$

or

$$u_\lambda^{(+)}(x) = e^{+w(\lambda)\,x}\, p_+(x;\lambda) \quad \text{and} \quad u_\lambda^{(-)}(x) = e^{+w(\lambda)\,x}\, \{x p_+(x;\lambda) + p_-(x;\lambda)\} \ ,$$

where both $p_+(\cdot;\lambda)$ and $p_-(\cdot;\lambda)$ are periodic functions with period L.

Remark 3.1.2. Sometimes, when there is no ambiguity, we will omit the dependence of $p_+(x)$ and $p_-(x)$ on the complex parameter λ.

The notion of stability is also important in the context of Floquet theory:

Definition 3.2. *A solution of the equation (3.1) is said to be stable if it is bounded and in* L^2*; unstable otherwise.*

Corollary 3.1 (Stability test). *Fix* $\lambda \in \mathbb{C}$ *and suppose* $\Delta(\lambda)$ *is real.*

(i) If $|\Delta(\lambda)| < 2$*, then all solutions of (3.1) are bounded on* $\mathbb{R}$*.*

(ii) If $|\Delta(\lambda)| > 2$*, then all non-trivial solutions are unbounded on* $\mathbb{R}$*.*

(iii) If $\Delta(\lambda) = 2$*, then there is at least one non-trivial solution that is periodic with period* L*. Moreover, if* $\phi'_\lambda(L) = 0 = \psi_\lambda(L)$*, then all solutions are periodic with period* L*. If either* $\phi'_\lambda(L) \neq 0$ *or* $\psi_\lambda(L) \neq 0$*, there do not exist two linearly independent periodic solutions.*

(iv) If $\Delta(\lambda) = -2$*, then there is at least one non-trivial solution that is semi-periodic with semi-period* L*. Moreover, if* $\phi'_\lambda(L) = 0 = \psi_\lambda(L)$*, all solutions are semi-periodic with semi-period* L*. If either* $\phi'_\lambda(L) \neq 0$ *or* $\psi_\lambda(L) \neq 0$*, there do not exist two linearly independent semi-periodic solution.*

If $\Delta(\lambda)$ *is not real, then all non-trivial solutions of (3.1) are unbounded on* $\mathbb{R}$*.*

The spectrum of the periodic Schrödinger operator can be characterized in terms of the quasi-momentum, as shown by:

Theorem 3.3. *The spectrum of the operator* H^{per} *is purely continuous and*

$$\sigma(\mathrm{H}_V^{per}) = \{\lambda \in \mathbb{C} \,:\, \mathrm{Re}\,(w(\lambda)) = 0\}\ ,$$

where $w(\lambda)$ *is the Floquet exponent associated with the equation (3.1).*

Corollary 3.2. *If* $\lambda \in \mathbb{C}$ *is not in* $\sigma(\mathrm{H}_V^{per})$*, then there are two linearly independent solutions of the spectral equation which can be written like in formula (3.5) of Theorem 3.2.*

Finally, the following theorem gives an explicit description of the structure of the spectrum of the periodic Schrödinger operator:

Theorem 3.4 (Bands-gaps structure). *Let V be also real-valued. Then, there exist two sequences of real numbers $\{\lambda_n\}_{n\in\mathbb{N}}$ and $\{\lambda'_n\}_{n\in\mathbb{N}}$, satisfying*

$$\lambda_0 < \lambda'_0 \le \lambda'_1 < \lambda_1 \le \lambda_2 < \lambda'_2 \le \lambda'_3 < \lambda_3 \le \lambda_4 < \dots$$

such that

$$\sigma(\mathrm{H}_V^{per}) = \bigcup_{n=0}^{\infty} \left([\lambda_{2n}, \lambda'_{2n}] \cup [\lambda'_{2n+1}, \lambda_{2n+1}] \right) .$$

We will often refer to the intervals $[\lambda_{2n}, \lambda'_{2n}]$ and $[\lambda'_{2n+1}, \lambda_{2n+1}]$ as *bands* of the spectrum of H^{per}, while the complementary intervals, including $]-\infty, \lambda_0[$, are called *gaps*. Recalling Section 1.5, this kind of structure for the spectrum represents one of the most typical case in which spectral pollution originates.

These are the results that we will need in what follows. Now we are ready to compute the Titchmarsh-Weyl function in the periodic perturbed case.

3.2 Spectrum of the perturbed periodic case

Let us consider now a periodic Schrödinger operator, i.e. fix a real-valued, periodic and essentially bounded function (the *potential*) $q : [0, +\infty[\longrightarrow \mathbb{R}$ with period $L > 0$. Our aim is now to study the spectrum of the non self-adjoint operator

$$\mathrm{H}_{R,\gamma}^{per} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\gamma\, \chi_R(x) = \mathrm{H}^{per} + i\gamma\, \chi_R(x) ,$$

on the Hilbert space $\mathrm{L}^2\left([0, +\infty[\right)$, where the parameters R, γ are positive and the domain of H^{per} is

$$\mathcal{D}\left(\mathrm{H}^{per}\right) = \left\{ u \in \mathrm{L}^2([0, +\infty[) \,:\, -u'' \in \mathrm{L}^2([0, +\infty[),\, u'(0) = 0 \right\} .$$

Remark 3.2.1. As already said in Chapter 1, this is not the most general assumption which can be made on the potential and on the domain of the operator H^{per}. Indeed, in order to get self-adjointness of H^{per}, the "best" (minimal) assumption is to consider $q \in \mathrm{L}^1_{loc}([0, +\infty[) \cap \mathrm{L}^1([0, \varepsilon])$ for some positive ε and take

$$\begin{aligned} \mathcal{D}\left(\mathrm{H}^{per}\right) \;=\; & \big\{ u \in \mathrm{L}^2([0, +\infty[) \cap H^2_{loc}([0, +\infty[) \,: \\ & \quad -u'' + q\, u \in \mathrm{L}^2([0, +\infty[), u'(0) = 0 \big\} . \end{aligned}$$

For details, see [2].

3.2.1 The Titchmarsh-Weyl function associated with the perturbed operator

We will use the same model of the free and compactly supported cases. Define:

- $\mathcal{H} = \mathrm{L}^2([0,+\infty[)$;
- $A := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\,\gamma\,\chi_R(x)$ with
$$\mathcal{D}(A) = \left\{u \in H^2\left([0,+\infty[\right) \,:\, u(0) = u'(0) = 0\right\} \;;$$
- $\tilde{A} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\,\gamma\,\chi_R(x)$, having domain $\mathcal{D}(\tilde{A}) = \mathcal{D}(A)$.

The respective adjoint operators are

$$A^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) - i\,\gamma\,\chi_R(x), \quad \tilde{A}^* = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) + i\,\gamma\,\chi_R(x) \;,$$

with domains $\mathcal{D}(A^*) = \mathcal{D}(\tilde{A}^*) = H^2\left([0,+\infty[\right)$, so that the operators A and $\tilde{A}$ form an adjoint pair. As in the case of compactly supported background potential, integrating by parts, we obtain that for $u \in \mathcal{D}(\tilde{A}^*)$ and $v \in \mathcal{D}(A^*)$:

$$(\tilde{A}^* u, v)_{\mathcal{H}} - (u, A^* v)_{\mathcal{H}} = u'(0)\bar{v}(0) - u(0)\bar{v}'(0) = (\Gamma_1 u, \Gamma_2 v)_{\mathbb{C}} - (\Gamma_2 u, \Gamma_1 v)_{\mathbb{C}} \;,$$

where $\Gamma_1 u := u'(0)$ and $\Gamma_2 u := u(0)$.
The Titchmarsh-Weyl function of interest is again the mapping

$$\Gamma_1 u \longmapsto \Gamma_2 u \;.$$

Once we have a global solution of the spectral equation

$$\mathrm{H}^{per}_{R,\gamma} u = \lambda\, u \;, \tag{3.6}$$

we may recover its value at 0, i.e. $\Gamma_2 u$, in terms of $\Gamma_1 u$.

