# Scattering Theory

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# Chapter 1

# Introduction

According to Reed and Simon [9], scattering theory is the study of an interacting system on a time and/or distance scale which is large compared to the scale of the actual interaction. This is a natural phenomenon occuring in several branches of physics; optics (think of the blue sky), acoustics, x-ray, sonar, particle physics,.... In this course we focus on the mathematical aspects of scattering theory, and on an important application in non-linear partial differential equations.

## 1.1 Scattering theory

As an example motivating the first chapters we consider the following situation occuring in quantum mechanics. Consider a particle of mass $m$ moving in three-dimensional space $\mathbb{R}^3$ according to a potential $V(\mathbf{x}, t)$, $\mathbf{x} \in \mathbb{R}^3$ the spatial coordinate and time $t \in \mathbb{R}$. In quantum mechanics this is modelled by a wave function $\psi(\mathbf{x}, t)$ satisfying $\int_{\mathbb{R}^3} |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} = 1$ for all time $t$, and the wave function is interpreted as a probability distribution for each time $t$. This means that for each time $t$, the probability that the particle is in the set $A \subset \mathbb{R}^3$ is given by $\int_A |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x}$. Similarly, the probability distribution of the momentum for this particle is given by $|\hat{\psi}(\mathbf{p}, t)|^2$, where

$$\hat{\psi}(\mathbf{p}, t) = \frac{1}{\left(\sqrt{2\pi}\right)^3} \int_{\mathbb{R}^3} e^{-i\mathbf{p}\cdot\mathbf{x}} \psi(\mathbf{x}, t) \, d\mathbf{x}$$

is the Fourier transform of the wave function with respect to spatial variable $\mathbf{x}$. (Here we have scaled Planck's constant $\hbar$ to 1.) Using the fact that the Fourier transform interchanges differentiation and multiplication the expected value for the momentum can be expressed in terms of a differential operator. The kinetic energy, corresponding to $|\mathbf{p}|^2/2m$, at time $t$ of the particle can be expressed as $\frac{-1}{2m}\langle \Delta\psi, \psi \rangle$, where we take the inner product corresponding to the Hilbert space $L^2(\mathbb{R}^3)$ and $\Delta$ is the three-dimensional Laplacian (i.e. with respect to the spatial coordinate $\mathbf{x}$).

The potential energy at time $t$ of the particle is described by $\langle V\psi, \psi\rangle$, so that (total) energy of the particle at time $t$ can be written as

$$E = \langle H\psi, \psi\rangle, \qquad H = \frac{-1}{2m}\Delta + V,$$

where we have suppressed the time-dependence. The operator $H$ is known as the energy operator, or as Hamiltonian, or as Schrödinger operator. In case the potential $V$ is independent of time and suitably localised in the spatial coordinate, we can view $H$ as a perturbation of the corresponding free operator $H_0 = \frac{-1}{2m}\Delta$. This can be interpreted that we have a 'free' particle scattered by the (time-independent) potential $V$. The free operator $H_0$ is a well-known operator, and we can ask how its properties transfer to the perturbed operator $H$. Of course, this will depend on the conditions imposed on the potential $V$. In Chapter 2 we study this situation in greater detail for the case the spatial dimension is 1, but the general perturbation techniques apply in more general situations as well. In general the potentials for which these results apply are called short-range potentials.

In quantum mechanics the time evolution of the wave function is determined by the time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(\mathbf{x}, t) \; = \; H\psi(\mathbf{x}, t). \tag{1.1.1}$$

We want to consider solutions that behave as solutions to the corresponding free time-dependent Schrödinger equation, i.e. (1.1.1) with $H$ replaced by $H_0$, for time to $\infty$ or $-\infty$. In case of the spatial dimension being 1 and for a time-independent potential $V$, we study this situation more closely in Chapter 3. We do this for more general (possibly unbounded) self-adjoint operators acting a Hilbert space.

Let us assume that $m = \frac{1}{2}$, then we can write the solution to the free time-dependent Schrödinger equation as

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} F(\mathbf{p})\, e^{i\mathbf{p}\cdot\mathbf{x}} e^{-i|\mathbf{p}|^2 t}\, d\mathbf{p},$$

where $F(\mathbf{p})$ denotes the distribution of the momenta at time $t = 0$ (up to a constant). This follows easily since the exponentials $e^{i\mathbf{p}\cdot\mathbf{x}}$ are eigenfunctions of $H_0 = -\Delta$ for the eigenvalue $|\mathbf{p}|^2$. For the general case the solution is given by

$$\psi(\mathbf{x}, t) = \int_{\mathbb{R}^3} F(\mathbf{p})\, \psi_{\mathbf{p}}(\mathbf{x})\, e^{-i|\mathbf{p}|^2 t}\, d\mathbf{p},$$

where $H\psi_{\mathbf{p}} = |\mathbf{p}|^2\, \psi_{\mathbf{p}}$ and where we can expect $\psi_{\mathbf{p}}(\mathbf{x}) \sim e^{i\mathbf{p}\cdot\mathbf{x}}$ if the potential $V$ is sufficiently 'nice'. We study this situation more closely in Chapter 4 in case the spatial dimension is one.

## 1.2 Inverse scattering method

As indicated in Section 4.2 we give an explicit relation between the potential $q$ in the Schrödinger operator $-\frac{d^2}{dx^2} + q$ and its scattering data consisting of the reflection and transition coefficient $R$ and $T$. To be specific, in Section 4.2 we discuss the transition $q \mapsto \{R, T\}$, which is called the direct problem, and in Section 4.4 we discuss the transition $\{R, T\} \mapsto q$, the inverse problem. In case we take a time-dependent potential $q(x, t)$, the scattering data also becomes time-dependent. It has been shown that certain non-linear partial differential equations (with respect to $t$ and $x$) for $q$ imply that the corresponding time evolution of the scattering data $R$ and $T$ is linear! Or, scattering can be used to linearise some non-linear partial differential equations.

The basic, and most famous, example is the Korteweg-de Vries equation, KdV-equation for short,

$$q_t(x,t) - 6\,q(x,t)\,q_x(x,t) + q_{xxx}(x,t) = 0,$$

which was introduced in 1894 in order to model the solitary waves encountered by James Scott Russell in 1834 while riding on horseback along the canal from Edinburgh to Glasgow. Although the Korteweg-de Vries paper "On the change of form of long waves advancing in a rectangular canal, and on a new type of long stationary waves", Philosophical Magazine, **39** (1895), 422–443, is now probably the most cited paper by Dutch mathematicians, the KdV-equation lay dormant for a long time until it was rediscovered by Kruskal and Zabusky in 1965 for the Fermi-Pasta-Ulam problem on finite heat conductivity in solids. Kruskal and Zabusky performed numerical experiments, and found numerical evidence for the solitary waves as observed by Scott Russell, which were named "solitons" by Kruskal and Zabusky. The fundamental discovery made by Gardner, Greene, Kruskal and Miura in 1967 is that if $q$ is a solution to the KdV-equation, then the spectrum of the Schrödinger with time-dependent potential $q$ is independent of time, and moreover, the time evolution for the scattering data, i.e. the reflection and transmission coefficient, is a simple linear differential equation. We discuss this method in Chapter 5. In particular, we discuss some of the soliton solutions.

This gave way to a solution method, nowadays called the inverse scattering method, or inverse spectral method, for classes of non-linear partial differential equations. Amongst others, similar methods work for well-known partial differential equations such as the modified KdV-equation $q_t - 6q^2 q_x + q_{xxx} = 0$, the sine-Gordon equation $q_{xt} = \sin q$, the non-linear Schrödinger equation $q_t = q_{xx} + |q|^2 q$, and many others. Nowadays, there are many families of partial differential equations that can be solved using similar ideas by realising them as conditions for isospectrality of certain linear problem. For the isospectrality we use the method of Lax pairs in Section 5.3.

There have been several approaches and extensions to the KdV-equations, notably as integrable systems with infinitely many conserved Poisson-commuting quantities. We refer to [1], [8].

## 1.3 Overview

The contents of these lecture notes are as follows. In Chapter 6 we collect some results from functional analysis, especially on unbounded self-adjoint operators and the spectral theorem, Fourier analysis, especially related to Sobolev and Hardy spaces. For these results not many proofs are given, since they occur in other courses. In Chapter 6 we also discuss some results on the spectrum and the essential spectrum, and for these results explicit proofs are given. So Chapter 6 is to be considered as an appendix.

In Chapter 2 we study first the Schrödinger operator $-\frac{d^2}{dx^2}+q$, and we give conditions on $q$ such that the Schrödinger operator is a unbounded self-adjoint operator with the Sobolev space as the domain which is also the domain for the unperturbed Schrödinger operator $-\frac{d^2}{dx^2}$. For this we use a classical result known as Rellich's perturbation theorem on perturbation of unbounded self-adjoint operators. We discuss the spectrum and the essential spectrum in this case. It should be noted that we introduce general results, and that the Schrödinger operator is merely an elaborate example.

In Chapter 3 the time-dependent Schrödinger operator is discussed. We introduce the notions of wave operators, scattering states and the scattering operator. Again this is a general procedure for two self-adjoint operators acting on a Hilbert space, and the Schrödinger operator is an important example.

In Chapter 4 the discussion is specific for the Schrödinger operator. We show how to determine the Jost solutions, and from this we discuss the reflection and transmission coefficient. The Gelfand-Levitan-Marchenko integral equation is derived, and the Gelfand-Levitan-Marchenko equation is the key step in the inverse scattering method.

In Chapter 5 we study the Korteweg-de Vries equation, and we discuss shortly the original approach of Gardner, Greene, Kruskal and Miura that triggered an enormous amount of research. We then discuss the approach by Lax, and we show how to construct the $N$-soliton solutions to the KdV-equation. We carry out the calculations for $N = 1$ and $N = 2$. This chapter is not completely rigorous.

The lecture notes end with a short list of references, and an index of important and/or useful notions which hopefully increases the readability. The main source of information for Chapter 2 is Schechter [10]. Schechter's book [10] is also relevant for Chapter 3, but for Chapter 3 also Reed and Simon [9] and Lax [7] have been used. For Chapter 4 several sources have been used; especially Eckhaus and van Harten [4], Reed and Simon [9] as well as an important original paper [3] by Deift and Trubowitz. For Chapter 5 there is an enormous amount of information available; introductory and readable texts are by Calogero and Degasperis [2], de Jager [6], as well as the original paper by Gardner, Greene, Kruskal and Miura [5] that has been so influential. As remarked before, Chapter 6 is to be considered as an appendix, and most of the results that are not proved can be found in general text books on functional analysis, such as Lax [7], Werner [11], or course notes for a course in Functional Analysis.

# Chapter 2

# Schrödinger operators and their spectrum

In Chapter 6 we recall certain terminology, notation and results that are being used in Chapter 2.

## 2.1 The operator $-\frac{d^2}{dx^2}$

**Theorem 2.1.1.** $-\frac{d^2}{dx^2}$ *with domain the Sobolev space* $W^2(\mathbb{R})$ *is a self-adjoint operator on* $L^2(\mathbb{R})$.

We occasionally denote $-\frac{d^2}{dx^2}$ by $L_0$, and then its domain by $D(L_0) = W^2(\mathbb{R})$. We first consider the operator $i\frac{d}{dx}$ on its domain $W^1(\mathbb{R})$.

**Lemma 2.1.2.** $i\frac{d}{dx}$ *with domain the Sobolev space* $W^1(\mathbb{R})$ *is self-adjoint.*

*Proof.* The Fourier transform, see Section 6.3, intertwines $i\frac{d}{dx}$ with the multiplication operator $M$ defined by $(Mf)(\lambda) = \lambda f(\lambda)$. The domain $W^1(\mathbb{R})$ under the Fourier transform is precisely $D(M) = \{f \in L^2(\mathbb{R}) \mid \lambda \mapsto \lambda f(\lambda) \in L^2(\mathbb{R})\}$, see Section 6.3. So $(i\frac{d}{dx}, W^1(\mathbb{R}))$ is unitarily equivalent to $(M, D(M))$.

Observe that $(M, D(M))$ is symmetric;

$$\langle Mf, g\rangle = \int_{\mathbb{R}} \lambda\, f(\lambda)\overline{g(\lambda)}\, d\lambda = \langle f, Mg\rangle, \qquad \forall f, g \in D(M).$$

Assume now $g \in D(M^*)$, or

$$D(M) \ni f \mapsto \langle Mf, g\rangle = \int_{\mathbb{R}} \lambda\, f(\lambda)\overline{g(\lambda)}\, d\lambda \in \mathbb{C}$$

is a continuous functional on $L^2(\mathbb{R})$. By taking complex conjugates, this implies the existence of a constant $C$ such that

$$\Big|\int_{\mathbb{R}} \lambda g(\lambda)\overline{f(\lambda)}\, d\lambda\Big| \leq C\|f\|, \qquad \forall f \in W^1(\mathbb{R}).$$

By the converse Hölder's inequality, it follows that $\lambda \mapsto \lambda g(\lambda)$ is square integrable, and $\|\lambda \mapsto \lambda g(\lambda)\| \leq C$. Hence, $D(M^*) \subset D(M)$, and since the reverse inclusion holds for any densely defined symmetric operator, we find $D(M) = D(M^*)$, and so $(M, D(M))$ is self-adjoint. This gives the result. □

Note that we actually have that the Fourier transform gives the spectral decomposition of $-i\frac{d}{dx}$. The functions $x \mapsto e^{i\lambda x}$ are eigenfunctions to $-i\frac{d}{dx}$ for the eigenvalue $\lambda$, and the Fourier transform of $f$ is just $\lambda \mapsto \langle f, e^{i\lambda\cdot}\rangle$, and the inverse Fourier transform states that $f$ is a continuous linear combination of the eigenvectors, $f = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \langle f, e^{i\lambda\cdot}\rangle e^{i\lambda\cdot}\, d\lambda$.

*Proof of Theorem 2.1.1.* Observe that by Lemma 2.1.2

$$(i\frac{d}{dx})^*(i\frac{d}{dx}) = -\frac{d^2}{dx^2}$$

as unbounded operators, since $\{f \in W^1(\mathbb{R}) \mid f' \in W^1(\mathbb{R})\} = W^2(\mathbb{R})$. Now the theorem follows from Lemma 6.2.4. □

**Theorem 2.1.3.** *$-\frac{d^2}{dx^2}$ with domain $W^2(\mathbb{R})$ has spectrum $\sigma = [0, \infty)$. There is no point spectrum.*

*Proof.* Let us first check for eigenfunctions, so we look for functions $-f'' = \lambda\, f$, or $f''+\lambda\, f = 0$. This equation is easily solved; $f$ is linear for $\lambda = 0$ and a combination of exponential functions $\exp(\pm x\sqrt{-\lambda})$ for $\lambda \neq 0$. There is no non-trivial combination that makes an eigenfunction square-integrable, hence $-\frac{d^2}{dx^2}$ has no eigenvalues.

By the proof of Theorem 2.1.1 and Lemma 6.2.4 it follows that the spectrum is contained in $[0, \infty)$. In order to show that the spectrum is $[0, \infty)$ we establish that any positive $\lambda$ is contained in the spectrum. Since the spectrum is closed, the result then follows.

So pick $\lambda > 0$ arbitrary. We use the description of Theorem 6.5.1, so we need to construct a sequence of functions, say $f_n \in W^2(\mathbb{R})$, of norm 1, such that $\| - f_n'' - \lambda\, f_n\| \to 0$. By the first paragraph $\psi(x) = \exp(i\gamma x)$, with $\gamma^2 = \lambda$, satisfies $\psi'' = \lambda\psi$, but this function is not in $L^2(\mathbb{R})$. The idea is to approximate this function in $L^2(\mathbb{R})$ using an approximation of the delta-function. The details are as follows. Put $\phi(x) = \sqrt[4]{2/\pi}\, \exp(-x^2)$, so that $\|\phi\| = 1$. Then define $\phi_n(x) = (\sqrt{n})^{-1}\phi(x/n)$ and define $f_n(x) = \phi_n(x)\exp(i\gamma x)$. Then $\|f_n\| = \|\phi_n\| = \|\phi\| = 1$, and since $f_n$ is infinitely differentiable and $f_n$ and all its derivatives tend to zero rapidly as $x \to \pm\infty$ (i.e. $f_n \in \mathcal{S}(\mathbb{R})$, the Schwartz space), it obviously is contained in the domain $W^2(\mathbb{R})$. Now

$$\begin{aligned} f_n'(x) &= \phi_n'(x)e^{i\gamma x} + i\gamma\phi_n(x)e^{i\gamma x} = \frac{1}{n\sqrt{n}}\phi'(\frac{x}{n})e^{i\gamma x} + i\gamma\phi_n(x)e^{i\gamma x} \\ f_n''(x) &= \frac{1}{n^2\sqrt{n}}\phi''(\frac{x}{n})e^{i\gamma x} + \frac{2i\gamma}{n\sqrt{n}}\phi'(\frac{x}{n})e^{i\gamma x} - \gamma^2\phi_n(x)e^{i\gamma x}, \end{aligned}$$

so that

$$\begin{aligned} \|f_n'' + \lambda f_n\| &\leq \frac{2|\gamma|}{n\sqrt{n}}\|\phi'(\frac{\cdot}{n})\| + \frac{1}{n^2\sqrt{n}}\|\phi''(\frac{\cdot}{n})\| \\ &= \frac{2|\gamma|}{n}\|\phi'\| + \frac{1}{n^2}\|\phi''\| \to 0, \qquad n \to \infty. \end{aligned}$$

So this sequence meets the requirements of Theorem 6.5.1, and we are done. □

Again we use the Fourier transform to describe the spectral decomposition of $-\frac{d^2}{dx^2}$. The functions $x \mapsto \cos(\lambda x)$ and $x \mapsto \sin(\lambda x)$ are the eigenfunctions of $-\frac{d^2}{dx^2}$ for the eigenvalue $\lambda^2 \in (0, \infty)$. Observe that the Fourier transform as in Section 6.3 preserves the space of even functions, and that for even functions we can write the transform pair as

$$\hat{f}(\lambda) = \frac{\sqrt{2}}{\sqrt{\pi}} \int_0^\infty f(x)\, \cos(\lambda x)\, dx, \qquad f(x) = \frac{\sqrt{2}}{\sqrt{\pi}} \int_0^\infty \hat{f}(\lambda)\, \cos(\lambda x)\, d\lambda,$$

which is known as the (Fourier-)cosine transform.

**Exercise 2.1.4.** Derive the (Fourier-)sine transform using odd functions. By splitting an arbitrary element $f \in L^2(\mathbb{R})$ into an odd and even part give the spectral decomposition of $-\frac{d^2}{dx^2}$.

**Exercise 2.1.5.** The purpose of this exercise is to describe the resolvent for $L_0 = -\frac{d^2}{dx^2}$. We obtain that for $z \in \mathbb{C}\backslash\mathbb{R}$, $z = \gamma^2$, $\Im\gamma > 0$, we get

$$(L_0 - z)^{-1} f(x) = \frac{-1}{2\gamma i} \int_{\mathbb{R}} e^{i\gamma|x-y|} f(y)\, dy$$

- Check that $u(x)$ defined by the right hand side satisfies $-u'' - zu = f$, for $f$ in a suitable dense subspace, e.g. $C_c^\infty(\mathbb{R})$. Show that $(L_0 - z)^{-1}$ extends to a bounded operator on $L^2(\mathbb{R})$ using Young's inequality for convolution products.