First, let us consider the spectral equation in $[R,+\infty[$:

$$-u'' + q(x)u = \lambda u \,, \tag{3.7}$$

where $\lambda \in \mathbb{C}$. If λ is not in the spectrum of H^{per}, there is a $\mathrm{L}^2([R,+\infty[)$ solution of the form:

$$u(x) = C\, p_-(x;\lambda) e^{-\tilde{w}(\lambda) x} \;, \tag{3.8}$$

where $p_-(\cdot;\lambda)$ is a periodic function with period L and $\tilde{w}(\lambda)$ is the Floquet quasi-momentum (chosen with positive real part) associated with the equation (3.7) with monodromy matrix

$$\tilde{M_\lambda}^{(R)} := \begin{pmatrix} \Phi_\lambda(R+L) & \Psi_\lambda(R+L) \\ \Phi'_\lambda(R+L) & \Psi'_\lambda(R+L) \end{pmatrix} .$$

Here Φ_λ and Ψ_λ are solutions of (3.7) such that

$$\begin{pmatrix} \Phi_\lambda(R) \\ \Phi'_\lambda(R) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \Psi_\lambda(R) \\ \Psi'_\lambda(R) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

However, taking R as an integer multiple of the period L, since we are interested in the limit as $R \to \infty$ the spectral equation (3.7) in $[R, +\infty[$ is translation-invariant, so equivalent to the same equation in $[0, +\infty[$; so, in this case, $\tilde{w}(\lambda)$ is the quasi-momentum $w(\lambda)$ associated with the standard monodromy matrix

$$M_\lambda := \begin{pmatrix} \phi_\lambda(L) & \psi_\lambda(L) \\ \phi'_\lambda(L) & \psi'_\lambda(L) \end{pmatrix} ,$$

where ϕ_λ and ψ_λ are solutions of (3.7) such that

$$\begin{pmatrix} \phi_\lambda(0) \\ \phi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \psi_\lambda(0) \\ \psi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

Let us make this assumption to simplify notation.

Remark 3.2.2. Note that, since λ is supposed to be not in the spectrum, then, by Theorem 3.3, $\mathrm{Re}(w(\lambda)) \neq 0$. The solution in (3.8) has to be in $H^2([0, +\infty[)$, thus we are allowed to choose $w(\lambda)$ in such a way that $\mathrm{Re}(w(\lambda)) > 0$.

Conversely, in the interval $[0, R]$ (let us suppose $R \geq L$) the spectral equation is

$$-u'' + (q(x) + i\gamma)\, u = \lambda u$$

that is

$$-u'' + q(x)\, u = (\lambda - i\gamma)\, u \; ; \tag{3.9}$$

it is clear that, comparing this equation with the spectral equation out of $[0, R]$, the difference is just a shift equal to $-i\gamma$ of the spectral parameter λ. Therefore, the general solution can be written as

$$u(x) = \alpha\, P_+(x) e^{+W(\lambda)x} + \beta\, P_-(x) e^{-W(\lambda)x} ,$$

where $P_\pm(\cdot) = p_\pm(\cdot; \lambda - i\gamma)$ are periodic functions with period L and the term $W(\lambda) := w(\lambda - i\gamma)$ is the quasi-momentum associated to the equation (3.9) with monodromy matrix $M_{\lambda - i\gamma}$. Note again that, if $\lambda - i\gamma$ does not belong to the spectrum of H^{per}, or equivalently if λ is not in the shifted spectrum $\sigma(\mathrm{H}^{per}) + i\gamma$, then we can choose $W(\lambda)$ such that $\mathrm{Re}(W(\lambda)) > 0$.

In order to find a global solution, let us impose the following "matching" condition at $x = R$:

$$\frac{u'(R-)}{u(R-)} = \frac{u'(R+)}{u(R+)} \ ,$$

that is

$$\begin{aligned}\frac{p'_-(R) - w(\lambda)p_-(R)}{p_-(R)} =& \frac{\alpha\left[e^{W(\lambda)R}\left(P'_+(R) + W(\lambda)P_+(R)\right)\right]}{\alpha P_+(R)e^{W(\lambda)R} + \beta P_-(R)e^{-W(\lambda)R}} \\ &+ \frac{\beta\left[e^{-W(\lambda)R}\left(P'_-(R) - W(\lambda)P_-(R)\right)\right]}{\alpha P_+(R)e^{W(\lambda)R} + \beta P_-(R)e^{-W(\lambda)R}} \ ,\end{aligned} \tag{3.10}$$

where it has been omitted the dependence of the functions p_-, P_+ and P_- on the respective spectral parameters.

Remark 3.2.3. Note that if λ is not real, $p_-(R)$ has to be non-zero, so that the expression above in the left hand side of (3.10) is well defined.
Indeed, let us suppose that $p_-(R) = 0$. Then, by periodicity of p_-, also $p_-(R+L) = 0$. These two conditions imply, in particular, that the solution u of (3.7) is 0 at the points $x = R$ and $x = R + L$. It is well known the regular Dirichlet problem

$$\begin{aligned} -u'' + q(x)\,u &= \lambda u \\ u(R) &= 0 \\ u(R+L) &= 0 \end{aligned}$$

is self-adjoint, therefore λ has to be a real number, in order to have a non-trivial eigenfunction u. This contradicts the hypothesis.

Calling

$$f(\lambda, R) := \frac{p'_-(R) - w(\lambda)p_-(R)}{p_-(R)} \tag{3.11}$$

and

$$G_\pm(\lambda, R) := P'_\pm(R) \pm P_\pm(R)\left(W(\lambda) \mp f(\lambda, R)\right) \ , \tag{3.12}$$

the condition (3.10) becomes

$$\alpha\, G_+(\lambda, R)e^{W(\lambda)R} + \beta\, G_-(\lambda, R)e^{-W(\lambda)R} = 0. \tag{3.13}$$

In order to construct the Titchmarsh-Weyl function, we also have to impose a generic Neumann condition at $x = 0$:

$$\alpha \left(P'_+(0) + W(\lambda)P_+(0)\right) + \beta \left(P'_-(0) - W(\lambda)P_-(0)\right) = z \ . \tag{3.14}$$

Let us define

$$F_\pm(\lambda - i\gamma) := p'_\pm(0; \lambda - i\gamma) \pm w(\lambda - i\gamma)p_\pm(0; \lambda - i\gamma) = P'_\pm(0) \pm W(\lambda)P_\pm(0) \ ,$$

so that the boundary condition (3.14) can be simply written as

$$\alpha \, F_+(\lambda - i\gamma) + \beta \, F_-(\lambda - i\gamma) = z \ . \tag{3.15}$$

Solving the system of two linear equations (3.13) and (3.15) by the Cramer's rule, we get

$$\alpha = \frac{-z \; G_-(\lambda, R) \, e^{-W(\lambda)R}}{G_+(\lambda, R) \cdot F_-(\lambda - i\gamma) \, e^{W(\lambda)R} - G_-(\lambda, R) \cdot F_+(\lambda - i\gamma) \, e^{-W(\lambda)R}} \tag{3.16}$$

and

$$\beta = \frac{z \; G_+(\lambda, R) \, e^{+W(\lambda)R}}{G_+(\lambda, R) \cdot F_-(\lambda - i\gamma) \, e^{W(\lambda)R} - G_-(\lambda, R) \cdot F_+(\lambda - i\gamma) \, e^{-W(\lambda)R}} \tag{3.17}$$

Therefore the Neumann-to-Dirichlet Titchmarsh Weyl function is the mapping

$$z \longmapsto \alpha \, P_+(0) + \beta \, P_-(0) \ ,$$

that is

$$z \longmapsto z \, \frac{P_-(0) \, G_+(\lambda, R) \, e^{+W(\lambda)R} - P_+(0) \, G_-(\lambda, R) \, e^{-W(\lambda)R}}{G_+(\lambda, R) \cdot F_-(\lambda - i\gamma) \, e^{W(\lambda)R} - G_-(\lambda, R) \cdot F_+(\lambda - i\gamma) \, e^{-W(\lambda)R}} \ . \tag{3.18}$$

Remark 3.2.4. At this point, it is important to notice that $w(\lambda)$, $P_+(\cdot\,; \lambda)$, $P_-(\cdot\,; \lambda)$, $F_+(\lambda - i\gamma)$, $F_-(\lambda - i\gamma)$, $G_+(\lambda, R)$ and $G_+(\lambda, R)$, viewed as functions of the complex variable λ, are analytic functions, at least inside the strip $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$. This comes from the theory of complex linear differential systems (see [10, Chap. 1, Sec. 8])

Our aim is now to show that the Titchmarsh-Weyl coefficient above in (3.18) is well defined. First, we notice that:

Lemma 3.1. *If λ is contained in the strip $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$, the functions P_+ and P_- are such that:*

- $P_\pm(0) \neq 0$;
- $F_\pm(\lambda - i\gamma) = P'_\pm(0) \pm W(\lambda) P_\pm(0) \neq 0$.

Proof. Let $\phi_{\lambda-i\gamma}$ and $\psi_{\lambda-i\gamma}$ solutions of the spectral equation

$$-u'' + q\,u = (\lambda - i\gamma)u$$

satisfying the initial conditions

$$\begin{pmatrix} \phi_{\lambda-i\gamma}(0) & \psi_{\lambda-i\gamma}(0) \\ \phi'_{\lambda-i\gamma}(0) & \psi'_{\lambda-i\gamma}(0) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

Let

$$g_+(x; \lambda - i\gamma) = P_+(x)\, e^{+w(\lambda - i\gamma)} .$$

Since $\phi_{\lambda-i\gamma}$ and $\psi_{\lambda-i\gamma}$ form a basis of solutions of the spectral equation above, g_+ can be expressed in the form

$$g_+(x) = c_1\, \phi_{\lambda-i\gamma}(x) + c_2\, \psi_{\lambda-i\gamma}(x) \;;$$

therefore also the derivative of g_+ can be written as

$$g'_+(x) = c_1\, \phi'_{\lambda-i\gamma}(x) + c_2\, \psi'_{\lambda-i\gamma}(x) \;.$$

Then, it is clear that

$$\begin{aligned} g_+(0) &= P_+(0) = c_1 \;, \\ g'_+(0) &= P'_+(0) + P_+(0)\, w(\lambda - i\gamma) = c_2 \;. \end{aligned}$$

According to the proof of Theorem 3.1, the vector $\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$ is an eigenvector of the monodromy matrix

$$M_{\lambda-i\gamma} = \begin{pmatrix} \phi_{\lambda-i\gamma}(L) & \psi_{\lambda-i\gamma}(L) \\ \phi'_{\lambda-i\gamma}(L) & \psi'_{\lambda-i\gamma}(L) \end{pmatrix}$$

with eigenvalue $e^{+w(\lambda-i\gamma)L}$, that is the vector $\begin{pmatrix} P_+(0) \\ P'_+(0) + P_+(0)\, w(\lambda - i\gamma) \end{pmatrix}$ solves the system

$$\begin{pmatrix} \phi_{\lambda-i\gamma}(L) - e^{w(\lambda-i\gamma)L} & \psi_{\lambda-i\gamma}(L) \\ \phi'_{\lambda-i\gamma}(L) & \psi'_{\lambda-i\gamma}(L) - e^{w(\lambda-i\gamma)L} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} .$$

Let us define

$$\mathbb{E}_{\lambda-i\gamma} := \begin{pmatrix} \phi_{\lambda-i\gamma}(L) - e^{w(\lambda-i\gamma)L} & \psi_{\lambda-i\gamma}(L) \\ \phi'_{\lambda-i\gamma}(L) & \psi'_{\lambda-i\gamma}(L) - e^{w(\lambda-i\gamma)L} \end{pmatrix} ;$$

therefore, the vector $\begin{pmatrix} P_+(0) \\ P'_+(0) + P_+(0)\, w(\lambda - i\gamma) \end{pmatrix}$ belongs to $\ker(\mathbb{E}_{\lambda-i\gamma})$. Note that

$$\det(\mathbb{E}_{\lambda-i\gamma}) = e^{2w(\lambda-i\gamma)L} - \big(\phi_{\lambda-i\gamma}(L) + \psi'_{\lambda-i\gamma}(L)\big)\, e^{w(\lambda-i\gamma)L} + 1 = 0 \ ,$$

because $e^{w(\lambda-i\gamma)L}$, eigenvalue of the monodromy matrix $M_{\lambda-i\gamma}$, is a solution of the characteristic equation of the linear system. Also, both $\phi'_{\lambda-i\gamma}(L)$ and $\psi_{\lambda-i\gamma}(L)$ are not 0: indeed, if -say- $\phi'_{\lambda-i\gamma}(L)$ were 0, then $\phi_{\lambda-i\gamma}$ would be solution of the self-adjoint (Neumann) problem:

$$\begin{aligned} -u'' + q(x)\, u &= (\lambda - i\gamma) u \\ u'(0) &= 0 \\ u'(L) &= 0 \quad ; \end{aligned}$$

this would imply, by self-adjointness, that $\lambda - i\gamma$ is real, but this is not possible by the hypothesis that $\lambda \in \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$. A similar argument is used to prove that $\psi_{\lambda-i\gamma}(L) \neq 0$.
Since $\det(\mathbb{E}_{\lambda-i\gamma}) = 0$, then all the entries of the matrix $\mathbb{E}_{\lambda-i\gamma}$ are not null. This means that

$$\ker(\mathbb{E}_{\lambda-i\gamma}) = \left\{ t \begin{pmatrix} \phi_{\lambda-i\gamma}(L) - e^{w(\lambda-i\gamma)L} \\ \psi_{\lambda-i\gamma}(L) \end{pmatrix} \,:\, t \in \mathbb{C} \right\}$$

and, in particular, $P_+(0) = 0$ if and only if $P'_+(0) + P_+(0)\, w(\lambda - i\gamma) = 0$.
A very similar proof also shows that $P_-(0) = 0$ if and only if $P'_-(0) - P_-(0)\, w(\lambda - i\gamma) = 0$. Finally, using periodicity and self-adjointness as we did above in Remark 3.2.3 to show that $p_-(R) \neq 0$, it follows that $P_+(0) \neq 0$, $P_-(0) \neq 0$ and, equivalently, $F_\pm(\lambda - i\gamma) \neq 0$. □

Lemma 3.2. *Let* $t \geq 0$, $\mu \in \mathbb{C} \setminus \sigma(\mathrm{H}^{per})$*; let* $g(x;\mu)$ *be the Jost solution (i.e. belonging to* $\mathcal{D}(\mathrm{H}^{per}) \subset \mathrm{L}^2([0, +\infty[)$*) of the spectral equation*

$$-u'' + q(x)\, u = \mu\, u \ .$$

Then,

$$\mathrm{Im}\left(\frac{g'(t;\mu)}{g(t;\mu)}\right)$$

has the same sign as $\mathrm{Im}(\mu)$*.*

Proof. By Floquet theory, it is known that $g(x) \equiv g(x;\mu)$ can be written as $p(x;\mu)e^{-w(\mu)x}$, where $\mathrm{Re}(w(\mu)) > 0$ and $p(t;\mu) \neq 0$, because μ is not in the spectrum of H^{per} (like in Remark 3.2.3); clearly g is such that

$$-g''(x) + q(x)\,g(x) = \mu\,g(x)\ . \tag{3.19}$$

Multiplying both sides of (3.19) by $\bar{g}(x)$ and integrating on $[t, +\infty[$, we get:

$$-\int_t^{+\infty} g''\bar{g}\,\mathrm{d}x + \int_t^{+\infty} q\,|g|^2\,\mathrm{d}x = \mu\int_t^{+\infty} |g|^2\,\mathrm{d}x\ ;$$

then, a suitable integration by parts on the first integral gives:

$$g'(t)\bar{g}(t) + \int_t^{+\infty} |g'|^2\,\mathrm{d}x + \int_t^{+\infty} q\,|g|^2\,\mathrm{d}x = \mu\int_t^{+\infty} |g|^2\,\mathrm{d}x\ . \tag{3.20}$$