- Instead of checking the result for $f \in C_c^\infty(\mathbb{R})$, we derive it by factoring the second order differential operator $-u'' - \gamma^2 u = f$ into two first order differential equations;

$$(i\frac{d}{dx} + \gamma)u = v, \qquad (i\frac{d}{dx} - \gamma)v = f.$$

  – Show that the second first order differential equation is solved by

$$v(x) = -i \int^x e^{-i\gamma(x-y)} f(y)\, dy.$$

  Argue that requiring $v \in L^2(\mathbb{R})$ gives $v(x) = i \int_x^\infty e^{-i\gamma(x-y)} f(y)\, dy$. Show that $\|v\| \le \frac{1}{|\Im\gamma|}\|f\|$.

  – Treat the other first order differential equation in a similar way to obtain the expression $u(x) = -i \int_{-\infty}^x e^{i\gamma(x-y)} v(y)\, dy$.

  – Finally, express $u$ in terms of $f$ to find the explicit expression for the resolvent operator.

## 2.2 The Schrödinger operator $-\frac{d^2}{dx^2} + q$

Consider the multiplication operator

$$Q\colon L^2(\mathbb{R}) \supset D(Q) \to L^2(\mathbb{R}), \qquad Q\colon f \to qf \tag{2.2.1}$$

with domain $D(Q) = \{f \in L^2(\mathbb{R}) \mid qf \in L^2(\mathbb{R})\}$ for some fixed function $q$. We follow the convention that the multiplication operator by a function, denoted by a small $q$, is denoted by the corresponding capital $Q$. We always assume that $q$ is a real-valued function and that $(Q, D(Q))$ is densely defined, i.e. $D(Q)$ is dense in $L^2(\mathbb{R})$.

Recall that we call a function $q$ locally square integrable if $\int_B |q(x)|^2\,dx < \infty$ for each bounded measurable subset $B$ of $\mathbb{R}$. So we see that in this case any function in $C_c^\infty(\mathbb{R})$, the space of infinitely many times differentiable functions having compact support, is in the domain $D(Q)$ of the corresponding multiplication operator $Q$. Since $C_c^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, we see that for such a potential $q$ the domain $D(Q)$ is dense.

We are only interested in so-called short range potentials. Loosely speaking, the potential only affects waves in a short range. Mathematically, we want the potential $q$ to have sufficient decay.

**Lemma 2.2.1.** *$(Q, D(Q))$ is a self-adjoint operator.*

**Exercise 2.2.2.** Prove Lemma 2.2.1. Hint: use the converse Hölder's inequality, cf. proof of Lemma 2.1.2.

**Exercise 2.2.3.**
1. Which conditions on the potential $q$ ensure that $Q\colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is actually a bounded operator?
2. Determine the spectrum of $Q$ in this case.

We study the Schrödinger[1] operator $-\frac{d^2}{dx^2} + q$ which has domain $W^2(\mathbb{R}) \cap D(Q)$. In this setting we call $q$ the potential of the Schrödinger operator. The first question to be dealt with is whether or not $-\frac{d^2}{dx^2} + q$ with this domain is self-adjoint or not. For this we use a 1939 perturbation Theorem 2.2.4 by Rellich[2], and then we give precise conditions on the potential function $q$ such that the conditions of Rellich's Perturbation Theorem 2.2.4 in this case are met.

**Theorem 2.2.4** (Rellich's Perturbation Theorem)**.** *Let $\mathcal{H}$ be a Hilbert space. Assume $T\colon \mathcal{H} \supset D(T) \to \mathcal{H}$ is a self-adjoint operator and $S\colon \mathcal{H} \supset D(S) \to \mathcal{H}$ is a symmetric operator, such that $D(T) \subset D(S)$ and $\exists\, a < 1,\, b \in \mathbb{R}$*

$$\|Sx\| \leq a\,\|Tx\| + b\,\|x\|, \qquad \forall\, x \in D(T),$$

*then $(T + S, D(T))$ is a self-adjoint operator.*

[1]Erwin Rudolf Josef Alexander Schrödinger, (12 August 1887 — 4 January 1961) Austrian physicist, who played an important role in the development of quantum mechanics, and is renowned for the cat in the box.

[2]Franz Rellich (14 September 1906 — 25 September 1955) German mathematician, who made contributions to mathematical physics and perturbation theory.

The infimum over all possible $a$ is called the $T$-bound of $S$.

Note that in case $S$ is a bounded self-adjoint operator, the statement is also valid. In this case the estimate is valid with $a = 0$ and $b = \|S\|$.

*Proof.* Note that $(T + S, D(T))$ is obviously a symmetric operator. Since $T$ is self-adjoint, $\mathrm{Ran}(T - z) = \mathcal{H}$ by Lemma 6.2.2 for all $z \in \mathbb{C}\backslash\mathbb{R}$ and $R(z;T) = (T - z)^{-1} \in B(\mathcal{H})$. In particular, take $z = i\lambda$, $\lambda \in \mathbb{R}\backslash\{0\}$, then, since $\langle Tx, x\rangle \in \mathbb{R}$,

$$\begin{aligned} \|(T - i\lambda)x\|^2 &= \|Tx\|^2 + 2\Re(i\lambda\langle Tx, x\rangle) + \lambda^2 \|x\|^2 \\ &= \|Tx\|^2 + \lambda^2 \|x\|^2, \qquad \forall x \in D(T). \end{aligned}$$

For $y \in \mathcal{H}$ arbitrary, pick $x \in D(T)$ such that $(T - i\lambda)x = y$, so that we get $\|y\|^2 = \|T(T - i\lambda)^{-1}y\|^2 + \lambda^2\|(T - i\lambda)^{-1}y\|^2$. This implies the basic estimates

$$\|y\| \geq \|T(T - i\lambda)^{-1}y\|, \qquad \|y\| \geq |\lambda| \, \|(T - i\lambda)^{-1}y\|.$$

Now $(T - i\lambda)^{-1}y = x \in D(T) \subset D(S)$ and

$$\begin{aligned} \|S(T - i\lambda)^{-1}y\| &\leq a\|T(T - i\lambda)^{-1}y\| + b\|(T - i\lambda)^{-1}y\| \\ &\leq a \,\|y\| + \frac{b}{|\lambda|} \,\|y\| = (a + \frac{b}{|\lambda|}) \,\|y\|, \end{aligned}$$

and, since $a + b/|\lambda| < 1$ for $|\lambda|$ sufficiently large, it follows that $\|S(T - i\lambda)^{-1}\| < 1$. In particular, $1 + S(T - i\lambda)^{-1}$ is invertible in $B(\mathcal{H})$, see Section 6.2. Now

$$(S + T) - i\lambda = (T - i\lambda) + S = \big(1 + S(T - i\lambda)^{-1}\big)(T - i\lambda),$$

(where the equality also involves the domains!) and we want to conclude that $\mathrm{Ran}(S + T - i\lambda) = \mathcal{H}$. So pick $x \in \mathcal{H}$ arbitrary, we need to show that there exists $y \in \mathcal{H}$ such that $\big((S + T) - i\lambda\big)y = x$, and this can be rephrased as $(T - i\lambda)y = \big(1 + S(T - i\lambda)^{-1}\big)^{-1}x$ by the invertibility for $|\lambda|$ sufficiently large. Since $\mathrm{Ran}(T - i\lambda) = \mathcal{H}$ such an element $y \in \mathcal{H}$ does exist.

Finally, since $S + T$ with dense domain $D(T)$ is symmetric, it follows by Lemma 6.2.2 that it is self-adjoint. □

The next exercise considers what happens if $a = 1$.

**Exercise 2.2.5.** Prove Wüst's theorem, which states the following. Assume $T\colon \mathcal{H} \supset D(T) \to \mathcal{H}$ is a self-adjoint operator and $S\colon \mathcal{H} \supset D(S) \to \mathcal{H}$ is a symmetric operator, such that $D(T) \subset D(S)$ and there exists $b \in \mathbb{R}$ such that

$$\|Sx\| \leq \|Tx\| + b\,\|x\|, \qquad \forall\, x \in D(T),$$

then $(T + S, D(T))$ is an essentially self-adjoint operator.

Proceed by showing that $\mathrm{Ker}((T + S)^* \pm i)$ is trivial using Lemma 6.2.2.

1. Show that we can use Rellich's Perturbation Theorem 2.2.4 to see that $T+tS$, $0<t<1$, is self-adjoint.
2. Take $x \in \mathrm{Ker}((T+S)^*-i)$, and show there exists $y_t \in D(T)$ such that $\|y_t\| \leq \|x\|$ and $(T+tS+i)y_t = x$. (Use Lemma 6.2.2.)
3. Define $z_t = x + (1-t)Sy_t$. Show that $\langle x, z_t\rangle = 0$.
4. Show that $(1-t)\|Ty_t\| \leq \|(T+tS)y_t\| + tb\|y_t\|$ and conclude that $(1-t)\|Ty_t\|$ is bounded as $t \nearrow 1$. Conclude next that $(1-t)\|Sy_t\|$ is bounded as $t \nearrow 1$, and hence $\|z_t\|$ is bounded.
5. Show that $x$ is the weak limit of $z_t$ as $t \nearrow 1$, and conclude that $\|x\| = 0$. (Hint consider $\langle z_t - x, u\rangle$ for $u \in D(T)$.)
6. Conclude that $(T+S, D(T))$ is an essentially self-adjoint operator.
7. Give an example to show that in general $(T+S, D(T))$ is not a self-adjoint operator.

We next apply Rellich's Perturbation Theorem 2.2.4 to the case $T$ equal $-\frac{d^2}{dx^2}$ and $S$ equal to $Q$. For this we need to rephrase the condition of Rellich's Theorem 2.2.4, see Theorem 2.2.6(5), into conditions on the potential $q$.

**Theorem 2.2.6.** *The following statements are equivalent:*

1. $W^2(\mathbb{R}) \subset D(Q)$,
2. $\exists\, C>0\ \|qf\|^2 \leq C\left(\|f''\|^2 + \|f\|^2\right),\ \forall\, f \in W^2(\mathbb{R})$,
3. $\displaystyle\sup_{y\in\mathbb{R}} \int_y^{y+1} |q(x)|^2\,dx < \infty$,
4. $\forall \varepsilon > 0\ \exists K > 0$ *with* $\|qf\|^2 \leq \varepsilon\,\|f''\|^2 + K\,\|f\|^2$, $\forall f \in W^2(\mathbb{R})$,
5. $\forall \varepsilon > 0\ \exists K > 0$ *with* $\|qf\| \leq \varepsilon\,\|f''\| + K\,\|f\|$, $\forall f \in W^2(\mathbb{R})$.

So the $-\frac{d^2}{dx^2}$-bound of $Q$ is zero.

**Corollary 2.2.7.** *If the potential $q$ satisfies Theorem 2.2.6(3), then the Schrödinger operator $-\frac{d^2}{dx^2} + q$ is self-adjoint on its domain $W^2(\mathbb{R})$. In particular, this is true for $q \in L^2(\mathbb{R})$.*

*Proof of Theorem 2.2.6.* (1) $\Rightarrow$ (2): Equip $W^2(\mathbb{R})$ with the graph norm of $L = -\frac{d^2}{dx^2}$, denoted by $\|\cdot\|_L$, see Section 6.2, which in particular means that $W^2(\mathbb{R})$ with this norm is complete. We claim that $Q\colon (W^2(\mathbb{R}), \|\cdot\|_L) \to L^2(\mathbb{R})$ is a closed operator, then the Closed Graph Theorem 6.2.1 implies that it is bounded, which is precisely (2). To prove the closedness, we take a sequence $\{f_n\}_{n=1}^\infty$ such that $f_n \to f$ in $(W^2(\mathbb{R}), \|\cdot\|_L)$ and $qf_n \to g$ in $L^2(\mathbb{R})$. We have to show that $f \in D(Q)$ and $qf = g$. First, since $f_n \to f$ and $(W^2(\mathbb{R}), \|\cdot\|_L)$ is complete, we have $f \in W^2(\mathbb{R}) \subset D(Q)$ by assumption (1). This assumption and Lemma 2.2.1 also gives $\langle qf_n, h\rangle = \langle f_n, qh\rangle$ for all $h \in W^2(\mathbb{R})$. Taking limits, $\langle g, h\rangle = \langle f, qh\rangle = \langle qf, h\rangle$ since convergence in $(W^2(\mathbb{R}), \|\cdot\|_L)$ implies convergence in $L^2(\mathbb{R})$ by $\|\cdot\| \leq \|\cdot\|_L$. Since $W^2(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, we may conclude $g = Q(f)$.

(2) $\Rightarrow$ (3): Put $\phi(x) = e^{1-x^2}$, so in particular $\phi \in W^2(\mathbb{R})$ and $\phi(x) \geq 1$ for $x \in [0,1]$. Put $\phi_y(x) = \phi(x-y)$ for the translated function, then

$$\int_y^{y+1} |q(x)|^2\,dx \leq \int_{\mathbb{R}} |q(x)\phi_y(x)|^2\,dx \leq C\big(\|\phi_y''\|^2 + \|\phi_y\|^2\big) = C\big(\|\phi''\|^2 + \|\phi\|^2\big) < \infty$$

since the integral is translation invariant.

(3) $\Rightarrow$ (4): By Sobolev's imbedding Lemma 6.3.1 we have $W^2(\mathbb{R}) \subset C^1(\mathbb{R})$, so we can apply the following lemma.

**Lemma 2.2.8.** *Take $f \in C^1(\mathbb{R})$, then for each $\varepsilon > 0$ and all intervals $I = [y, y+1]$ we have*

$$|f(x)|^2 \leq \varepsilon \int_I |f'(t)|^2\,dt + (1 + \frac{1}{\varepsilon}) \int_I |f(t)|^2\,dt, \qquad x \in I.$$

Denote by $C$ the supremum in (3). For $f \in W^2(\mathbb{R}) \subset C^1(\mathbb{R})$, we multiply the expression in Lemma 2.2.8 by $|q(x)|^2$ and integrate over the interval $I$, which gives

$$\int_I |q(x)f(x)|^2\,dx \leq C\varepsilon \int_I |f'(t)|^2\,dt + C(1+\varepsilon^{-1}) \int_I |f(t)|^2\,dt.$$

Since $\mathbb{R} = \cup I$, we find by summing

$$\|qf\|^2 \leq C\varepsilon\,\|f'\|^2 + C(1+\varepsilon^{-1})\,\|f\|^2.$$

In order to get the second (weak) derivative into play, we use the Fourier transform, see Section 6.3. In particular,

$$\begin{aligned}\|f'\|^2 &= \int_{\mathbb{R}} \lambda^2 |(\mathcal{F}f)(\lambda)|^2\,d\lambda \leq \frac{1}{2}\int_{\mathbb{R}} \lambda^4 |(\mathcal{F}f)(\lambda)|^2\,d\lambda + \frac{1}{2}\int_{\mathbb{R}} |(\mathcal{F}f)(\lambda)|^2\,d\lambda \\ &= \frac{1}{2}\int_{\mathbb{R}} |f''(t)|^2\,dt + \frac{1}{2}\int_{\mathbb{R}} |f(t)|^2\,dt\end{aligned}$$

using $2|\lambda|^2 \leq |\lambda|^4 + 1$. Plugging this back in gives

$$\|qf\|^2 \leq \frac{1}{2}C\varepsilon\,\|f''\|^2 + C(1 + \frac{1}{2}\varepsilon + \varepsilon^{-1})\,\|f\|^2,$$

which is the required estimate after renaming the constants.

(4) $\Rightarrow$ (5): Use

$$\begin{aligned}\|qf\|^2 &\leq \varepsilon\,\|f''\|^2 + K\,\|f\|^2 \leq \varepsilon\,\|f''\|^2 + 2\sqrt{\varepsilon K}\,\|f''\|\|f\| + K\,\|f\|^2 \\ &= \big(\sqrt{\varepsilon}\|f''\| + \sqrt{K}\,\|f\|\big)^2,\end{aligned}$$

which gives the result after taking square roots and renaming the constants.

(5) $\Rightarrow$ (1): For $f \in W^2(\mathbb{R})$ the assumption implies $qf \in L^2(\mathbb{R})$, or $f \in D(Q)$. $\square$

It remains to prove Lemma 2.2.8, which is the following exercise.

**Exercise 2.2.9.** 1. Show that, by reducing to real and imaginary parts, we can restrict to the case that $f$ is a real-valued function in $C^1(\mathbb{R})$.

2. Using $\frac{d(f^2)}{dx}(x) = 2f(x)f'(x)$, and $2ab \leq \varepsilon a^2 + \varepsilon^{-1}b^2$, show that

$$f(x)^2 - f(s)^2 \leq \varepsilon \int_I |f'(t)|^2 \, dt + \frac{1}{\varepsilon} \int_I |f(t)|^2 \, dt$$

for $x, s \in I$.

3. Show that for a suitable choice of $s \in I$ Lemma 2.2.8 follows.

**Exercise 2.2.10.** Consider the differential operator

$$-\frac{d^2}{dx^2} - 2\frac{p'}{p}\frac{d}{dx} + q - \frac{p''}{p}$$

for some strictly positive $p \in C^2(\mathbb{R})$. Show that this differential operator for real-valued $q$ is symmetric for a suitable choice of domain on the Hilbert space $L^2(\mathbb{R}, p(x)^2\, dx)$. Establish that this operator is unitarily equivalent to the Schrödinger operator $-\frac{d^2}{dx^2} + q$ on $L^2(\mathbb{R})$.

We have gone through some trouble to establish a suitable criterion in Corollary 2.2.7 such that the Schrödinger operator is a self-adjoint operator. It may happen that the potential is such that the corresponding Schrödinger operator defined on $W^2(\mathbb{R}) \cap D(Q)$ is not self-adjoint but a symmetric densely defined operator, and then one has to look for self-adjoint extensions. It can also happen that the potential is so 'bad', that $W^2(\mathbb{R}) \cap D(Q)$ is not dense. We do not go into this subject.

## 2.3 The essential spectrum of Schrödinger operators

The notion of essential spectrum is recalled in Section 6.5. From Theorem 6.5.5 and Theorem 2.1.3 it follows that the essential spectrum of $-\frac{d^2}{dx^2}$ is equal to its spectrum $[0, \infty)$. In this section we give a condition on the potential $q$ that ensures that the essential spectrum of $-\frac{d^2}{dx^2} + q$ is $[0, \infty)$ as well. In this section we assume that $-\frac{d^2}{dx^2} + q$ is a self-adjoint operator with domain the Sobolev space $W^2(\mathbb{R})$, which is the case if Theorem 2.2.6(3) holds.

We start with the general notion of $T$-compact operator, and next discuss the influence of a perturbation of $T$ by a $T$-compact operator $S$ on the essential spectrum.

**Definition 2.3.1.** *Let $(T, D(T))$ be a closed operator on a Hilbert space $\mathcal{H}$. The operator $(S, D(S))$ on the Hilbert space is compact relative to $T$, or $T$-compact, if $D(T) \subset D(S)$ and for any sequence $\{x_n\}_{n=1}^\infty$ satisfying $\|x_n\| + \|Tx_n\| \leq C$ the sequence $\{Sx_n\}_{n=1}^\infty$ has a convergent subsequence.*

Note that Definition 2.3.1 can be rephrased equivalently as $S\colon (D(T), \|\cdot\|_T) \to \mathcal{H}$ being compact, where $(D(T), \|\cdot\|_T)$ is the Hilbert space equipped with the graph norm.