In the same way, starting from the complex conjugate version of equation (3.19), we get:

$$\bar{g}'(t)g(t) + \int_t^{+\infty} |g'|^2\,\mathrm{d}x + \int_t^{+\infty} q\,|g|^2\,\mathrm{d}x = \bar{\mu}\int_t^{+\infty} |g|^2\,\mathrm{d}x\ . \tag{3.21}$$

Subtracting (3.20) and (3.21) and dividing both sides by $g(0)\cdot\bar{g}(0) \neq 0$, we have that:

$$\frac{g'(t)}{g(t)} - \frac{\bar{g}'(t)}{\bar{g}(t)} = \frac{(\mu - \bar{\mu})}{|g(t)|^2}\int_t^{+\infty} |g|^2\,\mathrm{d}x\ .$$

This is equivalent to

$$\mathrm{Im}\left(\frac{g'(t)}{g(t)}\right) = \mathrm{Im}\,(\mu)\,\frac{1}{|g(t)|^2}\int_t^{+\infty} |g|^2\,\mathrm{d}x\ ,$$

which finally proves the Lemma. □

Lemma 3.3. *If λ is contained in the strip $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, then*

$$G_-(\lambda, R) \neq 0\ .$$

Proof. Let us recall that

$$G_-(\lambda, R) = p'_-(R;\lambda - i\gamma) - p_-(R;\lambda - i\gamma)\,[w(\lambda - i\gamma) + f(\lambda, R)]$$

and

$$f(\lambda, R) = \frac{p'_-(R;\lambda) - w(\lambda)\,p_-(R;\lambda)}{p_-(R;\lambda)}$$

Suppose that $G_-(\lambda, R) = 0$, that is

$$\frac{p'_-(R;\lambda - i\gamma) - w(\lambda - i\gamma)\, p_-(R;\lambda - i\gamma)}{p_-(R;\lambda - i\gamma)} = \frac{p'_-(R;\lambda) - w(\lambda)\, p_-(R;\lambda)}{p_-(R;\lambda)} \, . \tag{3.22}$$

Let

$$g_-(x;\lambda) := p_-(x;\lambda)e^{-w(\lambda)}$$

and

$$g_-(x;\lambda - i\gamma) := p_-(x;\lambda - i\gamma)e^{-w(\lambda - i\gamma)} \, ,$$

respectively Jost solutions of

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

and

$$-u'' + q(x)\, u = (\lambda - i\gamma)u$$

on $[R, +\infty[$. By definition, the condition (3.22) can be rewritten as

$$\frac{g'_-(R;\lambda - i\gamma)}{g_-(R;\lambda - i\gamma)} = \frac{g'_-(R;\lambda)}{g_-(R;\lambda)} \, ,$$

in particular

$$\mathrm{Im}\left(\frac{g'_-(R;\lambda - i\gamma)}{g_-(R;\lambda - i\gamma)}\right) = \mathrm{Im}\left(\frac{g'_-(R;\lambda)}{g_-(R;\lambda)}\right) \, .$$

But this is not possible because, by Lemma 3.2

$$\mathrm{sgn}\left(\mathrm{Im}\left(\frac{g'_-(R;\lambda)}{g_-(R;\lambda)}\right)\right) = \mathrm{sgn}\left(\mathrm{Im}(\lambda)\right) > 0 \, ,$$

while

$$\mathrm{sgn}\left(\mathrm{Im}\left(\frac{g'_-(R;\lambda - i\gamma)}{g_-(R;\lambda - i\gamma)}\right)\right) = \mathrm{sgn}\left(\mathrm{Im}(\lambda - i\gamma)\right) < 0 \, .$$

□

According to the previous results, we may expect that the asymptotic behaviour of the M-function in this case is similar to the free case (and to the compactly supported case). However, there is no evidence that the coefficients of the exponentially growing terms, both in the numerator and in the denominator, are not zero.
As we are interested in the knowledge of this function for large R and we have chosen $R = nL$ (in order to guarantee translation invariance of the spectral

equation), we can simplify the notation, using periodicity of the functions p_-, P_+ and P_-: indeed

$$f(\lambda, nL) = \frac{p'_-(nL) - w(\lambda)p_-(nL)}{p_-(nL)} = \frac{p'_-(0) - w(\lambda)p_-(0)}{p_-(0)} = f(\lambda, 0)$$

and

$$G_\pm(\lambda, nL) = P'_\pm(nL) \pm P_\pm(nL)\,(W(\lambda) \mp f(\lambda, 0)) = G_\pm(\lambda, 0)\ .$$

Thus, if R is an integer multiple of the period L, the expression of the (Neumann-to-Dirichlet) Titchmarsh-Weyl function becomes much simpler, because the dependence on R is just in the argument of the exponentials:

$$z \longmapsto z\, \frac{P_-(0)\, G_+(\lambda, 0)\, e^{+n\,W(\lambda)L} - P_+(0)\, G_-(\lambda, 0)\, e^{-n\,W(\lambda)L}}{G_+(\lambda, 0) \cdot F_-(\lambda - i\gamma)\, e^{+n\,W(\lambda)L} - G_-(\lambda, 0) \cdot F_+(\lambda - i\gamma)\, e^{-n\,W(\lambda)L}}\ .$$

Unfortunately, as already said, it is not possible to apply the same procedure of Lemmata 3.2 and 3.3 to prove that

$$G_+(\lambda, 0) \neq 0\ ,$$

because the following holds true.

Lemma 3.4. *Let* $\mu \in \mathbb{C} \setminus \sigma(\mathrm{H}^{per})$*; let* $g_+(x;\mu)$ *be the Jost solution of the spectral equation*

$$-u'' + q(-x)\,u = \mu\,u$$

on $\mathrm{L}^2(]-\infty, 0])$*. Then,*

$$\mathrm{Im}\left(\frac{g'_+(0;\mu)}{g_+(0;\mu)}\right)$$

has the same sign as $-\mathrm{Im}(\mu)$*.*

Proof. The proof is very similar to the one of Lemma 3.2, except that the integration is made on $]-\infty, 0]$ and not on $[t, +\infty[$. □

Using the definition of G_+, the condition

$$G_+(\lambda, 0) = 0$$

is equivalent to

$$\frac{g'_-(0;\lambda)}{g_-(0;\lambda)} = \frac{g'_+(0;\lambda - i\gamma)}{g_+(0;\lambda - i\gamma)}\ , \tag{3.23}$$

which is not a contradiction in this case, at least according to Lemma 3.4.

Call
$$h_1(\lambda) := \frac{g'_-(0;\lambda)}{g_-(0;\lambda)}$$
and
$$h_2(\lambda) := \frac{g'_+(0;\lambda - i\gamma)}{g_+(0;\lambda - i\gamma)} \ .$$
Condition (3.23) thus becomes
$$h_1(\lambda) = h_2(\lambda) \ . \tag{3.24}$$
Since h_1 and h_2 are analytic functions, defined on $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$ (see Remark 3.2.4), by the identity principle we can say that the set of λ's such that (3.24) holds is (a priori) either discrete, with no finite accumulation point, or
$$h_1(z) = h_2(z)$$
for all z in the strip.