**Theorem 2.3.2.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and $(S, D(S))$ a closed symmetric $T$-compact operator. Then $(T + S, D(T))$ is a self-adjoint operator, and $\sigma_{ess}(T) = \sigma_{ess}(S + T)$.*

*Proof.* By Definition 2.3.1, $D(T) \subset D(S)$, so if we can check the condition in Rellich's Perturbation Theorem 2.2.4 we may conclude that $(T + S, D(T))$ is self-adjoint. We claim that for all $\varepsilon > 0$ there exists $K > 0$ such that

$$\|Sx\| \leq \varepsilon \,\|Tx\| + K\,\|x\|, \qquad \forall x \in D(T). \tag{2.3.1}$$

Then the first statement follows from Rellich's Theorem 2.2.4 by taking $\varepsilon < 1$.

To prove this claim we first prove a weaker claim, namely that there exists a constanst $C$ such that

$$\|Sx\| \leq C\,\big(\|Tx\| + \|x\|\big), \qquad \forall x \in D(T).$$

Indeed, if this estimate would not hold, we can find a sequence $\{x_n\}_{n=1}^\infty$ such that $\|Tx_n\| + \|x_n\| = 1$ and $\|Sx_n\| \to \infty$. But by $T$-compactness, $\{Sx_n\}_{n=1}^\infty$ has a convergent subsequence, say $Sx_{n_k} \to y$, so in particular $\|Sx_{n_k}\| \to \|y\|$ contradicting $\|Sx_n\| \to \infty$.

Now to prove the more refined claim (2.3.1) we argue by contradiction. So assume $\exists \varepsilon > 0$ such that we cannot find a $K$ such that (2.3.1) holds. So we can find a sequence $\{x_n\}_{n=1}^\infty$ in $D(T)$ such that $\|Sx_n\| > \varepsilon\|Tx_n\| + n\|x_n\|$. By changing $x_n$ to $x_n/(\|x_n\| + \|Tx_n\|)$ we can assume that this sequence satisfies $\|x_n\| + \|Tx_n\| = 1$. By the weaker estimate we have $\|Sx_n\| \leq C\big(\|Tx_n\| + \|x_n\|\big) \leq C$ and $C \geq \|Sx_n\| \geq \varepsilon\|Tx_n\| + n\|x_n\|$, so that $\|x_n\| \to 0$ and hence $\|Tx_n\| \to 1$ as $n \to \infty$. By $T$-compactness, the sequence $\{Sx_n\}_{n=1}^\infty$ has a convergent subsequence, which we also denote by $\{Sx_n\}_{n=1}^\infty$, say $Sx_n \to y$. Since we assume $(S, D(S))$ closed, we see that $x_n \to 0 \in D(S)$ and $y = S0 = 0$. On the other hand $\|y\| = \lim_{n\to\infty} \|Sx_n\| \geq \varepsilon \lim_{n\to\infty} \|Tx_n\| = \varepsilon > 0$. This gives the required contradiction.

In order to prove the equality of the essential spectrum, take $\lambda \in \sigma_{ess}(T)$, so we can take a sequence $\{x_n\}_{n=1}^\infty$ as in Theorem 6.5.4(3). Recall that this means that the sequence satisfies $\|x_n\| = 1$, $\langle x_n, y\rangle \to 0$ for all $y \in \mathcal{H}$ and $\|(T - \lambda)x_n\| \to 0$. We will show that $\lambda \in \sigma_{ess}(T + S)$.

In particular, $\|x_n\| + \|Tx_n\|$ is bounded, and by $T$-compactness it follows that $\{Sx_n\}_{n=1}^\infty$ has a convergent subsequence, say $Sx_{n_k} \to y$. We claim that $y = 0$. Indeed, for arbitrary $z \in D(T) \subset D(S)$ we have

$$\langle y, z\rangle = \lim_{k\to\infty} \langle Sx_{n_k}, z\rangle = \lim_{k\to\infty} \langle x_{n_k}, Sz\rangle = 0,$$

since $S$ is symmetric and using that $x_n \to 0$ weakly. By density of $D(T)$, we have $y = 0$. So $(S + T - \lambda)x_{n_k} \to 0$, and by Theorem 6.5.4(3) it follows that $\lambda \in \sigma_{ess}(S + T)$. Or $\sigma_{ess}(T) \subset \sigma_{ess}(S + T)$.

Conversely, we can use the above reasoning if we can show that $-S$ is $(T + S)$-compact, since then $\sigma_{ess}(S + T) \subset \sigma_{ess}(-S + T + S) = \sigma_{ess}(T)$. (Note that we already have shown that

$(T+S, D(T))$ is self-adjoint, and of course $-S$ is a closed symmetric operator.) It suffices to prove that $S$ is $(T+S)$-compact, since then $-S$ is also $(T+S)$-compact. We first observe that $S$ is $T$-compact implies the existence of a constant $C_0 > 0$ such that

$$\|x\| + \|Tx\| \leq C_0\big(\|x\| + \|(S+T)x\|\big). \tag{2.3.2}$$

Indeed, arguing by contradiction, if this is not true there exists a sequence $\{x_n\}_{n=1}^\infty$ such that $\|x_n\| + \|Tx_n\| = 1$ and $\|x_n\| + \|(S+T)x_n\| \to 0$, and by $T$-compactness of $S$ we have that there exists a convergent subsequence $\{Sx_{n_k}\}_{k=1}^\infty$ of $\{Sx_n\}_{n=1}^\infty$ converging to $x$. Then necessarily $Tx_{n_k} \to -x$ and $x_{n_k} \to 0$, and since $T$ is self-adjoint, hence closed, we have $x = 0$. This contradicts the assumption $\|x\| + \|Tx\| = 1$.

Now to prove that $S$ is $(T+S)$-compact, take a sequence $\{x_n\}_{n=1}^\infty$ satisfying $\|x_n\| + \|(T+S)x_n\| \leq C$, then by (2.3.2) we have $\|x_n\| + \|Tx_n\| \leq CC_0$, so by $T$-compactness the sequence $\{Sx_n\}_{n=1}^\infty$ has a convergent subsequence. Or $S$ is $(T+S)$-compact. □

**Exercise 2.3.3.** The purpose of this exercise is to combine Rellich's Perturbation Theorem 2.2.4 with Theorem 2.3.2 in order to derive the following statement: Let $(T, D(T))$ be a self-adjoint operator, and $S_1$, $S_2$ symmetric operators such that (i) $D(T) \subset D(S_1)$, (ii) $S_2$ is a closed $T$-compact operator, (iii) $\exists a < 1$, $b \geq 0$ such that $\|S_1 x\| \leq a\|Tx\| + b\|x\|$ for all $x \in D(T)$. Then $S_2$ is $(T+S_1)$-compact and $\sigma_{ess}(T+S_1+S_2) = \sigma_{ess}(T+S_1)$.

Prove this result using the following steps.

- Show $\|Tx\| \leq \|(T+S_1)x\| + a\|Tx\| + b\|x\|$ and conclude $(1-a)\|Tx\| \leq \|(T+S_1)x\| + b\|x\|$.
- Show that $S_2$ is $(T+S_1)$-compact.
- Conclude, using Theorem 2.3.2, that $\sigma_{ess}(T+S_1+S_2) = \sigma_{ess}(T+S_1)$.

We want to apply Theorem 2.3.2 to the Schrödinger operator $-\frac{d^2}{dx^2} + q$. Recall that we call a function $q$ locally square integrable if $\int_B |q(x)|^2\,dx < \infty$ for each bounded measurable subset $B$ of $\mathbb{R}$. Note that in particular any square integrable function, which we consider as an element of $L^2(\mathbb{R})$, is locally square integrable. The function $q(x) = 1$ is an example of a locally square integrable function that is not square integrable.

**Theorem 2.3.4.** *The operator $(Q, D(Q))$ is $-\frac{d^2}{dx^2}$-compact if and only if $q$ is a locally square integrable function satisfying*

$$\lim_{|y|\to\infty} \int_y^{y+1} |q(x)|^2\,dx \to 0.$$

**Corollary 2.3.5.** *If $q \in L^2(\mathbb{R})$, then the essential spectrum of $-\frac{d^2}{dx^2} + q$ is $[0,\infty)$.*

*Proof of Theorem 2.3.4.* First assume that the condition on the potential $q$ is not valid, then there exists a $\varepsilon > 0$ and a sequence of points $\{y_n\}_{n=1}^\infty$ such that $|y_n| \to \infty$ and $\int_{y_n}^{y_n+1} |q(x)|^2\,dx \geq \varepsilon$. Pick a function $\phi \in C_c^\infty(\mathbb{R})$ with the properties $\phi(x) \geq 1$ for $x \in [0,1]$ and $\mathrm{supp}(\phi) \subset [-1,2]$. Define the translated function $\phi_n(x) = \phi(x - y_n)$, then obviously

$\phi_n \in W^2(\mathbb{R})$ and $\|\phi_n''\| + \|\phi_n\| = \|\phi''\| + \|\phi\|$ is independent of $n$. Consequently, the assumption that $Q$ is $-\frac{d^2}{dx^2}$-compact implies that $\{Q\phi_n\}_{n=1}^\infty$ has a convergent subsequence, again denoted by $\{Q\phi_n\}_{n=1}^\infty$, say $Q\phi_n \to f$. Observe that

$$\int_{\mathbb{R}} |q(x)\phi_n(x)|^2\, dx \geq \int_{y_n}^{y_n+1} |q(x)|^2\, dx \geq \varepsilon,$$

so that $\|f\| \geq \sqrt{\varepsilon} > 0$. On the other hand, for any fixed bounded interval $I$ of length 1 we have $\phi_n|_I = 0$ for $n$ sufficiently large since $|y_n| \to \infty$, so that

$$\begin{aligned}\left(\int_I |f(x)|^2\, dx\right)^{\frac{1}{2}} &\leq \left(\int_I |f(x) - q(x)\phi_n(x)|^2\, dx\right)^{\frac{1}{2}} + \left(\int_I |q(x)\phi_n(x)|^2\, dx\right)^{\frac{1}{2}} \\ &= \left(\int_I |f(x) - q(x)\phi_n(x)|^2\, dx\right)^{\frac{1}{2}} \to 0, \qquad n \to \infty.\end{aligned}$$

This shows $\int_I |f(x)|^2\, dx = 0$, hence, by filling $\mathbb{R}$ with such intervals, $\|f\| = 0$, which is contradicting $\|f\| \geq \sqrt{\varepsilon} > 0$.

Now assume that the assumption on $q$ is valid. We start with some general remarks on $W^2(\mathbb{R})$. For $f \in W^2(\mathbb{R}) \subset C^1(\mathbb{R})$ (using the Sobolev inbedding Lemma 6.3.1) we have, using the Fourier transform and the Cauchy-Schwarz inequality (6.1.1),

$$\begin{aligned} f(x) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i\lambda x} (\mathcal{F}f)(\lambda)\, d\lambda \\ \Rightarrow |f(x)| &\leq \frac{1}{\sqrt{2\pi}} \|\lambda \mapsto \frac{1}{\sqrt{1+\lambda^2}}\| \, \|\lambda \mapsto \sqrt{1+\lambda^2}(\mathcal{F}f)(\lambda)\| = \frac{1}{2}\sqrt{2} \|\lambda \mapsto \sqrt{1+\lambda^2}(\mathcal{F}f)(\lambda)\| \end{aligned}$$

and similarly

$$|f'(x)| \leq \frac{1}{2}\sqrt{2}\|\lambda \mapsto \sqrt{1+\lambda^2}\lambda(\mathcal{F}f)(\lambda)\|.$$

Now, reasoning as in the proof of (3) $\Rightarrow$ (4) for Theorem 2.2.6 we see

$$\begin{aligned} \|\lambda \mapsto \sqrt{1+\lambda^2}(\mathcal{F}f)(\lambda)\|^2 &= \int_{\mathbb{R}} |(\mathcal{F}f)(\lambda)|^2\, d\lambda + \int_{\mathbb{R}} \lambda^2 |(\mathcal{F}f)(\lambda)|^2\, d\lambda \\ \leq \frac{3}{2} \int_{\mathbb{R}} |(\mathcal{F}f)(\lambda)|^2\, d\lambda &+ \frac{1}{2} \int_R \lambda^4 |(\mathcal{F}f)(\lambda)|^2\, d\lambda = \frac{3}{2}\|f\|^2 + \frac{1}{2}\|f''\|^2, \end{aligned}$$

and similarly

$$\|\lambda \mapsto \sqrt{1+\lambda^2}\lambda(\mathcal{F}f)(\lambda)\|^2 \leq \frac{1}{2}\|f\|^2 + \frac{3}{2}\|f''\|^2,$$

so, with $C = \sqrt{3}$,

$$|f(x)| + |f'(x)| \leq C\left(\|f''\| + \|f\|\right).$$

(So we have actually proved that the Sobolev inbedding $W^2(\mathbb{R}) \subset C^1(\mathbb{R})$ is continuous.)

If $\{f_n\}_{n=1}^{\infty}$ is now a sequence in $W^2(\mathbb{R})$ such that $\|f_n''\| + \|f_n\| \leq C_1$, then it follows that $f_n$ and $f_n'$ are uniformly bounded, this in particular implies that $M = \{f_n \mid n \in \mathbb{N}\}$ is uniformly continuous. Since $M$ is also bounded in the supremum norm, it follows by the Arzelà-Ascoli theorem that the closure of $M$ is compact in $C(\mathbb{R})$. In particular, there is a convergent subsequence, which is also denoted by $\{f_n\}_{n=1}^{\infty}$. This result, with the locally square integrability condition on $q$, now gives for each fixed $N > 0$

$$\int_{-N}^{N} |q(x)\big(f_n(x) - f_m(x)\big)|^2 \, dx \leq \|f_n - f_m\|_\infty^2 \int_{-N}^{N} |q(x)|^2 \, dx \to 0, \tag{2.3.3}$$

so this can be made arbitrarily small for $n, m$ large enough.

It remains to show that restricting the potential to the interval $[-N, N]$ does not affect $\{qf_n\}_{n=1}^{\infty}$ being a Cauchy sequence. Take $\varepsilon > 0$ arbitrary, and choose a corresponding $N$ such that $\int_y^{y+1} |q(x)|^2 \, dx < \varepsilon$ for all $|y| > N$. Denote by $q_N$ the function equal to $q$ for $|x| \leq N$ and $q_N(x) = 0$ for $|x| > N$. In (2.3.3) we have dealt with $q_N(f_n - f_m)$, the remaining part follows from the following claim. There exists constants $C_2$, $C_3$ independent of $N$ such that

$$\|(q - q_N)f\|^2 \leq \varepsilon \left(C_2 \, \|f''\|^2 + C_3 \, \|f\|^2\right), \qquad \forall\, f \in W^2(\mathbb{R}).$$

The claims follows from the reasoning after Lemma 2.2.8 by replacing $q$ and $C$ by $q - q_N$ and $\varepsilon$ (taking e.g. the $\varepsilon$ in the proof of Theorem 2.2.6 equal to 1, so we can take $C_2 = \frac{1}{2}$, $C_3 = \frac{5}{2}$). $\square$

**Exercise 2.3.6.** Consider the Schrödinger operator with a potential of the form $q_1 + q_2$, with $q_1(x) = a$, $q_2(x) = b\chi_I(x)$, where $\chi_I$ is the indicator function of the set $I$ (i.e. $\chi_I(x) = 1$ if $x \in I$ and $\chi_I(x) = 0$ if $x \notin I$) for $I$ the interval $I = [c, d]$. Use Exercise 2.3.3 to describe the essential spectrum, see also Section 2.5.1.

## 2.4 Bound states and discrete spectrum

We consider the Schrödinger operator $-\frac{d^2}{dx^2} + q$ for which we assume that the essential spectrum is $[0, \infty)$. So this is the case if $q$ satisfies the condition in Theorem 2.3.4, which we now assume throughout this section. This in particular means that any $\lambda < 0$ in the spectrum is isolated and contained in the point spectrum by Theorem 6.5.5. In this case there is an eigenfunction $f \in W^2(\mathbb{R})$ such that

$$-f''(x) + q(x)\, f(x) = \lambda\, f(x), \qquad \lambda < 0.$$

We count eigenvalues according to their multiplicity, i.e. the dimension of $\mathrm{Ker}(-\frac{d^2}{dx^2} + q - \lambda)$. In quantum mechanical applications an eigenfunction for the Schrödinger operator corresponding to an eigenvalue $\lambda < 0$ is called a bound state.

For a Schrödinger operator with essential spectrum $[0, \infty)$ the dimension of the space of bound states might be zero, finite or infinite. Note that the number of negative eigenvalues is denumerable by Theorem 6.5.5. We give a simple criterion that guarantees that there is at least a one-dimensional space of bound states. There are many more explicit criterions on the potential that imply explicit results for the dimension of the space of bound states.

We start with a general statement.

**Proposition 2.4.1.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$ such that $\sigma_{ess}(T) \subset [0, \infty)$. Then $T$ has negative eigenvalues if and only if there exists a non-trivial subspace $M \subset D(T) \subset \mathcal{H}$ such $\langle Tx, x\rangle < 0$ for all $x \in M\backslash\{0\}$.*

*Proof.* If $T$ has negative eigenvalues, then put $M = \bigoplus \mathrm{Ker}(T - \lambda)$, summing over all $0 > \lambda \in \sigma_p(T)$ and where we take only finite linear combinations.

If $T$ has no negative eigenvalues, then it follows by Theorem 6.5.5(ii) that $\sigma(T) \subset [0, \infty)$. By the Spectral Theorem 6.4.1, it follows that

$$\langle Tx, x\rangle = \int_{\sigma(T)} \lambda\, dE_{x,x}(\lambda), \qquad \forall x \in D(T),$$

and since $E_{x,x}$, $x \neq 0$, is a positive measure and $\sigma(T) \subset [0, \infty)$ the right hand side is obviously non-negative. So $M$ is trivial. $\square$

This principle can be used to establish a criterion for the occurrence of bound states.

**Theorem 2.4.2.** *Assume there exists $\alpha > 0$ such that*

$$\frac{1}{\alpha} \int_{\mathbb{R}} q(x) \exp(-2\alpha^2 (x-a)^2)\, dx < -\sqrt{\frac{\pi}{2}},$$

*then the Schrödinger operator $-\frac{d^2}{dx^2} + q$ has a negative eigenvalue.*

*Proof.* Take any function $f \in W^2(\mathbb{R}) \subset D(Q)$, then $\langle -f'', f\rangle = \langle f', f'\rangle = \|f'\|^2$. Hence, $\langle -f'' + qf, f\rangle = \|f'\|^2 + \int_{\mathbb{R}} q(x)|f(x)|^2\, dx$ and if this expression is (strictly) negative, Proposition 2.4.1 implies the result.

In order to obtain the result, we take $f(x) = \exp(-\alpha^2(x-a)^2)$, then $f'(x) = -2\alpha^2(x - a)\exp(-\alpha^2(x-a)^2)$, and

$$\|f'\|^2 = 4\alpha^4 \int_{\mathbb{R}} (x-a)^2 e^{-2\alpha^2(x-a)^2}\, dx = \frac{4\alpha^4}{2\alpha^3\sqrt{2}} \int_{\mathbb{R}} y^2 e^{-y^2}\, dy = \frac{2\alpha}{\sqrt{2}} \frac{1}{2}\sqrt{\pi} = \alpha\sqrt{\frac{\pi}{2}},$$

so for this $f$ we find

$$\|f'\|^2 + \int_{\mathbb{R}} q(x)|f(x)|^2\, dx = \alpha \left( \sqrt{\frac{\pi}{2}} + \frac{1}{\alpha} \int_{\mathbb{R}} q(x) e^{-2\alpha^2(x-a)^2}\, dx \right)$$

which is negative by assumption for suitable $\alpha$. $\square$

By applying this idea to other suitable functions, one can obtain other criteria for the existence of negative eigenvalues for Schrödinger operators.