Actually, we can say more:

Lemma 3.5. *Let*
$$D := \{z \in \mathbb{C} \, : \, (3.24) \text{ holds}\} \ . \tag{3.25}$$
Then
$$D \neq \{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\} \ .$$
and D is a discrete set, at most countable, having no accumulation point in $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$.

Proof. Suppose that D coincides with $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$.
Numerical range reasoning tells us that the real part of the spectrum is bounded below. Indeed,
$$\left(\mathrm{H}^{per}_{R,\gamma} u, u\right)_{\mathrm{L}^2} = \int_0^{+\infty} q(x) \, |u|^2 \, \mathrm{d}x + i\gamma \int_0^R |u|^2 \, \mathrm{d}x + \int_0^{+\infty} |u'|^2 \, \mathrm{d}x \ ,$$
which implies that $\mathrm{Re}(\lambda) \geq c$, where $c = -\|q\|_\infty$. Thus (3.24) cannot hold also for $\mathrm{Re}(\lambda) < c$.
The functions h_1 and h_2 are analytic on $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma, \, \mathrm{Re}(z) > c\}$ and have cut singularities on the lines $\{\lambda \in \mathbb{C} \, : \, \mathrm{Re}(\lambda) \geq c, \, \mathrm{Im}(\lambda) = 0\}$ and $\{\lambda \in \mathbb{C} \, : \, \mathrm{Re}(\lambda) \geq 0, \, \mathrm{Im}(\lambda) = \gamma\}$ (where the spectra of H^{per} and $\mathrm{H}^{per} + i\gamma$ are contained), so (3.24) has to hold everywhere in the complex plane except possibly on the two cut-lines. In particular, (3.24) holds for some λ such that $\mathrm{Re}(\lambda) < c$, which is impossible. So, by the identity principle for analytic functions, we can conclude that the set D has to be discrete with no accumulation point inside the strip $\{z \in \mathbb{C} \, : \, 0 < \mathrm{Im}(z) < \gamma\}$. $\square$

Therefore, we can state the following theorem about the spectrum of $\mathrm{H}_{R,\gamma}$ in the periodic case.

Theorem 3.5. *Let D be as in (3.25). For every compact set*

$$K \subset \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma,\, z \notin D\}\ ,$$

there exists $\bar{N} = \bar{N}_K$ such that for every $n \geq \bar{N}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}^{per}_{nL,\gamma}$ are such that

$$\sigma\left(\mathrm{H}^{per}_{nL,\gamma}\right) \cap K = \emptyset\ .$$

Proof. Using Lemmata 3.1 and 3.3, and the assumption that D is discrete, we are able to prove uniform positivity of the moduli of the denominator and of the numerator of the Titchmarsh-Weyl coefficient and its uniform boundedness. The proof is very close to the proofs of theorems 2.1 and 2.2. □

Example (The free case)**.** The potential $q(x) \equiv 0$ is, in particular, a periodic function, with arbitrary period L - say $L = 1$. We would like now to use all the notation of this section to study again the free case via the Floquet theory we have developed so far.

Let ϕ_λ and ψ_λ be solutions of

$$-u'' = \lambda\, u \tag{3.26}$$

such that

$$\begin{pmatrix} \phi_\lambda(0) \\ \phi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \begin{pmatrix} \psi_\lambda(0) \\ \psi'_\lambda(0) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}\ .$$

Solving the spectral equation above, we have that if $\lambda \neq 0$

$$\phi_\lambda(x) = \cos(\sqrt{\lambda}\, x)$$

and

$$\psi_\lambda(x) = \frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda}\, x)\ .$$

The monodromy matrix is thus

$$M_\lambda = \begin{pmatrix} \phi_\lambda(1) & \psi_\lambda(1) \\ \phi'_\lambda(1) & \psi'_\lambda(1) \end{pmatrix} = \begin{pmatrix} \cos(\sqrt{\lambda}) & \frac{1}{\sqrt{\lambda}} \sin(\sqrt{\lambda} x) \\ -\sqrt{\lambda}\, \sin(\sqrt{\lambda} x) & \cos(\sqrt{\lambda}) \end{pmatrix}\ .$$

Note that $\det M_\lambda = 1$. The eigenvalues $\rho_\pm$ of M_λ are solutions of the characteristic equation

$$\rho^2 - 2\cos(\sqrt{\lambda})\rho + 1 = 0 \ ,$$

that is

$$\rho_\pm = \cos(\sqrt{\lambda}) \pm \sqrt{\cos^2(\sqrt{\lambda}) - 1} = \cos(\sqrt{\lambda}) \pm i\sin(\sqrt{\lambda}) = e^{i\sqrt{\lambda}} \ ;$$

therefore, the quasi-momentum is

$$w(\lambda) = i\sqrt{\lambda} = \sqrt{-\lambda} \ ,$$

chosen with positive real part.
Also, we can find two linearly independent solutions of (3.26) which can be written in the form:

$$u_\lambda^{(\pm)} = p_\pm(x;\lambda)\, e^{\pm w(\lambda)x} = \pm e^{\pm\sqrt{-\lambda}\,x}$$

as stated in Theorem 3.2. Note that the periodic functions p_+ and p_- are in this case constant functions (we have assumed that $p_\pm \equiv \pm 1$).
The real part of the Floquet exponent is 0 if and only if $\lambda \geq 0$; according to Theorem 3.3, we discover again that

$$\sigma(\mathrm{H}^{free}) = [0, +\infty[\ .$$

The functions f, $F_\pm$ and $G_\pm$ are easy to compute. Indeed

$$\begin{aligned} F_\pm(\lambda - i\gamma) &= p_\pm'(0) \pm w(\lambda - i\gamma)p_\pm(0) = \sqrt{i\gamma - \lambda} \ , \\ f(\lambda, R) &= \frac{p_-'(R) - w(\lambda)p_-(R)}{p_-(R)} = -\sqrt{-\lambda} \ , \\ G_\pm(\lambda, R) &= p_\pm'(R) \pm p_\pm(R)\,(w(\lambda - i\gamma) \mp f(\lambda, R)) \\ &= \sqrt{i\gamma - \lambda} \pm \sqrt{-\lambda} \ . \end{aligned}$$

If λ is contained in the strip $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, we have that

$$F_\pm(\lambda - i\gamma) \neq 0$$

and

$$G_-(\lambda, 0) \neq 0 \ ,$$

as expected according to Lemmata 3.1 and 3.3. Also, in this case

$$G_+(\lambda, 0) \neq 0 \ ,$$

so the discrete set D is empty.

The "periodic" Titchmarsh-Weyl coefficient is then the same we have computed in the free case:

$$\frac{-\left[\left(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right)\, e^{+\sqrt{i\gamma-\lambda}R}+\left(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right)\, e^{-\sqrt{i\gamma-\lambda}R}\right]}{\sqrt{i\gamma-\lambda}\left[\left(\sqrt{i\gamma-\lambda}+\sqrt{-\lambda}\right)\, e^{+\sqrt{i\gamma-\lambda}R}-\left(\sqrt{i\gamma-\lambda}-\sqrt{-\lambda}\right)\, e^{-\sqrt{i\gamma-\lambda}R}\right]}\ .$$

3.3 Numerical experiments

In this section, we will show the results of some numerical experiments that, to some extent, justify the idea that the Titchmarsh-Weyl function in the general periodic case behaves exactly like in the free case, i.e. the term

$$G_+(\lambda,0)=p_+'(R)+p_+(R)\left(w(\lambda-i\gamma)-f(\lambda,R)\right)$$

is not 0 in the strip $\{z\in\mathbb{C}\,:\,0\le \mathrm{Im}(z)\le\gamma\}$. In order to do that, we will choose some periodic potentials on the real half-line, then build $G_+(\lambda)\equiv G_+(\lambda,0)$ for complex λ's and finally try to see if there can be zeros in the cases of study. In particular, we will show it by doing several "contour plots" of the function $|h|$, where

$$h(\lambda):=\frac{p_-'(0;\lambda)-w(\lambda)p_-(0;\lambda)}{p_-(0;\lambda)}-\frac{P_+'(0)+w(\lambda-i\gamma)P_+(0)}{P_+(0)}\ .$$

The code has been developed in Matlab (see Appendix A for details).