**Corollary 2.4.3.** *Assume the existence of a (measurable) set $B \subset \mathbb{R}$ such that $\int_B q(x)\,dx < 0$ and $q(x) \leq 0$ for $x \notin B$. Then the Schrödinger operator $-\frac{d^2}{dx^2} + q$ has at least one negative eigenvalue.*

The implicit assumption in Corollary 2.4.3 is that $q$ integrable is over the set $B$. Note that the standing assumption in this section is the assumption of Theorem 2.3.4. If $B$ is a bounded set, then the Hölder inequality implies $\int_B |q(x)|\,dx \leq \sqrt{|B|}\,\big(\int_B |q(x)|^2\,dx\big)^{1/2}$, so that the locally square integrability already implies this assumption. Here $|B|$ denotes the (Lebesgue) measure of the set $B$.

*Proof.* Note

$$\int_{\mathbb{R}} q(x)e^{-2\alpha^2x^2}\,dx \leq \int_B q(x)e^{-2\alpha^2x^2}\,dx \to \int_B q(x)\,dx < 0, \qquad \text{as } \alpha \downarrow 0,$$

so that $\frac{1}{\alpha}\int_{\mathbb{R}} q(x)e^{-2\alpha^2x^2}\,dx$ can be made arbitrarily negative, hence we can apply Theorem 2.4.2. Note that interchanging limit and integration is justifiable by the Dominated Convergence Theorem 6.1.3. □

In particular, the special case $B = \mathbb{R}$ of Corollary 2.4.3 gives the following result.

**Corollary 2.4.4.** *For $q \in L^1(\mathbb{R})$ such that $\int_{\mathbb{R}} q(x)\,dx < 0$ the Schrödinger operator $-\frac{d^2}{dx^2} + q$ has at least one negative eigenvalue.*

We also give without proof an estimate on the number of negative eigenvalues for the Schrödinger operator.

**Theorem 2.4.5.** *Assume that $q$ satisfies the condition in Theorem 2.3.4 and additionally that $\int_{\mathbb{R}} |x|\,|q(x)|\,dx < \infty$, then the number $N$ of eigenvalues of the Schrödinger operator is bounded by*

$$N \leq 2 + \int_{\mathbb{R}} |x|\,|q(x)|\,dx.$$

The argument used in the proof of Theorem 2.4.5 is an extension of a comparison argument for a Schrödinger operator on a finite interval, see [4].

## 2.5 Explicit examples of potentials

### 2.5.1 Indicator functions as potential

Consider first the potential $q(x) = a \in \mathbb{R}$, then using Exercise 2.3.3 or writing $q = aI$, $I$ identity operator in $B(L^2(\mathbb{R}))$, we see that the corresponding Schrödinger operator $L$ has $\sigma = \sigma_{ess} = [a, \infty)$. A somewhat more general statement is contained in the following exercise.

**Exercise 2.5.1.** Show that if the potential $q$ satisfies $q(x) \geq a$ almost everywhere, then $(-\infty, a)$ is contained in the resolvent $\rho(L)$. Rephrased, the spectrum $\sigma(L)$ is contained in $[a, \infty)$. Prove this using the following steps.

- Show that $\langle (L-\lambda)f, f\rangle = \langle -f'' + qf - \lambda f, f\rangle = \|f'\|^2 + \int_{\mathbb{R}} (q(x)-\lambda)|f(x)|^2\,dx$, $\forall f \in W^2(\mathbb{R})$.
- Conclude that for $\lambda < a$, $(a-\lambda)\|f\| \leq \|(L-\lambda)f\|$ for all $f \in W^2(\mathbb{R})$. Use Theorem 6.5.1 to conclude that $\lambda \in \rho(L)$.

**Exercise 2.5.2.** Assume that the potential $q \in L^2(\mathbb{R})$ satisfies $q(x) \geq a$ for $a < 0$. Show that $[a, 0]$ contains only finitely many points of the spectrum of the corresponding Schrödinger operator. (Hint: Use Theorem 6.5.5 and Exercise 2.5.1.)

Now consider $q(x) = a + b\chi_I(x)$, $b \in \mathbb{R}$, where we take for convenience $I = [0,1]$, and denote the corresponding Schrödinger operator again by $L$. By Exercise 2.3.3 we know that $\sigma_{ess}(L) = [a, \infty)$. In case $b > 0$, we have $\sigma_{ess}(L) = [a, \infty)$ by combining Exercise 2.3.3 and Theorem 2.3.4. Then Exercise 2.5.1 implies $\sigma(L) = [a, \infty)$.

We now consider the case $a = 0$, $b < 0$. By Corollary 2.4.3 or Corollary 2.4.4, there is negative point spectrum. On the other hand, the essential spectrum is $[0, \infty)$ and by Exercise 2.5.1 the spectrum is contained in $[b, \infty)$. We look for negative spectrum, which, by Theorem 6.5.5, is contained in the point spectrum and consists of isolated points. We put $\lambda = -\gamma^2$, $\sqrt{|b|} > \gamma > 0$ and we try to find solutions to $Lf = \lambda f$, or

$$\begin{cases} f'' - \gamma^2 f = 0, & x < 0, \\ f'' - (\gamma^2 + b)f = 0, & 0 < x < 1, \\ f'' - \gamma^2 f = 0, & x > 1. \end{cases}$$

The first and last equation imply $f(x) = A_- \exp(\gamma x) + B_- \exp(-\gamma x)$, $x < 0$, and $f(x) = A_+ \exp(\gamma x) + B_+ \exp(-\gamma x)$, $x > 1$, for constants $A_\pm, B_\pm \in \mathbb{C}$. Since we need $f \in L^2(\mathbb{R})$, we see that $B_- = 0$ and $A_+ = 0$, and because an eigenfunction (or bound state) can be changed by multiplication by a constant, we take $A_- = 1$, or $f(x) = \exp(\gamma x)$, $x < 0$, and $f(x) = B_+ \exp(-\gamma x)$, $x > 1$. Now $b + \gamma^2 < 0$, and we put $-\omega^2 = b + \gamma^2$, $\omega > 0$. It is left as an exercise to check that $\gamma^2 = -b$, i.e $\omega = 0$, does not lead to an eigenfunction. So the second equation gives $f(x) = A\cos(\omega x) + B\sin(\omega x)$, $0 < x < 1$. Since an eigenfunction $f \in W^2(\mathbb{R}) \subset C^1(\mathbb{R})$, we need to choose $A, B, B_+$ such that $f$ is $C^1$ at 0 and at 1. At 0 we need $1 = A$ for continuity and $\gamma = \omega B$ for continuity of the derivative. So $f(x) = \cos(\omega x) + \frac{\gamma}{\omega}\sin(\omega x)$, $0 < x < 1$, and we need $\cos(\omega) + \frac{\gamma}{\omega}\sin(\omega) = B_+ e^{-\gamma}$ for continuity at 1 –this then fixes $B_+$– and $-\omega\sin(\omega) + \gamma\cos(\omega) = -\gamma B_+ e^{-\gamma}$ for a continuous derivative at 1. In order that this has a solution we require

$$-\omega\sin(\omega) + \gamma\cos(\omega) = -\gamma\cos(\omega) - \frac{\gamma^2}{\omega}\sin(\omega) \;\Rightarrow\; \tan(\omega) = \frac{2\gamma\omega}{\omega^2 - \gamma^2}$$

and this gives an implicit requirement on the eigenvalue $\lambda = -\gamma^2$. Having a solution $\lambda \in [b, 0]$, we see from the above calculation that the corresponding eigenspace is at most one-dimensional, and that the corresponding eigenfunction or bound state is in $C^1(\mathbb{R})$. It remains to check that this eigenfunction is actually an element of $W^2(\mathbb{R})$ in order to be able to conclude that the corresponding $\lambda$ is indeed an eigenvalue.

**Exercise 2.5.3.** Show that the number $N$ of negative eigenvalues, i.e. the number of solutions to $\tan(\omega) = \frac{2\gamma\omega}{\omega^2-\gamma^2}$, is determined by the condition $N - 1 < \frac{\sqrt{-b}}{\pi} < N$ assuming $b \notin \pi^2\mathbb{Z}$. Show that the corresponding eigenfunction is indeed an element of the Sobolev space, so that there are $N$ eigenvalues. E.g. for $b = -10$, there are two bound states corresponding to $\gamma = 0.03244216751$, $\gamma = 2.547591633$.

The assumption in Exercises 2.5.3 is inserted to avoid bound states for the eigenvalue 0.

**Exercise 2.5.4.** Using the techniques above, discuss the spectrum of the Schrödinger operator with potential given by $q(x) = a$ for $x < x_1$, $q(x) = b$ for $x_1 < x < x_2$, $q(x) = c$ for $x_2 < x$ for $a, b, c \in \mathbb{R}$ and $x_1 < x_2$.

### 2.5.2 $\cosh^{-2}$-potential

The potentials discussed consist of an important special case for the theory in Chapter 5. They are closely related to soliton solutions of the Korteweg-de Vries equation, that are going to be obtained using the inverse scattering method.

Recall the hyperbolic cosine function $\cosh(x) = \frac{1}{2}(e^x + e^{-x})$, the hyperbolic sine function $\sinh(x) = \frac{1}{2}(e^x - e^{-x})$ and the relation $\cosh^2(x) - \sinh^2(x) = 1$. Obviously, $\frac{d}{dx}\cosh(x) = \sinh(x)$, $\frac{d}{dx}\sinh(x) = \cosh(x)$.

We take the potential $q(x) = a\cosh^{-2}(px)$, $a, p \in \mathbb{R}$, see Figure 2.1 for the case $a = -2$, $p = 1$. Since $q \in L^2(\mathbb{R})$, it follows from Corollary 2.2.7 and Corollary 2.3.5 that the corresponding Schrödinger operator $L = -\frac{d^2}{dx^2} + q$ is self-adjoint and $\sigma_{ess}(L) = [0, \infty)$. Since for $a > 0$ we have $\langle Lf, f\rangle = \|f'\| + \int_{\mathbb{R}} q(x)|f(x)|^2\, dx \geq 0$ for all $f \in W^2(\mathbb{R})$ it follows that $\sigma(L) = [0, \infty)$ as well. Since $\cosh^{-2} \in L^1(\mathbb{R})$, we can use Corollary 2.4.4 to see that for $a < 0$ there is at least one negative eigenvalue.

We consider a first example in the following exercise.

**Exercise 2.5.5.** Show that $f(x) = (\cosh(px))^{-1}$ satisfies

$$-f''(x) - \frac{2p^2}{\cosh^2(px)} f(x) = -p^2 f(x),$$

or $-p^2 \in \sigma_p(L)$ for the case $a = -2p^2$.

In Exercise 2.5.8 you have to show that in this case $\sigma = \{-p^2\} \cup [0, \infty)$ and that $\operatorname{Ker}(L + p^2)$ is one-dimensional.

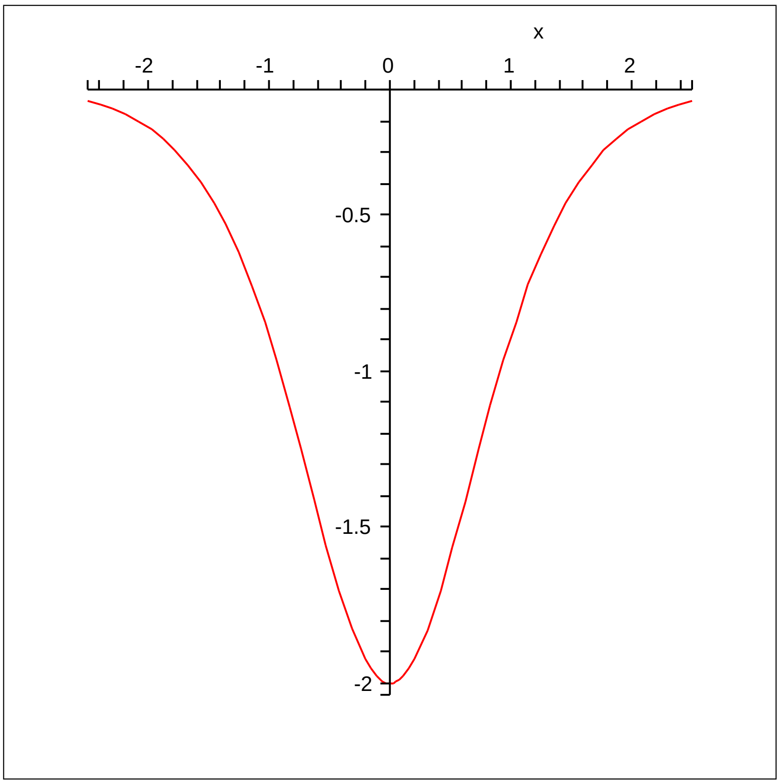


Figure 2.1: The potential $-2/\cosh^2(x)$.

**Exercise 2.5.6.** Consider a general potential $q \in L^2(\mathbb{R})$ and the corresponding Schrödinger operator $L_1$. Set $f_p(x) = f(px)$ for $p \neq 0$, and let $L_p$ denote the Schrödinger operator with potential $q_p$. Show that $\lambda \in \sigma(L_1) \Longleftrightarrow p^2\lambda \in \sigma(L_p)$ and similarly for the point spectrum and the essential spectrum.

Because of Exercise 2.5.6 we can restrict ourselves to the case $p = 1$. We transform the Schrödinger eigenvalue equation into the hypergeometric differential equation;

$$z(1-z)\,y_{zz} + \big(c - (1+a+b)z\big)\,y_z - ab\,y = 0 \tag{2.5.1}$$

for complex parameters $a, b, c$. In Exercise 2.5.7 we describe solutions to (2.5.1). This exercise is not essential, and is best understood within the context of differential equations on $\mathbb{C}$ with regular singular points.

Put $\lambda = \gamma^2$ with $\gamma$ real or purely imaginary, and consider $-f''(x) + a\cosh^{-2}(x)f(x) = \gamma^2 f(x)$. We put $z = \frac{1}{2}(1-\tanh(x)) = (1+\exp(2x))^{-1}$, where $\tanh(x) = \sinh(x)/\cosh(x)$. Note that $-\infty$ is mapped to 1 and $\infty$ is mapped to 0, and $x \mapsto z$ is invertible with $\frac{dz}{dx} = \frac{-1}{2\cosh^2(x)}$. So we have to deal with (2.5.1) on the interval $(0, 1)$.

Before transforming the differential equation, note that $\tanh(x) = 1 - 2z$ and $\cosh^{-2}(x) =$

$4z(1-z)$. Now we put $f(x) = (\cosh(x))^{i\gamma}\, y(z)$, then we have

$$\begin{aligned} f'(x) &= i\gamma(\cosh(x))^{i\gamma-1}\sinh(x)\, y(z) - \frac{1}{2}(\cosh(x))^{i\gamma-2}\, y_z(z),\\ f''(x) &= i\gamma(i\gamma-1)(\cosh(x))^{i\gamma-2}\sinh^2(x)\, y(z) + i\gamma(\cosh(x))^{i\gamma}\, y(z)\\ &\qquad -\frac{i}{2}\gamma(\cosh(x))^{i\gamma-3}\sinh(x)\, y_z(z) - \frac{1}{2}(i\gamma-2)(\cosh(x))^{i\gamma-3}\sinh(x)\, y_z(z)\\ &\qquad + \frac{1}{4}(\cosh(x))^{i\gamma-4}\, y_{zz}(z) \end{aligned}$$

Plugging this into $-f''(x)+a\cosh^{-2}(x)f(x) = \gamma^2 f(x)$ and multiplying by $(\cosh(x))^{2-i\gamma}$ gives,

$$-z(1-z)\, y_{zz}(z) + (1-2z)(i\gamma-1)\, y_z(z) + (a-\gamma^2-i\gamma)\, y(z) = 0.$$

This equation is of the hypergeometric differential type (2.5.1) if we set $(a,b,c)$ in (2.5.1) equal to $(\frac{1}{2}-i\gamma+\sqrt{\frac{1}{4}-a}, \frac{1}{2}-i\gamma-\sqrt{\frac{1}{4}-a}, 1-i\gamma)$.

Note that under this transformation the eigenvalue equation $-f''(x)+a\cosh^{-2}(x)f(x) = \gamma^2 f(x)$ is not transferred into another eigenvalue equation for the hypergeometric differential equation, since $\gamma$ also occurs in the coefficient of $y_z$.

**Exercise 2.5.7.** 1. Define the Pochhammer symbol

$$(a)_n = a(a+1)(a+2)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}, \qquad a\in\mathbb{C}$$

so that $(1)_n = n!$ and $(a)_0 = 1$. Define the hypergeometric function

$${}_2F_1\left(\begin{matrix} a,\, b \\ c \end{matrix}\,;z\right) = \sum_{n=0}^{\infty} \frac{(a)_n(b)_n}{(c)_n\, n!} z^n.$$

Show that the radius of convergence is 1 and that it gives an analytic solution to (2.5.1). Check that this is a well-defined function for $c\notin\{\cdots,-3,-2,-1,0\}$, and that $\frac{1}{\Gamma(c)}\,{}_2F_1\left(\begin{smallmatrix} a,b \\ c \end{smallmatrix}\,;z\right)$ is well-defined for $c\in\mathbb{C}$.

2. Show that

$$z^{1-c}\,{}_2F_1\left(\begin{matrix} a-c+1,\, b-c+1 \\ 2-c \end{matrix}\,;z\right)$$

is also a solution to (2.5.1). (We define $z^{1-c} = \exp\bigl((1-c)\bigl(\ln|z| + i\arg(z)\bigr)\bigr)$ with $|\arg(z)|<\pi$, so that the complex plane is cut along the negative real axis.) Show that for $c\notin\mathbb{Z}$ we have obtained two linearly independent solutions to (2.5.1).

3. Rewrite (2.5.1) by switching to $w = 1-z$, and observe that this is again a hypergeometric differential equation. Use this to observe that

$${}_2F_1\left(\begin{matrix} a,\, b \\ a+b+1-c \end{matrix}\,;1-z\right), \qquad (1-z)^{c-a-b}\,{}_2F_1\left(\begin{matrix} c-a,\, c-b \\ c+1-a-b \end{matrix}\,;1-z\right)$$

are also solutions to (2.5.1). These are linearly independent solutions in case $c-a-b\notin\mathbb{Z}$.

4. Use Exercise 2.5.5 to obtain an expression for $\cosh^{-1}(x)$ in terms of a hypergeometric function.

Since we are interested in negative eigenvalues we assume that $a < 0$ and $\lambda = \gamma^2 < 0$; we put $\gamma = i\beta$ with $\beta > 0$. Then the eigenfunction $f$ satisfies

$$|f(x)|^2 = \frac{1}{\cosh^{2\beta}(x)} \, |y(\frac{1}{1+e^{2x}})|^2,$$

so that square integrability for $x \to \infty$ gives a condition on $y$ at 0. We call a function $f$ square integrable at $\infty$ if $\int_a^\infty |f(x)|^2 \, dx < \infty$ for some $a \in \mathbb{R}$. Note that any $f \in L^2(\mathbb{R})$ is square integrable at $\infty$. Square integrability at $-\infty$ is defined analogously. Note that ${}_2F_1\left({a, b \atop c}\, ; z\right)$ equals 1 at $z = 0$, so is bounded and the corresponding eigenfunction is then square integrable at $\infty$. For the other solution we get

$$|f(x)|^2 = \frac{1}{\cosh^{2\beta}(x)} |(1+e^{2x})|^{2\beta} \left| {}_2F_1\left( {a-c+1,\, b-c+1 \atop 2-c} \, ; \frac{1}{1+e^{2x}} \right) \right|^2$$

(with $a, b, c$ of the hypergeometric function related to $a, \gamma = i\beta$ as above) and this is not square integrable for $x \to \infty$. So we conclude that the eigenfunction for the eigenvalue $-\beta^2$ that is square integrable for $x \to \infty$ is a multiple of

$$f_+(x) = \frac{1}{\cosh^{\beta}(x)} \, {}_2F_1\left( {\frac{1}{2} + \beta + (\frac{1}{4} - a)^{1/2},\, \frac{1}{2} + \beta - (\frac{1}{4} - a)^{1/2} \atop 1+\beta} \, ; \frac{1}{1+e^{2x}} \right). \tag{2.5.2}$$

This already implies that the possible eigenspace is at most one-dimensional, since there is a one-dimensional space of eigenfunctions that is square integrable at $\infty$.