First, let us start with sin as background potential. Figure 3.1 shows a contour plot of the function $|h|$ around the strip

$$\{z\in\mathbb{C}\,:\,0\le\mathrm{Re}(z)\le 4,\ 0\le\mathrm{Im}(z)\le\gamma\}\ .$$

According to Figure 3.1, it seems that h never has null modulus in the strip. There are some (apparently) critical points on the lines $\{z\in\mathbb{C}\,:\,\mathrm{Im}(z)=0\}$ and $\{z\in\mathbb{C}\,:\,\mathrm{Im}(z)=\gamma\}$, but they are local maxima for the function $|h|$ (see Figure 3.2). The function h has been also computed over a given mesh with vertical and horizontal steps equal to 10^{-3} and it does not show significant changes of signs both in the real and in the imaginary part.

A similar experiment has been repeated choosing cos as background potential (see Figure 3.3). Again, there are some points close to the lines $\{z\in\mathbb{C}\,:\,\mathrm{Im}(z)=0\}$ and $\{z\in\mathbb{C}\,:\,\mathrm{Im}(z)=\gamma\}$, which are local maxima of the modulus of h.

According to these examples, we may formulate the following Conjecture, which has already been proven in the free background case.

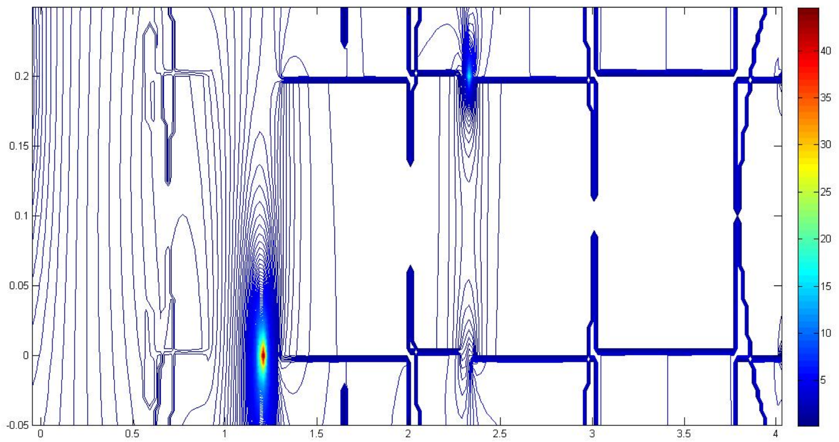

Figure 3.1: Contour plot of $|h|$ associated with sin for $\gamma = 0.2$

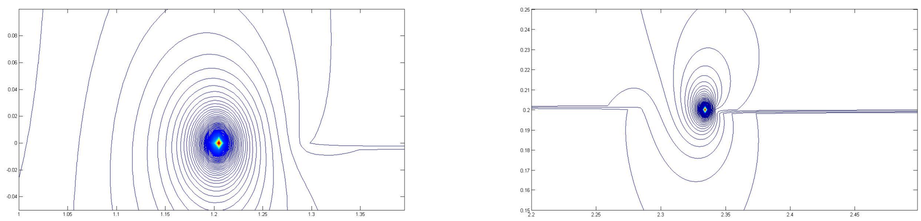

Figure 3.2: Zoom around the local maxima of $|h|$

Conjecture 3.1. *If λ is contained in the strip $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$, then*

$$G_+(\lambda, R) \neq 0 \ .$$

Equivalently

Conjecture 3.2. *The set D defined in Section 3.2 is empty.*

Conjectures 3.1 and 3.2 lead to Conjecture 3.3, which has a completely similar form to Theorem 2.1 for free background potentials.

Conjecture 3.3 (Spectrum of the perturbed periodic operator)**.** *For every compact set*

$$K \subset \{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$$

there exists $\bar{N} = \bar{N}_K$ such that for every $n \geq \bar{N}$ both the Neumann and the Dirichlet spectra of the operator $\mathrm{H}^{per}_{nL,\gamma}$ are such that

$$\sigma\left(\mathrm{H}^{per}_{nL,\gamma}\right) \cap K = \emptyset \ .$$

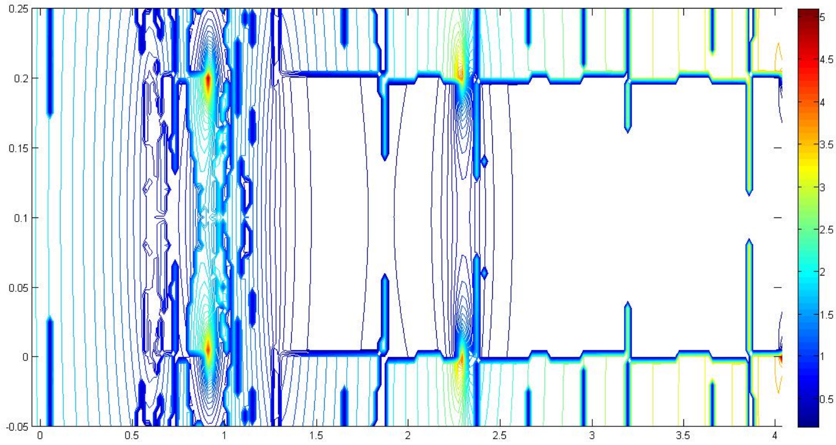

Figure 3.3: Contour plot of $|h|$ associated with cos for $\gamma = 0.2$

3.4 A characterization in terms of a $\mathcal{PT}$- symmetric Schrödinger operator on the real line

In this section, we are able to say something more about our problem and about Conjecture 3.1, under the additional assumption that the periodic potential q is defined on all $\mathbb{R}$ and it is an even function, i.e. extending q as follows:

$$q(-x) := q(x) \quad \forall\, x > 0 \ .$$

In this way, the condition

$$\frac{g'_-(0;\lambda)}{g_-(0;\lambda)} \neq \frac{g'_+(0;\lambda - i\gamma)}{g_+(0;\lambda - i\gamma)} \ , \tag{3.27}$$

which is equivalent to Conjecture 3.1 (see Section 3.2), brings to a new, equivalent:

Conjecture 3.4. *Let*

$$Q_\gamma(x) := \begin{cases} q(x) & , if \quad x > 0 \\ q(x) + i\gamma & , if \quad x < 0 \end{cases} .$$

The spectral problem

$$-u''(x) + Q_\gamma(x)\, u(x) = \lambda\, u(x) \tag{3.28}$$

on $\mathrm{L}^2(\mathbb{R})$ *has no eigenvalues in the strip* $\{z \in \mathbb{C} \,:\, 0 < \mathrm{Im}(z) < \gamma\}$.