Similarly, using the solutions of Exercise 2.5.7(3) we can look at eigenfunctions that are square integrable for $x \to -\infty$, and we see that these are a multiple of

$$f_-(x) = \frac{1}{\cosh^{\beta}(x)} \, {}_2F_1\left( {\frac{1}{2} + \beta + (\frac{1}{4} - a)^{1/2},\, \frac{1}{2} + \beta - (\frac{1}{4} - a)^{1/2} \atop 1+\beta} \, ; \frac{e^{2x}}{1+e^{2x}} \right). \tag{2.5.3}$$

So we actually find an eigenfunction in case $f_+$ is a multiple of $f_-$. Since the four hypergeometric functions in Exercise 2.5.7 are solutions to the same second order differential equation, there are linear relations between them. We need,

$$\begin{gathered} {}_2F_1\left( {a,\, b \atop a+b-c+1} \, ; 1-z \right) = A \, {}_2F_1\left( {a,\, b \atop c} \, ; z \right) + B \, z^{1-c} \, {}_2F_1\left( {a-c+1,\, b-c+1 \atop 2-c} \, ; z \right), \\ A = \frac{\Gamma(a+b+1-c)\Gamma(1-c)}{\Gamma(a-c+1)\Gamma(b-c+1)}, \qquad B = \frac{\Gamma(a+b+1-c)\Gamma(c-1)}{\Gamma(a)\Gamma(b)}. \end{gathered} \tag{2.5.4}$$

So we find that $f_-$ is a multiple of $f_+$ in case the $B$ in (2.5.4) vanishes, or

$$\frac{\Gamma(1+\beta)\Gamma(\beta)}{\Gamma(\frac{1}{2} + \beta + (\frac{1}{4} - a)^{1/2})\Gamma(\frac{1}{2} + \beta - (\frac{1}{4} - a)^{1/2})} = 0.$$

This can only happen if the Γ-functions in the denominator have poles. Since the Γ-functions have poles at the $\{\cdots,-2,-1,0\}$ and $\beta>0$ and $a<0$ we see that this can only happen if $\frac{1}{2}+\beta-\sqrt{\frac{1}{4}-a}=-n\leq 0$ for $n$ a non-negative integer, or $\beta=\sqrt{\frac{1}{4}-a}-\frac{1}{2}-n$.

It remains to check that in this case the eigenfunctions are indeed elements of the Sobolev space $W^2(\mathbb{R})$. We leave this to the reader.

**Exercise 2.5.8.** Show that the number of (strictly) negative eigenvalues of the Schrödinger operator for the potential $a/\cosh^2(x)$ is given by the integer $N$ satisfying $N(N-1)<-a<N(N+1)$. Show that for the special case $-a=m(m+1)$, $m\in\mathbb{N}$, one of the points $\beta$ corresponds to zero, and in this case $N=m$. Conclude that the spectrum of the Schrödinger operator in Exercise 2.5.5 has spectrum $\{-p^2\}\cup[0,\infty)$ and that there is a one-dimensional space of eigenfunctions, or bound states, for the eigenvalue $-p^2$.

### 2.5.3 Exponential potential

We consider the potential $q(x)=a\exp(-2|x|)$, then it is clear from Corollary 2.2.7 and Corollary 2.3.5 that the Schrödinger operator is self-adjoint and that its essential spectrum is $[0,\infty)$, and for $a>0$ we see from Exercise 2.5.1 that its spectrum is $[0,\infty)$ as well. See Figure 2.2 for the case $a=-2$, and compare with Figure 2.1.

The eigenvalue equation $f''(x)+(\lambda-a\exp(-2|x|))f(x)=0$ can be transformed into a well-known differential equation. For the transformation we consider the intervals $(-\infty,0)$ and $(0,\infty)$ separately. For $x<0$ we put $z=\sqrt{-a}\exp(x)$, and for $x>0$ we put $z=\sqrt{-a}\exp(-x)$ and put $y(z)=f(x)$, then the eigenvalue equation is transformed into the Bessel differential equation

$$z^2\,y_{zz}+z\,y_z+(z^2-\nu^2)\,y=0,$$

where we have put $\lambda=-\nu^2$. Note that $(-\infty,0)$ is transformed into $(0,\sqrt{-a})$ and $(0,\infty)$ into $(\sqrt{-a},0)$, and so we need to glue solutions together at $x=0$ or $z=\sqrt{-a}$ in a $C^1$-fashion.

**Exercise 2.5.9.** 1. Check the details of the above transformation.

2. Define the Bessel function

$$J_\nu(z)=\frac{(z/2)^\nu}{\Gamma(\nu+1)}\sum_{n=0}^{\infty}\frac{(-1)^n}{(\nu+1)_n}\frac{z^{2n}}{4^n\,n!}=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!\,\Gamma(\nu+n+1)}\Big(\frac{z}{2}\Big)^{\nu+2n}.$$

Show that the power series in the middle defines an entire function. Show that $J_\nu(z)$ is a solution to Bessel differential equation. Conclude that $J_{-\nu}$ is also a solution.

3. Show that for $\nu\notin\mathbb{Z}$ the Bessel functions $J_\nu$ and $J_{-\nu}$ are linearly independent solutions to the Bessel functions. (Hint: show that for any pair of solutions $y_1,y_2$ of the Bessel differential equation the Wronskian $W(z)=y_1(z)y_2'(z)-y_1'(z)y_2(z)$ satisfies a first order differential equation that leads to $W(z)=C/z$. Show that for $y_1(z)=J_\nu(z)$, $y_2(z)=J_{-\nu}(z)$ the constant $C=-2\sin(\nu\pi)/\pi$.)

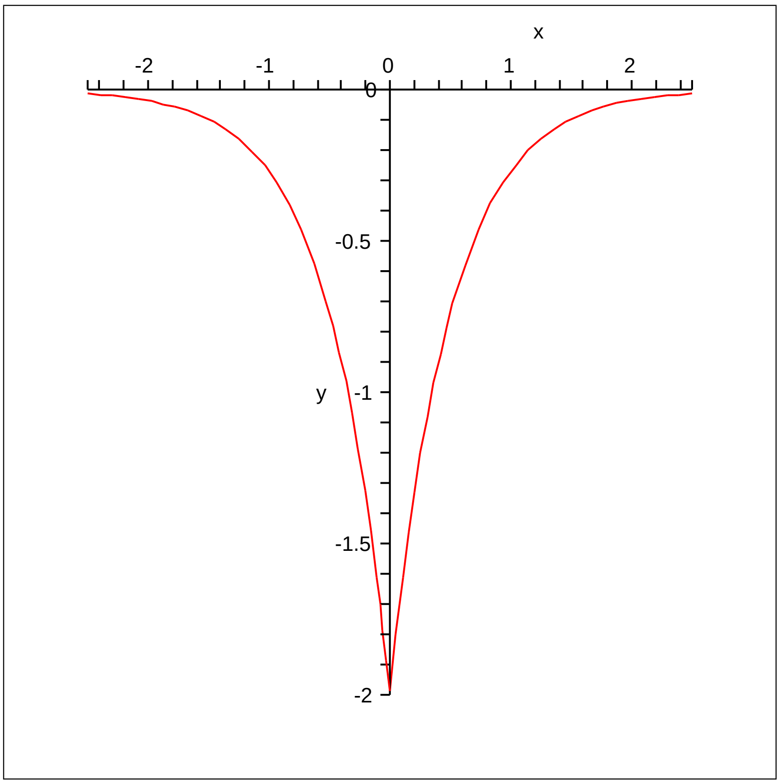


Figure 2.2: The potential $-2\exp(-2|x|)$.

The reduction to the Bessel differential equation works for arbitrary $a$, but we now stick to the case $a<0$. In case $a<0$ we want to discuss the discrete spectrum. We consider eigenfunctions $f$ for eigenvalue $\lambda=-\nu^2<0$, so we have $\nu\in\mathbb{R}$ and we assume $\nu>0$. We now put $c=\sqrt{-a}$. For negative $x$ it follows $|f(x)|^2=|y(ce^x)|^2$, and since $J_\nu(z)=\frac{(z/2)^\nu}{\Gamma(\nu+1)}\big(1+\mathcal{O}(z)\big)$ as $z\to 0$ for $\nu\notin-\mathbb{N}$, it follows that $f$ is a multiple of $J_\nu(ce^x)$ for $x<0$ in order to be square integrable at $\infty$. In order to extend $f$ to a function for $x>0$, we put $f(x)=A\,J_\nu(ce^{-x})+B\,J_{-\nu}(ce^{-x})$, so that it is a solution to the eigenvalue equation for $x>0$. Since $f$ has to be in $W^2(\mathbb{R})\subset C^1(\mathbb{R})$ we need to impose a $C^1$-transition at $x=0$, this gives

$$\begin{cases} A\,J_\nu(c)+B\,J_{-\nu}(c)=J_\nu(c), \\ -cA\,J'_\nu(c)-cB\,J'_{-\nu}(c)=cJ'_\nu(c) \end{cases} \Longrightarrow \begin{pmatrix} J_\nu(c) & J_{-\nu}(c) \\ J'_\nu(c) & J'_{-\nu}(c)\end{pmatrix}\begin{pmatrix} A \\ B\end{pmatrix}=\begin{pmatrix} J_\nu(c) \\ -J'_\nu(c)\end{pmatrix}$$

$$\Longrightarrow \begin{pmatrix} A \\ B\end{pmatrix} = -\frac{\pi}{2\sin(\nu\pi)}\begin{pmatrix} J'_{-\nu}(c) & -J_{-\nu}(c) \\ -J'_\nu(c) & J_\nu(c)\end{pmatrix}\begin{pmatrix} J_\nu(c) \\ -J'_\nu(c)\end{pmatrix},$$

since the determinant of the matrix is precisely the Wronskian of the Bessel functions $J_\nu$ and $J_{-\nu}$, see Exercise 2.5.9(3), and where we now assume $\nu\notin\mathbb{Z}$.

Similarly, for $x>0$ we have $|f(x)|^2=|y(ce^{-x})|^2$ is square integrable at $\infty$ if only if $y$ equals $J_\nu$, so that $f$ is a multiple of $J_\nu(ce^{-x})$ for $x>0$ in order to be square integrable. So we can only have a square integrable eigenfunction (or bound state) in case $B$ in the previous calculation vanishes, or $J_\nu(c)J'_\nu(c) = 0$. Given $a$, hence $c$, we have to solve this equation for $\nu$ yielding the corresponding eigenvalues $\lambda = -\nu^2$ for the Schrödinger operator. This equation cannot be solved easily in a direct fashion, and requires knowledge about Bessel functions, its derivatives and its zeros. Since the negative spectrum has to be contained in $[-c^2, 0]$ we conclude that the smallest positive zero of $\nu \mapsto J_\nu(c)$ and $\nu \mapsto J'_\nu(c)$ is less than $c$. (This is a classical result, due to Riemann.)

# Chapter 3

# Scattering and wave operators

## 3.1 Time-dependent Schrödinger equation

Consider a self-adjoint Schrödinger operator $L$ acting on $L^2(\mathbb{R})$. The time-dependent Schrödinger equation is

$$i\psi'(t) = L\psi(t), \qquad \psi\colon D \subset \mathbb{R} \to L^2(\mathbb{R})$$

on some time domain $D$. The derivative with respect to time $t$ is defined by

$$\lim_{h\to 0} \|\frac{1}{h}\big(\psi(t+h) - \psi(t)\big) - \psi'(t)\| = 0$$

whenever the limit exists. The solution of the time-dependent Schrödinger equation can be solved completely using the Spectral Theorem 6.4.1 and the corresponding functional calculus.

**Theorem 3.1.1.** *Assume $L$ is a self-adjoint operator on $L^2(\mathbb{R})$, then the system*

$$i\psi'(t) = L\psi(t), \qquad \psi(0) = \psi_0 \in D(L) \tag{3.1.1}$$

*has a unique solution $\psi(t)$, $t \in \mathbb{R}$, given by $\psi(t) = \exp(-itL)\psi_0$ which satisfies $\|\psi(t)\| = \|\psi_0\|$.*

*Proof.* Let us first show existence. We use the Spectral Theorem 6.4.1 to establish the operator $U(t) = \exp(-itL)$, which is a one-parameter group of unitary operators on the Hilbert space $L^2(\mathbb{R})$. Define $\psi(t) = U(t)\psi_0$. This is obviously defined for all $t \in \mathbb{R}$ and $\psi(0) = U(0)\psi_0 = \psi_0$, since $U(0) = 1$ in $B(\mathcal{H})$. Note that this can be defined for any $\psi_0$, i.e. for this construction the requirement $\psi_0 \in D(L)$ is not needed.

In order to show that the differential equation is fulfilled we consider

$$\|\frac{1}{h}\big(U(t+h)\psi_0 - U(t)\psi_0\big) + iLU(t)\psi_0\|^2$$

and to see that $U(t)\psi_0 \in D(L)$ we note that, by the Spectral Theorem 6.4.1, it suffices to note that $\int_{\mathbb{R}} \lambda^2 dE_{U(t)\psi_0,U(t)\psi_0}(\lambda) < \infty$ which follows from

$$\langle E(A)U(t)\psi_0, U(t)\psi_0\rangle = \langle U(t)E(A)\psi_0, U(t)\psi_0\rangle = \langle E(A)\psi_0, \psi_0\rangle,$$

since $\psi_0 \in D(L)$, $U(t)$ commutes with $L$ and $U(t)$ is unitary by the Spectral Theorem 6.4.1. Since all operators are functions of the self-adjoint operator $L$, it follows that this equals

$$\begin{aligned}\|\Big(\frac{1}{h}\big(e^{-i(t+h)L} - e^{-itL}\big) + iLe^{-itL}\Big)\psi_0\|^2 &= \int_{\mathbb{R}} \big|\frac{1}{h}\big(e^{-i(t+h)\lambda} - e^{-it\lambda}\big) + i\lambda e^{-it\lambda}\big|^2 \, dE_{\psi_0,\psi_0}(\lambda) \\ = \int_{\mathbb{R}} \big|e^{-it\lambda}\Big(\frac{1}{h}\big(e^{-ih\lambda} - 1\big) + i\lambda\Big)\big|^2 \, dE_{\psi_0,\psi_0}(\lambda) &= \int_{\mathbb{R}} \big|\frac{1}{h}\big(e^{-ih\lambda} - 1\big) + i\lambda\big|^2 \, dE_{\psi_0,\psi_0}(\lambda).\end{aligned}$$

Since $\frac{1}{h}\big(e^{-ih\lambda} - 1\big) + i\lambda \to 0$ as $h \to 0$, we only need to show that we can interchange the limit with the integration. In order to do so we use $|\frac{1}{h}\big(e^{-i\lambda h} - 1\big)| \leq |\lambda|$, so that the integrand can be estimated by $4|\lambda|^2$ independent of $h$. So we require $\int_{\mathbb{R}} |\lambda|^2 \, dE_{\psi_0,\psi_0}(\lambda) < \infty$, or $\psi_0 \in D(L)$, see the Spectral Theorem 6.4.1.

To show uniqueness, assume that $\psi(t)$ and $\phi(t)$ are solutions to (3.1.1), then their difference $\varphi(t) = \psi(t) - \phi(t)$ is a solution to $i\varphi'(t) = L\varphi(t)$, $\varphi(0) = 0$. Consider

$$\begin{aligned}\frac{d}{dt}\|\varphi(t)\|^2 &= \frac{d}{dt}\langle\varphi(t), \varphi(t)\rangle = \langle\varphi'(t), \varphi(t)\rangle + \langle\varphi(t), \varphi'(t)\rangle \\ &= \langle -iL\varphi(t), \varphi(t)\rangle + \langle\varphi(t), -iL\varphi(t)\rangle = -i\Big(\langle L\varphi(t), \varphi(t)\rangle - \langle\varphi(t), L\varphi(t)\rangle\Big) = 0\end{aligned}$$

since $L$ is self-adjoint. So $\|\varphi(t)\|$ is constant and $\|\varphi(0)\| = 0$, it follows that $\varphi(t) = 0$ for all $t$ and uniqueness follows. □

It follows that the time-dependent Schrödinger equation is completely determined by the time-independent self-adjoint Schrödinger operator $L$.

**Exercise 3.1.2.** We consider the setting of Theorem 3.1.1. Show that $\psi(t) = e^{-i\lambda t}u$, $u \in L^2(\mathbb{R})$, $\lambda \in \mathbb{R}$ fixed, is a solution to the time-dependent Schrödinger equation (3.1.1) if and only if $u \in D(L)$ is an eigenvector of $L$ for the eigenvalue $\lambda$.

## 3.2 Scattering and wave operators

Let $L_0$ be the unperturbed Schrödinger operator $-\frac{d^2}{dx^2}$ with its standard domain $W^2(\mathbb{R})$ and let $L$ be the perturbed Schrödinger operator $-\frac{d^2}{dx^2} + q$. We assume that $L$ is self-adjoint, e.g. if the potential $q$ satisfies the conditions of Theorem 2.3.4. However, it should be noted that the set-up in this section is much more general and works for any two operators $L$ and $L_0$ which are (possibly unbounded) self-adjoint operators on a Hilbert space $\mathcal{H}$, and in this situation we now continue.

**Definition 3.2.1.** *The solution $\psi$ to* (3.1.1) *for a general self-adjoint operator $(L, D(L))$ on a Hilbert space $\mathcal{H}$ has an incoming asymptotic state $\psi^-(t) = \exp(-itL_0)\psi^-(0)$ for a self-adjoint operator $(L_0, D(L_0))$ on $\mathcal{H}$ if*

$$\lim_{t\to-\infty} \|\psi(t) - \psi^-(t)\| = 0.$$

*The solution $\psi$ to* (3.1.1) *has an outgoing asymptotic state* $\psi^+(t) = \exp(-itL_0)\psi^+(0)$ *if*

$$\lim_{t\to\infty} \|\psi(t) - \psi^+(t)\| = 0.$$

*The solution $\psi$ to* (3.1.1) *is a scattering state if it has an incoming asymptotic state and an outgoing asymptotic state.*

Define the operator $W(t) = e^{itL}e^{-itL_0}$, which is an element in $B(\mathcal{H})$. Note that $t \mapsto e^{itL}$ and $t \mapsto e^{-itL_0}$ are one-parameter groups of unitary operators. In particular, they are isometries, i.e. preserve norms. Also note that in general $e^{itL}e^{-itL_0} \neq e^{it(L-L_0)}$, unless $L$ and $L_0$ commute. Assuming the solution $\psi$ to (3.1.1) has an incoming state, then we have

$$\lim_{t\to-\infty} W(t)\psi^-(0) = \psi(0).$$

To see that this is true, write

$$\begin{aligned}\|W(t)\psi^-(0) - \psi(0)\| &= \|e^{itL}e^{-itL_0}\psi^-(0) - \psi(0)\| = \|e^{-itL_0}\psi^-(0) - e^{-itL}\psi(0)\| \\ &= \|\psi^-(t) - \psi(t)\| \to 0, \qquad t \to -\infty.\end{aligned}$$

Similarly, if the solution $\psi$ to (3.1.1) has an outgoing state, then we have

$$\lim_{t\to\infty} W(t)\psi^+(0) = \psi(0).$$

**Definition 3.2.2.** *The wave operators $W^\pm$ are defined as the strong limits of $W(t)$ as $t \to \pm\infty$. So its domain is*

$$D(W^\pm) = \{f \in \mathcal{H} \mid \lim_{t\to\pm\infty} W(t)f \ \textit{exists}\}$$

*and $W^\pm f = \lim_{t\to\pm\infty} W(t)f$ for $f \in D(W_\pm)$.*

**Exercise 3.2.3.** In Definition 3.2.2 we take convergence in the strong operator topology. To see that the operator norm is not suited, show that $\lim_{t\to\infty} W(t) = V$ exists in operator norm if and only if $L = L_0$, and in this case $V$ is the identity. Show first that $e^{itL}V = Ve^{itL_0}$ for all $t \in \mathbb{R}$. (Hint: if $V$ exists, observe that $\|e^{i(s+t)L}e^{-i(s+t)L_0} - e^{isL}Ve^{-isL_0}\| = \|e^{itL}e^{-itL_0} - V\| \to 0$ as $t \to \infty$, and hence, by uniqueness of the limit, $V = e^{isL}Ve^{-isL_0}$. Conclude that $\|e^{itL}e^{-itL_0} - V\| = \|1 - V\|$.)

Since $W(t)$ is a composition of unitaries, it is in particular an isometry. So $\|W(t)f\| = \|f\|$, so that the wave operators $W^\pm$ are partial isometries. The wave operators relate the initial values of the incoming, respectively outgoing, asympotic states for the unperturbed problem to the initial value for the perturbed problem. So $D(W^-)$, respectively $D(W^+)$, consists of initial values for the unperturbed time-dependent Schrödinger equation that occur as incoming, respectively outgoing, asymptotic states for solutions to (3.1.1). Its range $\mathrm{Ran}(W^-)$, respectively $\mathrm{Ran}(W^+)$, consists of initial values for the perturbed time-dependent Schrödinger equation (3.1.1) that have an incoming, respectively outgoing, asymptotic state.

Note that for a scattering state $\psi$, the wave operators completely determine the incoming and outgoing asymptotic states. Indeed, assume $W^{\pm}\psi^{\pm}(0) = \psi(0)$, then we can define $\psi^{\pm}(t) = \exp(-itL_0)\psi^{\pm}(0)$ and $\psi(t) = \exp(-itL)\psi(0)$. It then follows that

$$\lim_{t\to\pm\infty} \|\psi(t) - \psi^{\pm}(t)\| = \lim_{t\to\pm\infty} \|\psi(0) - W(t)\psi^{\pm}(0)\| = 0,$$

so that $\psi^{\pm}(t)$ are the incoming and outgoing asymptotic states. In physical models it is important to have as many scattering states as possible, preferably $\mathrm{Ran}(W^{\pm})$ is the whole Hilbert space $\mathcal{H}$. Note that scattering states have initial values in $\mathrm{Ran}\, W^+ \cap \mathrm{Ran}\, W^-$.

**Proposition 3.2.4.** *Assume that $L$ has an eigenvalue $\lambda$ for the eigenvalue $u \in D(L)$, and consider the solution $\psi(t) = \exp(-i\lambda t)u$ to* (3.1.1)*, see Exercise 3.1.2. Then $\psi$ has no (incoming or outgoing) asymptotic states unless $u$ is an eigenvector for $L_0$ for the same eigenvalue $\lambda$.*

*Proof.* Assume $\psi(t) = \exp(-i\lambda t)u$ has an incoming asymptotic state, so that there exists a $v \in \mathcal{H}$ such that $W^- v = u$ or $\lim_{t\to-\infty} W(t)v = u = \psi(0)$. This means $\| \exp(-itL_0)v - \exp(-itL)u\| = \| \exp(-itL_0)v - \exp(-it\lambda)u\| \to 0$ as $t \to -\infty$, and using the isometry property this gives $\| v - \exp(-it(\lambda - L_0))u\| \to 0$ as $t \to -\infty$. For $s \in \mathbb{R}$ fixed we get

$$\|e^{-i(t+s)(\lambda-L_0)}u - e^{-it(\lambda-L_0)}u\| \le \|e^{-i(t+s)(\lambda-L_0)}u - v\| + \|v - e^{-it(\lambda-L_0)}u\| \to 0, \quad t \to -\infty,$$

and so $\|e^{-is(\lambda-L_0)}u - u\| \to 0$ as $t \to -\infty$, but since the expression is independent of $t$, we actually have $e^{-is(\lambda-L_0)}u = u$ for arbitrary $s$, so that by Exercise 3.1.2, we have $L_0 u = \lambda u$. A similar reasoning applies to outgoing states. □

**Exercise 3.2.5.** Put $W(L, L_0)$ as the strong operator limit of $e^{itL}e^{-itL_0}$ to stress the dependence on the self-adjoint operators $L$ and $L_0$. Investigate how $W^{\pm}(L_0, L)$ and $W^{\pm}(L, L_0)$ are related. Show also that $W^{\pm}(A, B) = W^{\pm}(A, C)W^{\pm}(C, B)$ for self-adjoint $A, B, C \in B(\mathcal{H})$ assuming that the domains of all wave operators involved equal the Hilbert space $\mathcal{H}$. (See also Proposition 3.4.4.)

**Theorem 3.2.6.** *$D(W^{\pm})$ and $\mathrm{Ran}(W^{\pm})$ are closed subspaces of $\mathcal{H}$.*

*Proof.* Consider a convergent sequence $\{f_n\}_{n=1}^{\infty}$, $f_n \to f$ in $\mathcal{H}$ with $f_n \in D(W^+)$. We need to show that $f \in D(W^+)$. Recall that $W(t) \in B(\mathcal{H})$ and consider

$$\begin{aligned}\|W(t)f - W(s)f\| &\le \|W(t)(f - f_n)\| + \|W(s)(f_n - f)\| + \|\big(W(t) - W(s)\big)f_n\| \\ &= 2\,\|f - f_n\| + \|\big(W(t) - W(s)\big)f_n\|\end{aligned}$$

using that $W(t)$ and $W(s)$ are isometries. For $\varepsilon > 0$ arbitrary, we can find $N \in \mathbb{N}$ such that for $n \ge N$ we have $\|f - f_n\| \le \frac{\varepsilon}{2}$, since $f_n \to f$ in $\mathcal{H}$. And since $f_N \in D(W^+)$ we have $\lim_{t\to\infty} W(t)f_N$ exists, so there exists $T > 0$ such that for $s, t \ge T$ we have $\|\big(W(t) - W(s)\big)f_N\| \le \frac{\varepsilon}{2}$. So $\|W(t)f - W(s)f\| \le \varepsilon$, hence $\lim_{t\to\infty} W(t)f$ exists, and $f \in D(W^+)$. Similarly, $D(W^-)$ is closed.

Next take a convergent sequence $\{f_n\}_{n=1}^{\infty}$, $f_n \in \mathrm{Ran}(W^+)$, $f_n \to f$ in $\mathcal{H}$. Take $g_n \in D(W^+)$ with $W^+ g_n = f_n$, then

$$\|g_n - g_m\| \;=\; \|W^+(g_n - g_m)\| \;=\; \|f_n - f_m\|,$$

since $W^+$ is an isometry. So $\{g_n\}_{n=1}^{\infty}$ is a Cauchy sequence in $D(W^+) \subset \mathcal{H}$, hence convergent to, say, $g \in D(W^+)$, since $D(W^+)$ is closed. Now

$$\|f_n - W^+ g\| \;=\; \|W^+(g_n - g)\| \;=\; \|g_n - g\| \to 0, \qquad n \to \infty,$$

so $f = W^+ g \in \mathrm{Ran}(W^+)$. Similarly, $\mathrm{Ran}(W^-)$ is closed. □

So a scattering state $\psi$ has an incoming state and an outgoing state, and their respective values for $t = 0$ are related by the wave operators;

$$W^+\psi^+(0) \;=\; \psi(0) \;=\; W^-\psi^-(0).$$

Since the wave operator $W^-$ is an isometry from its domain to its range, it is injective, and we can write

$$\psi^+(0) \;=\; S\psi^-(0), \qquad S = (W^+)^{-1}W^-.$$

$S$ is the scattering operator; it relates the incoming asymptotic state $\psi^-$ with the outgoing asymptotic state $\psi^+$ for a scattering state $\psi$. Note that $S = (W^+)^{-1}W^-$ with

$$D(S) = \{f \in D(W^-) \mid W^- f \in \mathrm{Ran}(W^+)\}.$$

**Theorem 3.2.7.** $D(S) = D(W^-)$ *if and only if* $\mathrm{Ran}(W^-) \subset \mathrm{Ran}(W^+)$ *and* $\mathrm{Ran}(S) = D(W^+)$ *if and only if* $\mathrm{Ran}(W^+) \subset \mathrm{Ran}(W^-)$.

**Corollary 3.2.8.** $S\colon D(W^-) \to D(W^+)$ *is unitary if and only if* $\mathrm{Ran}(W^+) = \mathrm{Ran}(W^-)$.

So we can rephrase Corollary 3.2.8 as $S$ is unitary if and only if all solutions with an incoming asymptotic state also have an outgoing asymptotic state and vice versa. Loosely speaking, there are only scattering states.

*Proof of Theorem 3.2.7.* Consider the first statement. If $\mathrm{Ran}(W^-) \subset \mathrm{Ran}(W^+)$, then $D(S) = \{f \in D(W^-) \mid W^- f \in \mathrm{Ran}(W^+)\} = D(W^-)$ since the condition is true. Conversely, if $D(S) = D(W^-)$, we have by definition $W^- f \in \mathrm{Ran}(W^+)$ for all $f \in D(W^-)$, or $\mathrm{Ran}(W^-) \subset \mathrm{Ran}(W^+)$.

For the second statement, note that $Sf = g$ means $f \in D(S)$ and $W^+ g = W^- f$, so $\mathrm{Ran}(S) = \{g \in D(W^+) \mid W^+ g \in \mathrm{Ran}(W^-)\}$. So if $\mathrm{Ran}(W^+) \subset \mathrm{Ran}(W^-)$, the condition is void and $\mathrm{Ran}(S) = D(W^+)$. Conversely, if $\mathrm{Ran}(S) = D(W^+)$, we have $W^+ g \in \mathrm{Ran}(W^-)$ for all $g \in D(W^+)$ or $\mathrm{Ran}(W^+) \subset \mathrm{Ran}(W^-)$. □

The importance of the wave operators is that they can be used to describe possible unitary equivalences of the operators $L$ and $L_0$.

**Exercise 3.2.9.** Let $L$, $L_0$ be (possibly unbounded) self-adjoint operators with $LU = UL_0$ for some unitary operator $U$. Show that all spectra $\sigma$, $\sigma_p$, $\sigma_{pp}$, $\sigma_{ess}$, $\sigma_{ac}$, $\sigma_{sc}$ for $L$ and $L_0$ are the same. See Chapter 6, and in particular Section 6.6 for the notation.

Such self-adjoint operators which are unitarily equivalent have the same spectrum, knowing the wave operators plus the spectral decomposition of one of the operators gives the spectral decomposition of the other operator. However, the situation is not that nice, since the wave operators may not be defined on the whole Hilbert space or the range of the wave operators may not be the whole Hilbert space. So we need an additional definition, see also Section 6.2 for unexplained notions and notation.

**Definition 3.2.10.** *A closed subspace $V$ of an Hilbert space $\mathcal{H}$ is said to reduce, or to be a reducing subspace for, the operator $(T, D(T))$ if the orthogonal projection $P$ onto $V$ preserves the domain of $T$, $P\colon D(T) \to D(T)$, and commutes with $T$, $PT \subset TP$.*

Note that for a self-adjoint operator $(T, D(T))$ and a reducing subspace $V$, the orthocomplement $V^\perp$ is also a reducing subspace for $(T, D(T))$.

We first discuss reduction of the bounded operators $e^{-itL_0}$ and $e^{-itL}$, and from this, using Stone's Theorem 6.4.2, for the unbounded self-adjoint operators $L_0$ and $L$.

**Theorem 3.2.11.** *For each $t \in \mathbb{R}$ we have*

$$e^{-itL_0}\colon D(W^+) \to D(W^+), \qquad e^{-itL_0}\colon D(W^-) \to D(W^-),$$
$$e^{-itL}\colon \mathrm{Ran}(W^+) \to \mathrm{Ran}(W^+), \qquad e^{-itL}\colon \mathrm{Ran}(W^-) \to \mathrm{Ran}(W^-)$$

*and*

$$W^+ e^{-itL_0} = e^{-itL} W^+, \qquad W^- e^{-itL} = e^{-itL_0} W^-.$$

Since $\big(e^{-itL_0}\big)^* = e^{itL_0}$ and $\big(e^{-itL}\big)^* = e^{itL}$ by the self-adjointness of $L$ and $L_0$, we obtain

$$e^{-itL_0}\colon D(W^+)^\perp \to D(W^+)^\perp, \qquad e^{-itL_0}\colon D(W^-)^\perp \to D(W^-)^\perp,$$
$$e^{-itL}\colon \mathrm{Ran}(W^+)^\perp \to \mathrm{Ran}(W^+)^\perp, \qquad e^{-itL}\colon \mathrm{Ran}(W^-)^\perp \to \mathrm{Ran}(W^-)^\perp.$$

By Theorem 3.2.6 the subspaces $D(W^\pm)$, $\mathrm{Ran}(W^\pm)$ are closed, and since orthocomplements are closed as well, we can rephrase the first part of Theorem 3.2.11.

**Corollary 3.2.12.** *$D(W^\pm)$ and $D(W^\pm)^\perp$ reduce $e^{-itL_0}$ and $\mathrm{Ran}(W^\pm)$ and $\mathrm{Ran}(W^\pm)^\perp$ reduce $e^{-itL}$.*

*Proof of Theorem 3.2.11.* Take $f \in D(W^+)$ and put $g = W^+ f$ and consider

$$\begin{aligned} W(t)e^{-isL_0}f - e^{-isL}g &= e^{itL}e^{-itL_0}e^{-isL_0}f - e^{-isL}g = e^{itL}e^{-i(s+t)L_0}f - e^{-isL}g \\ &= e^{-isL}e^{i(s+t)L}e^{-i(s+t)L_0}f - e^{-isL}g = e^{-isL}W(t+s)f - e^{-isL}g = e^{-isL}\big(W(t+s)f - g\big) \end{aligned}$$

and since $e^{-isL}$ is an isometry we find, for $s \in \mathbb{R}$ fixed,

$$\|W(t)e^{-isL_0}f - e^{-isL}g\| = \|W(t+s)f - g\| \to 0, \qquad t \to \infty.$$

In particular, $e^{-isL_0}f \in D(W^+)$ and $W^+e^{-isL_0}f = e^{-isL}g = e^{-isL}W^+f$. This proves that $e^{-isL_0}$ preserves $D(W^+)$ and that $e^{-isL}$ preserves $\mathrm{Ran}(W^+)$ and $W^+e^{-isL_0} = e^{-isL}W^+$.

The statement for $W^-$ is proved analogously. $\square$

In order to see that these spaces also reduce $L$ and $L_0$ we need to consider the orthogonal projections on $D(W^\pm)$ and $\mathrm{Ran}(W^\pm)$ in relation to the domains of $L$ and $L_0$. We use the characterisation of the domain of $L$, respectively $L_0$, as those $f \in \mathcal{H}$ for which the limit $\lim_{t\to 0} \frac{1}{t}\big(\exp(-itL)f - f\big)$, respectively $\lim_{t\to 0} \frac{1}{t}\big(\exp(-itL_0)f - f\big)$, exists, see Stone's Theorem 6.4.2.

**Theorem 3.2.13.** *$D(W^+)$ and $D(W^-)$ reduce $L_0$ and $\mathrm{Ran}(W^+)$ and $\mathrm{Ran}(W^-)$ reduce $L$.*

*Proof.* We show that first statement. Let $P^+ \colon \mathcal{H} \to \mathcal{H}$ be the orthogonal projections on $D(W^+)$. Then we have to show first that $P^+$ preserves the domain $D(L_0)$. Take $f \in D(L_0)$, then for all $t \in \mathbb{R}\backslash\{0\}$ we have

$$\frac{1}{t}\big(e^{-itL_0}P^+f - P^+f\big) = P^+\Big(\frac{1}{t}\big(e^{-itL_0}f - f\big)\Big)$$

by Corollary 3.2.12. For $f \in D(L_0)$ the right hand side converges as $t \to 0$ by Stone's Theorem 6.4.2 and continuity of $P^+$. Hence the left hand side converges. By Stone's Theorem 6.4.2 it follows that $P^+f \in D(L_0)$.

For $f \in D(L_0)$ we multiply this identity by $i$ and take the limit $t \to 0$. Again by Stone's Theorem 6.4.2 it follows that $L_0P^+f = P^+L_0f$ for all $f \in D(L_0)$. Since $D(L_0) = D(P^+L_0) \subset D(L_0P^+) = \{f \in \mathcal{H} \mid P^+f \in D(L_0)\}$ we get $P^+L_0 \subset L_0P^+$. $\square$

**Exercise 3.2.14.** Prove the other cases of Theorem 3.2.13.

In view of Theorems 3.2.11 and 3.2.13 we may expect that the wave operators intertwine $L$ and $L_0$. This is almost true, and this is the content of the following Theorem 3.2.15.

**Theorem 3.2.15.** *Let $P$ be the orthogonal projection on $\mathrm{Ker}(L_0)^\perp$, then $LW^+P = W^+L_0$ and $LW^-P = W^-L_0$.*

Note that this is a statement for generally unbounded operators, so that this statement also involves the domains of the operators. In case $L_0$ has trivial kernel, we see that $W^+$ and $W^-$ intertwine the self-adjoint operators. In particular, in case the wave operators are unitary, we see that $L$ and $L_0$ are unitarily equivalent, and so by Exercise 3.2.9 have the same spectrum.

*Proof.* Observe first that $\mathrm{Ker}(L_0)^\perp = \overline{\mathrm{Ran}(L_0)}$. Indeed, we have for arbitrary $f \in \mathrm{Ker}(L_0)$ and for arbitrary $g \in D(L_0)$ the identity $0 = \langle L_0f, g\rangle = \langle f, L_0g\rangle$, since $L_0$ is self-adjoint.

Next we note that, with the notation $P^\pm$ for the orthogonal projection on the domains $D(W^\pm)$ for the wave operators as in Theorem 3.2.13, we have $PP^\pm P = P^\pm P$. Indeed, this is obviously true on $\mathrm{Ker}(L_0)$ since both sides are zero. For any $f \in \mathrm{Ran}(L_0)$ put $f = L_0g$, so that $PP^+Pf = PP^+f = PP^+L_0g = PL_0P^+g = L_0P^+g = P^+L_0g = P^+f = P^+Pf$ by Theorem

3.2.13 (twice) and the observation $PL_0 = L_0$. So the result follows for any $f \in \mathrm{Ran}(L_0)$, and since orthogonal projections are bounded operators the result follows for $\overline{\mathrm{Ran}(L_0)}$ by continuity of the projections. The case for $P^-$ is analogous.