Indeed, if (3.27) were false, this would mean that the function

$$U(x) = \begin{cases} g_-(x;\lambda) & \text{, if} \quad x \geq 0 \\ g_+(x;\lambda - i\gamma) & \text{, if} \quad x < 0 \end{cases}$$

is an eigenvector (in $\mathrm{L}^2(\mathbb{R})$) of (3.28) with eigenvalue λ, since the Jost functions

$$g_-(x;\lambda) = p_-(x;\lambda)e^{-w(\lambda)} \in \mathrm{L}^2([0,+\infty[) \ ,$$
$$g_+(x;\lambda - i\gamma) = p_+(x;\lambda - i\gamma)e^{+w(\lambda - i\gamma)} \in \mathrm{L}^2(]-\infty, 0])$$

"match" with (second order) derivability at $x = 0$

$$\frac{g'_-(0;\lambda)}{g_-(0;\lambda)} = \frac{g'_+(0;\lambda - i\gamma)}{g_+(0;\lambda - i\gamma)} \ . \tag{3.29}$$

We have thus proven the equivalence between conjectures 3.1 and 3.4, that is:

Theorem 3.6. *If q is a periodic even function with period L, the function $G_-(\cdot, 0)$, defined in (3.12), is never null if, and only if, problem (3.28) on the real line has no eigenvalues.*

Problem (3.28) has some interesting properties, which are typical in the context of $\mathcal{PT}$-symmetric operators[1].
First, one can show that the eigenvalues of the Schrödinger operator on $\mathrm{L}^2(\mathbb{R})$

$$\mathrm{H}^{per}_{Q_\gamma} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + Q_\gamma(x) \ ,$$

having domain $\mathcal{D}(\mathrm{H}^{per}_{Q_\gamma}) = \mathcal{D}(\mathrm{H}^{per})$, occur in complex pairs which are symmetric with respect to the line $\left\{z \in \mathbb{C} \,:\, \mathrm{Im}(z) = \frac{\gamma}{2}\right\}$.

Proposition 3.1. *If λ is an eigenvalue of the problem (3.28), so is $\tilde{\lambda} := \bar{\lambda} + i\gamma$.*

Proof. Let λ be eigenvalue of the problem (3.28) with eigenvector $u \in \mathrm{L}^2(\mathbb{R})$, i.e. u is such that

$$\begin{cases} -u''(x) + q(x)\,u(x) &= \lambda\, u(x) & \text{if} \quad x > 0 \\ -u''(x) + q(x)\,u(x) &= (\lambda - i\gamma)\, u(x) & \text{if} \quad x < 0 \end{cases} ;$$

[1]A $\mathcal{PT}$-symmetric operator is an operator which has the property of space-time reflection symmetry. For example a Schr̆odinger operator $\mathrm{H} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + Q(x)$ is $\mathcal{PT}$-symmetric if the potential is such that $Q(x) = \overline{Q(-x)}$.

clearly, u also satisfies

$$\begin{cases} -\bar{u}''(x) + q(x)\,\bar{u}(x) &= \bar{\lambda}\,\bar{u}(x) \qquad \text{if} \quad x > 0 \\ -\bar{u}''(x) + q(x)\,\bar{u}(x) &= (\bar{\lambda} + i\gamma)\,\bar{u}(x) \qquad \text{if} \quad x < 0 \end{cases} .$$

Call $v(x) := \bar{u}(-x)$; then v belongs to $\mathrm{L}^2(\mathbb{R})$ and is such that

$$\begin{cases} -v''(-x) + q(x)\,v(-x) &= (\tilde{\lambda} - i\gamma)\,v(-x) \qquad \text{if} \quad x > 0 \\ -v''(-x) + q(x)\,v(-x) &= \tilde{\lambda}\,v(-x) \qquad \text{if} \quad x < 0 \end{cases} .$$

Since q is an even function, v satisfies

$$\begin{cases} -v''(x) + q(x)\,v(x) &= \tilde{\lambda}\,v(x) \qquad \text{if} \quad x > 0 \\ -v''(x) + q(x)\,v(x) &= (\tilde{\lambda} - i\gamma)\,v(x) \qquad \text{if} \quad x < 0 \end{cases}$$

i.e. v is an eigenvector for problem (3.28) associated with the eigenvalue $\tilde{\lambda}$. □

Remark 3.4.1. If we consider a shift of λ, such that the new spectral parameter is $z := \lambda - i\frac{\gamma}{2}$ and $\tilde{\lambda}$ becomes $\tilde{\lambda} - i\frac{\gamma}{2} = \bar{\lambda} + i\frac{\gamma}{2} = \bar{z}$, equation (3.28) can be rewritten as

$$-u''(x) + \tilde{Q}_\gamma(x)\,u(x) = z\,u(x) \ ,$$

where $\tilde{Q}_\gamma(x) := Q_\gamma(x) - i\frac{\gamma}{2}$. For every $x \in \mathbb{R}$, $\tilde{Q}_\gamma$ is such that

$$\tilde{Q}_\gamma(-x) = \overline{\tilde{Q}_\gamma(x)} \ ; \tag{3.30}$$

so, according to (refeq:ptsympot) the Schrödinger operator

$$\mathrm{H}^{per}_{\tilde{Q}_\gamma} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \tilde{Q}_\gamma(x)$$

is in the class of $\mathcal{PT}$-symmetric operators. Note that its eigenvalues occur in complex conjugate pairs.

Now, note that, according to the assumption on q, the spectral equation on $\mathrm{L}^2(\mathbb{R})$

$$-u''(x) + q(x)\,u(x) = \mu\,u(x)$$

is symmetric with respect to the real axis, therefore it is enough to consider it on $\mathrm{L}^2([0, +\infty[)$; also, we have that $g_-(x;\mu) = g_+(-x;\mu)$, in particular for $\mu = \lambda$ and $\mu = \lambda - i\gamma$. Then the matching condition (3.29) becomes

$$\frac{g_-'(0;\lambda)}{g_-(0;\lambda)} = -\frac{g_-'(0;\lambda - i\gamma)}{g_-(0;\lambda - i\gamma)} \ .$$

Define for $z \in \mathbb{C}$

$$m(\mu) = \frac{g'_-(0;\mu)}{g_-(0;\mu)} \ ;$$

it can be seen as the multiplicative coefficient of a Dirichlet-to-Neumann Titchmarsh-Weyl function (see Section 1.4). Equation (3.29) is then equivalent to

$$m(\lambda) = -m(\lambda - i\gamma) \ . \tag{3.31}$$

We have seen that solutions of (3.31), if they exist, occur in complex pairs.

So far, in our analysis, the non-negative parameter γ has been kept fixed; now we will show that, moving γ so that it is sufficiently small, the relation (3.31) may not be valid under some limiting hypotheses.

Suppose that, for sufficiently small γ, equation (3.31) has a pair of solutions λ_γ and $\tilde{\lambda}_\gamma = \bar{\lambda}_\gamma + i\gamma$. Suppose also that there exists λ_0 such that

$$\lim_{\gamma \downarrow 0} \lambda_\gamma = \lambda_0 \ ,$$

i.e. for every ε there exists $\delta > 0$ such that $|\gamma| < \delta$ implies that $|\lambda_\gamma - \lambda_0| < \varepsilon$. The same has to hold for $\tilde{\lambda}$: $\tilde{\lambda}_\gamma \longrightarrow \bar{\lambda}_0$.
Suppose that λ_0 is not in the essential spectrum; in particular it has to belong to $\mathbb{R} \setminus \sigma_{ess}(\mathrm{H}^{per})$, i.e. $\lambda_0 = \bar{\lambda}_0$. This implies that

$$\mathrm{dist}(\lambda_\gamma, \tilde{\lambda}_\gamma) = 2\left|\mathrm{Im}(\lambda_\gamma) - \frac{\gamma}{2}\right|$$

tends to 0 as $\gamma \downarrow 0$.
Consider a regular open subset of the strip $\{z \in \mathbb{C} : 0 < \mathrm{Im}(z) < \gamma\}$, containing λ_γ and $\tilde{\lambda}_\gamma$: for example, a ball centered at $c := \mathrm{Re}(\lambda_\gamma) + i\frac{\gamma}{2}$ with radius $\rho := \left|\mathrm{Im}(\lambda_\gamma) - \frac{\gamma}{2}\right| + a\gamma$, where a is a constant chosen to ensure that the ball is strictly contained in the strip for every γ. Let us now define the closed curve

$$\Gamma_\gamma := \partial B(c, \rho) \ ,$$

oriented counter-clockwisely. Note that as γ tends to 0, Γ_γ shrinks to $\Gamma_0 = \{\lambda_0\}$.
Let

$$h(\lambda) = m(\lambda) + m(\lambda - i\gamma) \ .$$

Since $h(\cdot)$ is an analytic function having two zeros λ_γ and $\tilde{\lambda}_\gamma$ inside Γ_γ, by the argument principle it is known that

$$\frac{1}{2\pi i}\oint_{\Gamma_\gamma} \frac{h'(z)}{h(z)}\,\mathrm{d}z = 2 \ .$$

By dominated convergence

$$\frac{1}{2\pi i}\oint_{\Gamma_\gamma}\frac{h'(z)}{h(z)}\,\mathrm{d}z \xrightarrow{\gamma\downarrow 0} \oint_{\{\lambda_0\}}\frac{h'(z)}{h(z)}\,\mathrm{d}z = 0 \ ,$$

which leads to a contradiction. We have thus proved:

Proposition 3.2. *For small γ's, equation (3.31)*

$$m(\lambda) = -m(\lambda - i\gamma)$$

has no zeros with real part $\mathrm{Re}(\lambda) \notin \sigma_{ess}(\mathrm{H}^{per})$.