We first show that $LW^+P \supset W^+L_0$. So take $f \in D(W^+L_0) = \{f \in D(L_0) \mid L_0 f \in D(W^+)\}$. Then $f = Pf + (1-P)f$, so that $f \in D(L_0)$, $(1-P)f \in \mathrm{Ker}(L_0) \subset D(L_0)$ shows that $Pf \in D(L_0)$. Since with $D(W^+)$, also $D(W^+)^\perp$, reduces $L_0$, we see that $(1-P^+)Pf \in D(L_0)$ and

$$L_0(1-P^+)Pf = (1-P^+)L_0 Pf = (1-P^+)L_0 f$$

since $L_0 Pf = L_0 f + L_0(1-P)f = L_0 f$ as $1-P$ projects onto $\mathrm{Ker}(L_0)$. Since $f \in D(W^+L_0)$, we have $L_0 f \in D(W^+)$, so that $(1-P^+)L_0 f = 0$. We conclude that $(1-P^+)Pf \in \mathrm{Ker}(L_0)$ and $P(1-P^+)Pf = 0$ or $Pf = P^2 f = PP^+Pf = P^+Pf$, where the last equality follows from the second observation in this proof. Now $Pf = P^+Pf$ says $Pf \in D(W^+)$ or $f \in D(W^+P)$.

As a next step we show that $W^+Pf \in D(L)$, and for this we use Stone's Theorem 6.4.2. So, using Theorem 3.2.11,

$$\frac{1}{t}\big(e^{-itL} - 1\big)W^+Pf = W^+\frac{1}{t}\big(e^{-itL_0} - 1\big)Pf. \tag{3.2.1}$$

Since $Pf \in D(L_0)$, $\lim_{t\to 0} \frac{1}{t}\big(e^{-itL} - 1\big)Pf$ exists and since the domain of $W^+$ is closed it follows that the right hand side has a limit $-iW^+LPf$ as $t \to 0$. So the left hand side has a limit, and by Stone's Theorem 6.4.2, we have $W^+Pf \in D(L)$ and the limit is $-iLW^+Pf$. So $f \in D(LW^+P)$ and $LW^+Pf = W^+L_0Pf$, and since $L_0Pf = L_0 f$ we have $W^+L_0 \subset LW^+P$.

Conversely, to show $LW^+P \subset W^+L_0$, take $f \in D(LW^+P)$, or $Pf \in D(W^+)$ and $W^+Pf \in D(L)$. So, again by Stone's Theorem 6.4.2, $\lim_{t\to 0} \frac{1}{t}(e^{-itL} - 1)W^+Pf$ exists, and since (3.2.1) is valid, we see that $W^+\frac{1}{t}(e^{-itL_0} - 1)Pf$ converges to, say, $g = -iLW^+Pf$. Since $W^+$ is continuous, $g \in \overline{\mathrm{Ran}(W^+)} = \mathrm{Ran}(W^+)$ by Theorem 3.2.6. So $g = W^+h$ for some $h \in \mathcal{H}$, and

$$\|\frac{1}{t}\big(e^{-itL_0} - 1\big)Pf - h\| = \|W^+\frac{1}{t}\big(e^{-itL_0} - 1\big)Pf - W^+h\| = \|W^+\frac{1}{t}\big(e^{-itL_0} - 1\big)Pf - g\| \to 0,$$

as $t \to \infty$. Again, by Stone's Theorem 6.4.2, $Pf \in D(L_0)$ and $-iL_0Pf = h$, and thus $W^+L_0Pf = iW^+h = ig = LW^+Pf$. As before, with $Pf \in D(L_0)$ it follows $f \in D(L_0)$ and $L_0Pf = L_0f$, so that we have $f \in D(W^+L_0)$ and $LW^+Pf = W^+L_0f$. This proves $LW^+P \subset W^+L$.

The case $W^-$ is analogous. □

**Exercise 3.2.16.** Consider the operator $L_0 = i\frac{d}{dx}$ with domain $W^1(\mathbb{R})$, then $L_0$ is an unbounded self-adjoint operator on $L^2(\mathbb{R})$, see Lemma 2.1.2. For $L$ we take $i\frac{d}{dx} + q$, for some potential function $q$.

- Show that $U(t) = e^{itL_0}$ is a translation operator, i.e. $\big(U(t)f\big)(x) = f(x-t)$.
- Define $M$ to be the multiplication operator by a function $m$. Show that for $im' = qm$ we have $L_0 M = M L$. What conditions on $q$ imply that $M\colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is a unitary operator? Give a domain $D(L)$ such that $(L, D(L))$ is an unbounded self-adjoint operator on $L^2(\mathbb{R})$.

- Assume these conditions on $m$. Conclude that $e^{itL} = M^* e^{itL_0} M = M^* U(t) M$, and $W(t) = M^* U(t) M U(-t)$ is a multiplication operator.

- What conditions on $q$ ensure that $W^{\pm}$ exist? What are $W^{\pm}$ in this case? Describe the scattering operator $S = (W^+)^{-1} W^-$ as well in this case. (Hint: $S$ is a multiple of the identity.)

## 3.3 Domains of the wave operators for the Schrödinger operator

In Sections 3.1, 3.2 the situation was completely general. In this section we discuss conditions on the potential $q$ of the Schrödinger equation $L = -\frac{d^2}{dx^2} + q$, such that $D(W^{\pm})$ equal the whole Hilbert space $L^2(\mathbb{R})$.

The idea of the method, due to Cook, is based on the observation that for a $f \in C^1(\mathbb{R})$ with integrable derivative, $f' \in L^1(\mathbb{R})$, the limit $\lim_{t\to\infty} f(t)$ exists. This follows from the estimate

$$|f(t) - f(s)| = |\int_s^t f'(x)\,dx| \leq \int_s^t |f'(x)|\,dx \to 0$$

for $s < t$ and $s$, $t$ tend to $\infty$. Similarly, the limit $\lim_{t\to-\infty} f(t)$ exists. Cook's idea is also used in Theorem 3.4.9. This gives rise to the following description.

**Proposition 3.3.1.** *Assume that* $\exp(-itL_0)f \in D(L_0) \cap D(L)$ *for all* $t \geq a$ *for some* $a \in \mathbb{R}$, *and that*

$$\int_a^\infty \|(L - L_0)e^{-itL_0} f\|\,dt < \infty,$$

*then* $f \in D(W^+)$. *Similarly, if* $\exp(-itL_0)g \in D(L_0) \cap D(L)$ *for all* $t \leq b$ *for some* $b \in \mathbb{R}$, *and that*

$$\int_{-\infty}^b \|(L - L_0)e^{-itL_0} g\|\,dt < \infty,$$

*then* $g \in D(W^-)$.

*Proof.* Recalling $W(t)f = e^{itL}e^{-itL_0}f$, we see that

$$W'(t)f = iL\,e^{itL}e^{-itL_0}f - ie^{itL}L_0e^{-itL_0}f,$$

where we need $\exp(-itL_0)f \in D(L)$, $f \in D(L_0)$, cf. Theorem 3.1.1. Since this shows $\exp(-itL_0)f \in D(L) \cap D(L_0)$ we have $W'(t)f = i\exp(itL)\big(L - L_0\big)\exp(-itL_0)f$ and hence $\|W'(t)f\| = \|(L - L_0)\exp(-itL_0)f\|$.

Apply now the previous observation to get for arbitrary $u \in L^2(\mathbb{R})$,

$$|\langle W(t)f, u\rangle - \langle W(s)f, u\rangle| \leq \int_s^t |\langle W'(x)f, u\rangle|\,dx \leq \|u\| \int_s^t \|W'(x)f\|\,dx,$$

which shows that

$$\|W(t)f - W(s)f\| \le \int_s^t \|W'(x)f\|\,dx \le \int_s^t \|(L-L_0)\exp(-ixL_0)f\|\,dx.$$

By assumption for $t > s \ge a$, the right hand side integrated over $[a,\infty)$ is finite. Hence, $\lim_{t\to\infty} W(t)f$ exists, or $f \in D(W^+)$. □

**Theorem 3.3.2.** *Let $L$ be the Schrödinger operator, where the potential $q$ satisfies the conditions of Corollary 2.2.7, and $L_0$ is the unperturbed operator $-\frac{d^2}{dx^2}$ with domain $W^2(\mathbb{R})$. If $x \mapsto (1+|x|)^\alpha q(x)$ is an element of $L^2(\mathbb{R})$ for some $\alpha > \frac{1}{2}$, then $D(W^+) = L^2(\mathbb{R}) = D(W^-)$.*

The following gives a nice special case of the theorem.

**Corollary 3.3.3.** *Theorem 3.3.2 holds true if the potential $q$ is locally square integrable and for some $\beta > 1$ the fuction $x \mapsto |x|^\beta q(x)$ is bounded for $|x| \to \infty$.*

**Exercise 3.3.4.** Prove Corollary 3.3.3 from Theorem 3.3.2.

*Proof of Theorem 3.3.2.* The idea is to show that we can use Proposition 3.3.1 for sufficiently many functions. Consider the function $f_s(\lambda) = \lambda\exp(-\lambda^2 - is\lambda)$ for $s \in \mathbb{R}$. Then $f_s \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$. We want to exploit the fact that the Fourier transform diagonalises $L_0 = -\frac{d^2}{dx^2}$, see Theorem 2.1.1 and its proof. We consider $u_s = \mathcal{F}^{-1} f_s$, then

$$\begin{aligned}\big(e^{-itL_0}u_s\big)(x) &= \mathcal{F}^{-1}\big(e^{-it\lambda^2} f_s(\lambda)\big)(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{i\lambda(x-s)-\lambda^2(1+it)} \lambda d\lambda \\ &= \frac{\exp\big(\frac{-(x-s)^2}{4(1+it)}\big)}{\sqrt{2\pi}} \int_{\mathcal{C}} e^{-z^2}\Big(\frac{z}{\sqrt{1+it}} + \frac{i(x-s)}{2(1+it)}\Big)\frac{dz}{\sqrt{1+it}}\end{aligned}$$

by switching to $z = \big(\sqrt{1+it}\big)\big(\lambda - \frac{i}{2}\frac{x-s}{1+it}\big)$. Here the square root is $\sqrt{z} = \sqrt{|z|}e^{i\frac{1}{2}\arg z}$ for $|\arg z| < \pi$, and the contour $\mathcal{C}$ in the complex plane is a line corresponding to the image of the real line under this coordinate transformation.

**Lemma 3.3.5.** $\int_{\mathcal{C}} e^{-z^2}dz = \sqrt{\pi}$, $\int_{\mathcal{C}} e^{-z^2} z dz = 0$.

Using Lemma 3.3.5 we see that

$$\big(e^{-itL_0}u_s\big)(x) = \frac{i(x-s)}{\big(\sqrt{2+2it}\big)^3} \exp\big(\frac{-(x-s)^2}{4(1+it)}\big),$$

so

$$\big|\big(e^{-itL_0}u_s\big)(x)\big| \le \frac{|x-s|}{\big(4+4t^2\big)^{3/4}} \exp\big(\frac{-(x-s)^2}{4(1+t^2)}\big).$$

Now we have

$$\|(L-L_0)e^{-itL_0}u_s\|^2 = \|qe^{-itL_0}u_s\|^2 = \int_{\mathbb{R}} \frac{|q(x)(x-s)|^2}{\big(4+4t^2\big)^{3/2}} \exp\big(\frac{-(x-s)^2}{2(1+t^2)}\big)\,dx,$$

which we have to integrate with respect to $t$ in order to be able to apply Proposition 3.3.1.

Using the estimate $e^{-x} \leq (1+\frac{x}{a})^{-a}$ for $x \geq 0$ and $a \geq 0$, we get

$$\begin{aligned}\exp\big(\frac{-(x-s)^2}{2(1+t^2)}\big) &\leq \Big(1+\frac{(x-s)^2}{2a(1+t^2)}\Big)^{-a} = (2a)^a(1+t^2)^a\big(2a(1+t^2)+(x-s)^2\big)^{-a} \\ &\leq (2a)^a(1+t^2)^a|x-s|^{-2a}\end{aligned}$$

so that

$$\|(L-L_0)e^{-itL_0}u_s\|^2 \leq C(1+t^2)^{a-\frac{3}{2}} \int_{\mathbb{R}} |q(x)|^2|x-s|^{2-2a}\,dx$$

and noting $|x-s| \leq (1+|x|)(1+|s|)$ and inserting this estimate gives, assuming $a \leq 1$,

$$\|(L-L_0)e^{-itL_0}u_s\|^2 \leq C(1+t^2)^{a-3/2} \int_{\mathbb{R}} |q(x)|^2(1+|x|)^{2-2a}\,dx$$

with the constant $C$ independent of $x$ and $t$, but depending on $s$ and $a$. Hence,

$$\int_{\mathbb{R}} \|(L-L_0)e^{-itL_0}u_s\|\,dt \leq C\int_{\mathbb{R}}(1+t^2)^{a/2-3/4}\,dt\Big(\int_{\mathbb{R}}|q(x)|^2(1+|x|)^{2-2a}\,dx\Big)^{1/2}$$

and the integral with respect to $t$ is finite for $\frac{3}{2}-a>1$ or $a<\frac{1}{2}$ and the integral with respect to $x$ is the $L^2(\mathbb{R})$-norm of $x \mapsto q(x)(1+|x|)^{1-a}$, and this is finite by assumption if $1-a \leq \alpha$. Since we need $0 \leq a < \frac{1}{2}$, we see that the integral is finite for a suitable choice of $a$ if $\alpha > \frac{1}{2}$. By Proposition 3.3.1 we see that $u_s \in D(W^{\pm})$ for arbitrary $s \in \mathbb{R}$.

**Lemma 3.3.6.** *$\{u_s \mid s \in \mathbb{R}\}$ is dense in $L^2(\mathbb{R})$.*

Now Lemma 3.3.6 and Theorem 3.2.6 imply that $D(W^+) = L^2(\mathbb{R}) = D(W^-)$. $\square$

**Exercise 3.3.7.** Prove Lemma 3.3.5 and Lemma 3.3.6. For the proof of Lemma 3.3.5 use that the lemma is true if $\mathcal{C} = \mathbb{R}$ and Cauchy's theorem from Complex Function Theory on shifting contours for integrals of analytic functions. For the proof of Lemma 3.3.6 proceed as follows; take $g \in L^2(\mathbb{R})$ orthogonal to any $u_s$, then

$$0 = \langle g, u_s\rangle = \langle \mathcal{F}g, \mathcal{F}u_s\rangle = \int_{\mathbb{R}} \big(\mathcal{F}g\big)(\lambda)\lambda e^{-\lambda^2}e^{is\lambda}\,d\lambda$$

for any $s$, i.e. the Fourier inverse of $\big(\mathcal{F}g\big)(\lambda)\lambda e^{-\lambda^2}$ equals zero. Conclude that $g$ has to be zero in $L^2(\mathbb{R})$.

## 3.4 Completeness

As stated in Section 3.2 we want as many scattering states as possible. Moreover, by Proposition 3.2.4, the discrete spectrum is not be expected to be related to scattering states, certainly not for the Schrödinger operator $L$ and unperturbed Schrödinger operator $-\frac{d^2}{dx^2}$, since for the last one $\sigma_p = \emptyset$, whereas the discrete spectrum of the Schrödinger operator $L$ may be non-trivial. For this reason we need to exclude eigenvectors, and we go even one step further by restricting to the subspace of absolute continuity, see Section 6.6. Again, we phrase the results for self-adjoint operators $L$ and $L_0$ acting on a Hilbert space $\mathcal{H}$, but the main example is the case of the Schrödinger operators on $L^2(\mathbb{R})$.

We assume that the domains of the wave operator $W^\pm$ at least contain the absolute continuous subspace $\mathcal{H}_{ac}(L_0)$ for the operator $L_0$.

**Exercise 3.4.1.** Show that for the unperturbed Schrödinger operator $-\frac{d^2}{dx^2}$ the subspace of absolute continuity is equal to $\mathcal{H}$, so $P_{ac} = 1$.

**Definition 3.4.2.** *Let $L$ and $L_0$ be self-adjoint operators on the Hilbert space $\mathcal{H}$. The generalised wave operators $\Omega^\pm = \Omega^\pm(L, L_0)$ exist if $\mathcal{H}_{ac}(L_0) \subset D(W^\pm)$, and $\Omega^\pm = W^\pm P_{ac}(L_0)$.*

We first translate some of the results of the wave operators obtain in Section 3.2 to the generalised wave operators $\Omega^\pm$.

**Proposition 3.4.3.** *Assume that $\Omega^\pm$ exist, then*

1. *$\Omega^\pm$ are partial isometries with inital space $\mathrm{Ran}(P_{ac}(L_0))$ and final space $\mathrm{Ran}(\Omega^\pm)$,*
2. *$\Omega^\pm(D(L_0)) \subset D(L)$ and $L\,\Omega^\pm = \Omega^\pm L_0$,*
3. *$\mathrm{Ran}(\Omega^\pm) \subset \mathrm{Ran}(P_{ac}(L))$.*

*Proof.* The first statement follows from the discussion following Definition 3.2.2. The second statement follows from Theorem 3.2.13 and Theorem 3.2.15 and the observation that $\mathrm{Ker}(L_0) \subset \mathrm{Ran}\, P_{pp}(L_0) \subset \big(\mathrm{Ran}\, P_{ac}(L_0)\big)^\perp$ and Theorem 6.6.2. By the second result we see that the generalised wave operators intertwine $L\big|_{\mathrm{Ran}(\Omega^\pm)}$ with $L_0\big|_{\mathrm{Ran}(P_{ac}(L_0))}$ and by the first statement this equivalence is unitary. So $L\big|_{\mathrm{Ran}(\Omega^\pm)}$ has only absolutely continuous spectrum or $\mathrm{Ran}(\Omega^\pm) \subset P_{ac}(L)$, see Section 6.6. $\square$

The next proposition should be compared to Exercise 3.2.5, and because we take into account the projection onto the absolutely continuous subspace some more care is needed.

**Proposition 3.4.4.** *Let $A, B, C$ be self-adjoint operators, and assume that $\Omega^\pm(A, B)$ and $\Omega^\pm(B, C)$ exist, then $\Omega^\pm(A, C)$ exist and $\Omega^\pm(A, C) = \Omega^\pm(A, B)\Omega^\pm(B, C)$.*

In particular, $\Omega^\pm(A, A) = P_{ac}(A)$, which follows by definition.