So, we have seen that if the projection of λ on the real axis (call it $\pi(\lambda)$) lies in the spectral gaps of the periodic background operator

$$m(\lambda) = -m(\lambda - i\gamma)$$

cannot be true for small γ's. Also, this holds if $\pi(\lambda)$ is in the interior of the spectral bands (which are closed intervals, see Theorem 3.4), as shown by the following:

Proposition 3.3. *Let $\lambda \in \mathbb{C}$ such that $\pi(\lambda) \in \mathrm{int}(\sigma_{ess}(\mathrm{H}^{per}))$. Then, for sufficiently small γ*

$$m(\lambda) \neq -m(\lambda - i\gamma) \ .$$

Proof. Suppose that there exists λ_γ such that

$$m(\lambda_\gamma) = -m(\lambda_\gamma - i\gamma) \ .$$

Then also $\tilde{\lambda}_\gamma$ is a solution of the equation. By hypothesis, the real point $\mathrm{Re}(\lambda_\gamma) = \mathrm{Re}(\tilde{\lambda}_\gamma)$ belongs to the essential spectrum of H^{per}, in particular to one of the (infinitely many) spectral bands. Call l the width of this spectral band.

Denote by $B^+(c;\rho)$ the upper half of the ball $B(c,\rho)$ in the complex plane, having center at

$$c := \left(\mathrm{Re}(\lambda_\gamma) + \frac{i\gamma}{2}\right) + \frac{i}{100}\left|\mathrm{Im}(\lambda_\gamma) - \frac{\gamma}{2}\right|$$

and radius

$$\rho := \inf\left(\left|\mathrm{Im}(\lambda_\gamma) - \frac{\gamma}{2}\right| + \gamma,\, l\right) \ ,$$

where a is chosen in order to guarantee that $B^+(c;\rho)$ is a strict subset of $\left\{z \in \mathbb{C} \,:\, \frac{\gamma}{2} < \mathrm{Im}(z) < \gamma\right\}$. Consider the following closed path surrounding λ_γ:

$$\Gamma_\gamma := \partial B^+(c;\rho) \cup \{z \in \mathbb{C} \,:\, |\mathrm{Re}(z-c)| \leq \rho \text{ and } \mathrm{Im}(z) = \mathrm{Im}(c)\} \ .$$

Similarly for $\tilde{\lambda}_\gamma$, define

$$\tilde{\Gamma}_\gamma := \partial B^-(\tilde{c};\rho) \cup \{z \in \mathbb{C} \,:\, |\mathrm{Re}(z-\tilde{c})| \leq \rho \text{ and } \mathrm{Im}(z) = \mathrm{Im}(\tilde{c})\} \ ,$$

where

$$\tilde{c} = \left(\mathrm{Re}(\lambda_\gamma) + \frac{i\gamma}{2}\right) - \frac{i}{100}\left|\mathrm{Im}(\lambda_\gamma) - \frac{\gamma}{2}\right| \ .$$

As γ tends to 0, both Γ_γ and $\tilde{\Gamma}_\gamma$ shrink to $\pi(\lambda_\gamma)$.
Again, by Cauchy's formula

$$\frac{1}{2\pi i}\oint_{\Gamma_\gamma} \frac{h'(z)}{h(z)}\,\mathrm{d}z = 1$$

and

$$\frac{1}{2\pi i}\oint_{\tilde{\Gamma}_\gamma} \frac{h'(z)}{h(z)}\,\mathrm{d}z = 1$$

But this is a contradiction, because both the integrals above converge to zero as $\gamma \downarrow 0$. $\square$

Appendix A

Codes

In this section we would like to present the MATLAB codes which have been written for the purposes of Section 3.3. The aim was to construct the function $G_+(\lambda, 0)$ defined in Chapter 3 for some given periodic potentials and see if it could be null somewhere in the strip. We conject that it is never 0.

First of all, the following function called 'monodromy' computes the monodromy matrix associated with a potential q:

```
function M=monodromy(lambda,q)

  phi_0=1; Dphi_0=0;       % initial values phi
  psi_0=0; Dpsi_0=1;       % initial values psi
  per=2*pi;                % chosen period
  time_span=[0,2*per];     % time interval for the solution

   function  xp= A(x,Y)     % 1-dim vector field
     xp=zeros(2,1);
     xp(1)=Y(2);
     xp(2)=(q(x)-lambda)*Y(1);
   end;

  sol=ode45(@A,time_span,[phi_0,Dphi_0]);
  Phi=deval(sol,per);

  sol=ode45(@A,time_span,[psi_0,Dpsi_0]);
  Psi=deval(sol, per);

  M=[Phi Psi];
```

```
end;
```

The function 'eigenratioM' produces the value of the ratio

$$\frac{g'_-(0;z)}{g_-(0;z)}$$

for $x \in \mathbb{C}$.

```
function r=eigenratioM(z,q)

  [V D]=eig(monodromy(z,q));
  a=D(1,1);

  if real(a)<0
     r=V(2,1)/V(1,1);
  else
     r=V(2,2)/V(1,2);
  end;

end;
```

Similarly, the ratio

$$\frac{g'_+(0;z)}{g_+(0;z)}$$

can be computed as follows by 'eigenratioP'.

```
function r=eigenratioP(z,q)

  [V D]=eig(monodromy(z,q));
  a=D(1,1);

  if real(a)>0
    r=V(2,1)/V(1,1);
  else
    r=V(2,2)/V(1,2);
  end;

end;
```

Then, let us define, for $\lambda \in \mathbb{C}$

$$h(\lambda) := \frac{g'_-(0;\lambda)}{g_-(0;\lambda)} - \frac{g'_+(0;\lambda - i\gamma)}{g_+(0;\lambda - i\gamma)} \ .$$

```
function x=h(lambda,q,gamma)

  x=eigenratioM(lambda,q)-eigenratioP(lambda-gamma*i,q);

end;
```

That $G_+(\lambda, 0) = 0$ is equivalent to $h(\lambda) = 0$. In order to prove or disprove it, in Section 3.3 we made a contour plot of the absolute value of the function h. Actually, the function 'graphcont' written here below does this job: it returns a matrix of values of the function h in a given rectangular domain and plots the "contour" of the absolute value $|h|$.

```
function L=graphcont(q,gamma,xmin,xmax,ymin,ymax,stx,sty)

nx=floor(1+(xmax-xmin)/stx);
ny=floor(1+(ymax-ymin)/sty);
x=(0:nx-1)*stx+xmin;
y=(0:ny-1)*sty+ymin;
L=zeros(ny,nx);

for h=1:ny
    for k=1:nx
       param=xmin+(k-1)*stx+i*(ymin+(h-1)*sty);
       L(h,k)=h( param, q, gamma );
    end;
end;

contour(x,y,abs(L));
end;
```

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Padua, 1 October 2011 *Gianluigi Potente*