*Proof.* Since $\Omega^+(B, C)$ exists, it follows from the third statement of Proposition 3.4.3 that $\mathrm{Ran}(\Omega^+(B, C)) \subset \mathrm{Ran}(P_{ac}(B))$, so for any $\psi \in \mathcal{H}$ we have $\big(1 - P_{ac}(B)\big)\Omega^+(B, C)\psi = 0$, or

$$\lim_{t\to\infty} \|\big(1 - P_{ac}(B)\big)e^{itB}e^{-itC}\psi\| = 0.$$

Now

$$\begin{aligned} e^{itA}e^{-itC}P_{ac}(C)\psi &= e^{itA}e^{-itB}e^{itB}e^{-itC}P_{ac}(C)\psi \\ &= e^{itA}e^{-itB}P_{ac}(B)e^{itB}e^{-itC}P_{ac}(C)\psi + e^{itA}e^{-itB}(1-P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\psi. \end{aligned}$$

Put $\Omega^+(B,C)\psi = \phi$, and $\Omega^+(A,B)\phi = \xi$, then

$$\begin{aligned} &\|e^{itA}e^{-itC}P_{ac}(C)\psi - \xi\| \leq \|e^{itA}e^{-itB}P_{ac}(B)e^{itB}e^{-itC}P_{ac}(C)\psi - \xi\| \\ &\qquad + \|e^{itA}e^{-itB}(1-P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\psi\| \\ &\leq \|e^{itA}e^{-itB}P_{ac}(B)e^{itB}e^{-itC}P_{ac}(C)\psi - e^{itA}e^{-itB}P_{ac}(B)\phi\| + \|e^{itA}e^{-itB}P_{ac}(B)\phi - \xi\| \\ &\qquad + \|(1-P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\psi\| \\ &\leq \|e^{itB}e^{-itC}P_{ac}(C)\psi - \phi\| + \|e^{itA}e^{-itB}P_{ac}(B)\phi - \xi\| + \|(1-P_{ac}(B))e^{itB}e^{-itC}P_{ac}(C)\psi\| \end{aligned}$$

and since each of these three terms tends to zero as $t \to \infty$, the result follows. □

Completeness is related to the fact that we only have scattering states, i.e. any solution to the time-dependent Schrödinger equation with an incoming asymptotic state also has an outgoing asymptotic state and vice versa. This is known as weak asymptotic completeness, and for the generalised wave operators this means $\mathrm{Ran}(\Omega^+(L,L_0)) = \mathrm{Ran}(\Omega^-(L,L_0))$. We have strong asymptotic completeness if $\mathrm{Ran}(\Omega^+(L,L_0)) = \mathrm{Ran}(\Omega^-(L,L_0)) = \big(P_{pp}(L)\mathcal{H}\big)^\perp$. Here $P_{pp}(L)$ is the projection on the closure of the subspace of consisting of all eigenvectors of $L$, see Section 6.6. In this section we have an intermediate notion for completeness, and here $P_{ac}(L)$ denotes the orthogonal projection onto the absolutely continuous subspace for $L$, see Section 6.6.

**Definition 3.4.5.** *Assume $\Omega^\pm(L,L_0)$ exist, then we say that the generalised wave operators are complete if* $\mathrm{Ran}(\Omega^+(L,L_0)) = \mathrm{Ran}(\Omega^-(L,L_0)) = \mathrm{Ran}(P_{ac}(L))$.

Note that completeness plus empty singular continous spectrum of $L$, see Section 6.6, is equivalent to strong asymptotic completeness.

**Theorem 3.4.6.** *Assume $\Omega^\pm(L,L_0)$ exist. Then the generalised wave operators $\Omega^\pm(L,L_0)$ are complete if and only if the generalised wave operators $\Omega^\pm(L_0,L)$ exist.*

*Proof.* Assume first that $\Omega^\pm(L,L_0)$ and $\Omega^\pm(L_0,L)$ exist. By Proposition 3.4.4 we have

$$P_{ac}(L) = \Omega^\pm(L,L) = \Omega^\pm(L,L_0)\Omega^\pm(L_0,L),$$

so that $\mathrm{Ran}(P_{ac}(L)) \subset \mathrm{Ran}(\Omega^\pm(L,L_0))$. Since Proposition 3.4.3 gives the reverse inclusion, we have $\mathrm{Ran}(P_{ac}(L)) = \mathrm{Ran}(\Omega^\pm(L,L_0))$, and so the generalised wave operators are complete.

Conversely, assume completeness of the wave operators $\Omega^\pm(L,L_0)$. For $\phi \in P_{ac}(L) = \mathrm{Ran}(\Omega^+(L,L_0))$ we have $\psi$ such that $\phi = \Omega^+(L,L_0)\psi$, or

$$\|e^{itL}e^{-itL_0}P_{ac}(L_0)\psi - \phi\| = \|e^{-itL_0}P_{ac}(L_0)\psi - e^{-itL}\phi\| = \|P_{ac}(L_0)\psi - e^{itL_0}e^{-itL}\phi\|$$

tends to zero as $t \to \infty$. It follows that strong limit of $e^{itL_0}e^{-itL}$ exists on the absolutely continuous subspace for $L$, hence $\Omega^+(L_0,L)$ exists. □

Theorem 3.4.6 gives a characterisation that is usually hard to establish. The reason is that $L_0$ is the unperturbed "simple" operator, and we can expect to have control on its absolutely continuous subspace and its spectral decomposition, but in order to apply Theorem 3.4.6 one also needs to know these properties of the perturbed operator, which is much harder. There are many theorems (the so-called Kato-Birman theory) on the existence of the generalised wave operators if $L$ and $L_0$ (or $f(L)$ and $f(L_0)$ for a suitable function $f$) differ by a trace-class operator. This is less applicable for the Schrödinger operators.

In the remainder of this Chapter 3 we use the notion of $T$-smooth operators in order to study wave operators for the Schrödinger operators. However, the proof is too technical to consider in detail, and we only discuss the main ingredients.

**Definition 3.4.7.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. A closed operator $(S, D(S))$ on $\mathcal{H}$ is $T$-smooth if there exists a constant $C$ such that for all $x \in \mathcal{H}$ the element $e^{itT}x \in D(S)$ for almost all $t \in \mathbb{R}$ and*

$$\frac{1}{2\pi} \int_{\mathbb{R}} \|Se^{itT}\, x\|^2 \, dt \leq C\, \|x\|^2.$$

Note that the identity operator is never $T$-smooth for any operator $T$.

The notion of $T$-smooth is stronger than the assumption occuring in the Rellich Perturbation Theorem 2.2.4.

**Proposition 3.4.8.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and the closed operator $(S, D(S))$ on $\mathcal{H}$ be $T$-smooth. Then for all $\varepsilon > 0$ there exists a $K$ such that*

$$\|Sx\| \leq \varepsilon\, \|Tx\| + K\, \|x\|, \qquad \forall x \in D(T).$$

*Moreover,* $\overline{\mathrm{Ran}(S^*)} \subset \mathcal{H}_{ac}(T)$.

*Proof.* Use the functional calculus and the formula

$$\frac{1}{x-a} = i \int_0^\infty e^{-ixt} e^{iat}\, dt, \qquad \Im a > 0,$$

to find for $y \in D(S^*)$, $x \in \mathcal{H}$, $a = \lambda + i\varepsilon$, the expression

$$-i\, \langle R(\lambda + i\varepsilon)x, S^*y\rangle = \int_0^\infty \langle e^{-itT}x, S^*y\rangle\, e^{i\lambda t} e^{-\varepsilon t}\, dt = \int_0^\infty \langle Se^{-itT}x, y\rangle\, e^{i\lambda t} e^{-\varepsilon t}\, dt$$

for all $\varepsilon > 0$, where $R(z) = (T - z)^{-1}$, $z \in \rho(T)$, is the resolvent for $T$, see Section 6.4. To estimate this expression we use the Cauchy-Schwarz inequality (6.1.1) in $L^2(0, \infty)$;

$$\begin{aligned} |\langle R(\lambda + i\varepsilon)x, S^*y\rangle| &\leq \|y\| \int_0^\infty \|Se^{-itT}x\| e^{-\varepsilon t}\, dt \\ &\leq \|y\| \left( \int_0^\infty \|Se^{-itT}x\|^2\, dt \right)^{\frac{1}{2}} \left( \int_0^\infty e^{-2\varepsilon t}\, dt \right)^{\frac{1}{2}} \leq \frac{\|y\|}{\sqrt{2\varepsilon}} \sqrt{2\pi C}\, \|x\|, \end{aligned}$$

since $S$ is $T$-smooth. It follows that $y \mapsto \langle S^* y, R(\lambda+i\varepsilon)x\rangle$ is continuous, so that $R(\lambda+i\varepsilon)x \in D(S^{**}) = D(S)$, since $S$ is closed, and $\|SR(\lambda+i\varepsilon)x\| \leq \sqrt{\frac{\pi C}{\varepsilon}}\,\|x\|$. Since $\mathrm{Ran}(R(z)) = D(T)$, see Lemma 6.2.2, we see that $D(T) \subset D(S)$. Now for $x \in D(T)$ write

$$\|Sx\| = \|SR(\lambda+i\varepsilon)(T-(\lambda+i\varepsilon))\,x\| \leq \sqrt{\frac{\pi C}{\varepsilon}}\,\|(T-(\lambda+i\varepsilon))\,x\| \leq \sqrt{\frac{\pi C}{\varepsilon}}\Big(\|Tx\|+\sqrt{\lambda^2+\varepsilon^2}\|x\|\Big)$$

and take $\varepsilon$ big in order to obtain the result.

Next, use the closedness of $\mathcal{H}_{ac}$ to reduce to proving $\mathrm{Ran}(S^*) \subset \mathcal{H}_{ac}(T)$. Take $x = S^*y \in \mathrm{Ran}(S^*)$ and consider almost everywhere

$$\sqrt{2\pi}\,F(t) = \int_{\mathbb{R}} e^{-itu}\,dE_{x,x}(u) = \langle e^{-itT}x, x\rangle = \langle e^{-itT}x, S^*y\rangle = \langle Se^{-itT}x, y\rangle,$$

where $E$ is the spectral measure for the self-adjoint operator $T$. Now estimate $|F(t)| \leq \|Se^{-itT}x\|\|y\|$ to see that $F \in \mathcal{H}$. Since $F$ is the Fourier transform of the measure $E_{x,x}$ we see from the Plancherel Theorem, see Section 6.3, that $E_{x,x}$ is absolutely continuous by $E_{x,x}(B) = \int_B \big(\mathcal{F}^{-1}F\big)(\lambda)\,d\lambda$, $B$ Borel set. Hence, $x$ is in the absolutely continuous subspace for $T$. $\square$

**Theorem 3.4.9.** *Assume $L$ and $L_0$ are self-adjoint operators such that $L = L_0 + A^*B$ in the following sense; $D(L) \subset D(A)$, $D(L_0) \subset D(B)$ and for all $x \in D(L)$, $y \in D(L_0)$*

$$\langle Lx, y\rangle = \langle x, L_0 y\rangle + \langle Ax, By\rangle.$$

*Assume that $A$ is $L$-smooth and $B$ is $L_0$-smooth, then the wave operators $W^\pm$ exist as unitary operators.*

In particular, $\mathrm{Ran}\,W^+ = \mathrm{Ran}\,W^- = \mathcal{H}$. Note that Theorem 3.4.9 does not deal yet with generalised wave operators, so it cannot be applied to the Schrödinger operators once the perturbed Schrödinger operator has discrete spectrum, cf. Proposition 3.2.4. Moreover, it still has the problem that there is a smoothness condition with respect to the perturbed operator $L$. The proof of Theorem 3.4.9 is based on the idea of Cook as for Proposition 3.3.1.

*Proof.* Take $x \in D(L_0)$ and consider $w(t) = e^{itL}e^{-itL_0}x$. Take $y \in D(L)$ and consider

$$\begin{aligned}\frac{d}{dt}\langle w(t), y\rangle &= \frac{d}{dt}\langle e^{-itL_0}x, e^{-itL}y\rangle = -i\langle L_0\,e^{-itL_0}x, e^{-itL}y\rangle + i\langle e^{-itL_0}x, L\,e^{-itL}y\rangle \\ &= i\langle B\,e^{-itL_0}x, A\,e^{-itL}y\rangle\end{aligned}$$

since $e^{-itL_0}x \in D(L)$, $e^{itL}y \in D(L_0)$. Consequently, for $t > s$

$$\begin{aligned}&|\langle w(t)-w(s), y\rangle| \leq \int_s^t |\langle B\,e^{-iuL_0}x, A\,e^{-iuL}y\rangle|\,du \leq \int_s^t \|B\,e^{-iuL_0}x\|\,\|A\,e^{-iuL}y\|\,du \\ &\leq \left(\int_s^t \|B\,e^{-iuL_0}x\|^2\,du\right)^{\frac12}\left(\int_s^t \|A\,e^{-iuL}y\|^2\,du\right)^{\frac12} \\ &\leq \left(\int_s^t \|B\,e^{-iuL_0}x\|^2\,du\right)^{\frac12}\left(\int_{\mathbb{R}} \|A\,e^{-iuL}y\|^2\,du\right)^{\frac12} \leq C\|y\|\,\left(\int_s^t \|B\,e^{-iuL_0}x\|^2\,du\right)^{\frac12}\end{aligned}$$

for some constant $C$ since $A$ is $L$-smooth. In particular, we see

$$\|w(t) - w(s)\| \leq C \left( \int_s^t \|B\, e^{-iuL_0} x\|^2\, du \right)^{\frac{1}{2}} \tag{3.4.1}$$

and since the integrand is integrable over $\mathbb{R}$ we see that $w(s)$ is Cauchy as $s \to \infty$. So the domain of $W^+$ contains the dense subset $D(L_0)$, and since $D(W^+)$ is closed by Theorem 3.2.6 it follows that $D(W^+)$ is the whole Hilbert space. Similarly for $W^-$.

Since the problem is symmetric in $L$ and $L_0$, i.e. $L_0 = L - B^*A$ it follows that the strong limits of $e^{itL_0}e^{-itL}$ also exist for $t \to \pm\infty$. Since these are each others inverses, unitarity follows. □

Theorem 3.4.9 can be used to discuss completeness for the Schrödinger operator $-\frac{d^2}{dx^2} + q$, but the details are complicated. We only discuss globally the proof of Theorem 3.4.13. For this we first give a condition on the resolvent of $T$ and $S$ for $S$ to be a $T$-smooth operators using the Fourier transform.

First recall, that for $F\colon \mathbb{R} \to \mathcal{H}$ a a Hilbert space valued function, such that $\int_{\mathbb{R}} \|F(t)\|\, dt < \infty$ (and $t \mapsto \langle F(t), y\rangle$ is measurable for all $y \in \mathcal{H}$) we can define $\int_{\mathbb{R}} F(t)\, dt \in \mathcal{H}$. Indeed, $y \mapsto \int_{\mathbb{R}} \langle y, F(t)\rangle\, dt$ is bounded and now use Riesz's representation theorem. Note that $\left\| \int_{\mathbb{R}} F(t)\, dt \right\| \leq \int_{\mathbb{R}} \|F(t)\|\, dt$. For such a function $F$ we define its Fourier transform as $\big(\mathcal{F}F\big)(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\lambda t} F(t)\, dt$ as an element of $\mathcal{H}$.

**Lemma 3.4.10.** *Let $(S, D(S))$ be a closed operator on $\mathcal{H}$, then*

$$\int_{\mathbb{R}} \|S\big(\mathcal{F}F\big)(\lambda)\|^2\, d\lambda = \int_{\mathbb{R}} \|SF(t)\|^2\, dt,$$

*where the left hand side is set to $\infty$ in case $\mathcal{F}F(\lambda) \notin D(S)$ almost everywhere, and similarly for the right hand side.*

**Exercise 3.4.11.** Prove Lemma 3.4.10 according to the following steps.

- First take $S$ bounded, then for any $x \in \mathcal{H}$ we see that $\langle S\mathcal{F}F(\lambda), x\rangle = \langle \mathcal{F}F(\lambda), S^*x\rangle$ is the (ordinary) Fourier transform of $\langle SF(t), x\rangle = \langle F(t), S^*x\rangle$. Use Plancherel and next take $x$ elements of an orthonormal basis of the Hilbert space (we assume $\mathcal{H}$ separable) Deduce $\int_{\mathbb{R}} \|S\mathcal{F}F(\lambda)\|^2\, d\lambda = \int_{\mathbb{R}} \|SF(t)\|^2\, dt$.

- Next assume $(S, D(S))$ self-adjoint with spectral decomposition $E$. Use the previous result for $SE(-n, n)$ and use that if $F(t) \in D(S)$ almost everywhere $\|SE(-n, n)\, F(t)\|^2$ converges monotonically to $\|SF(t)\|^2$ as $n \to \infty$. Now use the monotone convergence theorem.

- For arbitrary $(S, D(S))$ we take its polar decomposition $S = U\,|S|$ with $D(|S|) = D(S)$, $(|S|, D(|S|))$ self-adjoint and $\|\,|S|x\| = \|Sx\|$ for all $x \in D(S) = D(|S|)$.

Apply Lemma 3.4.10 (with the Fourier transform replaced by the inverse Fourier transform) to $F(t) = e^{-\varepsilon t}e^{-itT}x$ for $t \geq 0$, $F(t) = 0$ for $t < 0$. Using the functional calculus as in the beginning of the proof of Proposition 3.4.8 we get, for $\varepsilon > 0$ and $R(z)$ the resolvent for $T$,

$$\int_{\mathbb{R}} \|SR(\lambda + i\varepsilon)x\|^2 \, d\lambda = 2\pi \int_0^\infty e^{-2\varepsilon t} \|Se^{-itT}x\|^2 \, dt.$$

Similarly, we obtain for $\varepsilon > 0$

$$\int_{\mathbb{R}} \|SR(\lambda - i\varepsilon)x\|^2 \, d\lambda = 2\pi \int_{-\infty}^0 e^{2\varepsilon t} \|Se^{-itT}x\|^2 \, dt.$$

Using the Parseval version, or by polarizing, one can also derive

$$\int_{\mathbb{R}} \langle SR(\lambda + i\varepsilon)x, SR(\lambda - i\varepsilon)y\rangle \, d\lambda = 0$$

assuming the integral exists. In particular, we get

$$\begin{aligned} 4\varepsilon^2 \int_{\mathbb{R}} \|SR(\lambda + i\varepsilon)R(\lambda - i\varepsilon)x\|^2 \, d\lambda &= \int_{\mathbb{R}} \|S\big(R(\lambda + i\varepsilon) - R(\lambda - i\varepsilon)\big)x\|^2 \, d\lambda \\ &= 2\pi \int_{\mathbb{R}} e^{-2\varepsilon|t|} \|Se^{-itT}x\|^2 \, dt. \end{aligned}$$

using the resolvent equation $R(\mu) - R(\lambda) = (\mu - \lambda)R(\mu)R(\lambda)$.

**Proposition 3.4.12.** *$S$ is a $T$-smooth operator if and only if for all $x \in \mathcal{H}$ we have $R(\lambda \pm i\varepsilon)x \in D(S)$ for allmost all $\lambda \in \mathbb{R}$ and*

$$\sup_{\|x\|=1,\ \varepsilon>0} \int_{\mathbb{R}} \|SR(\lambda + i\varepsilon)x\|^2 + \|SR(\lambda - i\varepsilon)x\|^2 \, d\lambda < \infty.$$

*If $\varepsilon\|SR(\lambda + i\varepsilon)\|^2 \leq C$ or if $\varepsilon\|SR(\lambda - i\varepsilon)\|^2 \leq C$ independently of $\varepsilon > 0$, $\lambda \in \mathbb{R}$, then $S$ is $T$-smooth.*

*Proof.* For the first statement we use the two equations following Exercise 3.4.11 to obtain

$$\int_{\mathbb{R}} \|SR(\lambda + i\varepsilon)x\|^2 + \|SR(\lambda - i\varepsilon)x\|^2 \, d\lambda = 2\pi \int_{\mathbb{R}} e^{-2\varepsilon|t|} \|Se^{-itT}x\|^2 \, dt.$$

In case $S$ is a $T$-smooth operator the right hand side is bounded for $\varepsilon \geq 0$, so the supremum of the left hand side is finite. In case the supremum of the left hand side is finite, it follows from the monotone convergence theorem that $\int_{\mathbb{R}} \|Se^{-itT}x\|^2 \, dt < \infty$.

For the second statement we use

$$2\pi \int_{\mathbb{R}} e^{-2\varepsilon|t|} \|Se^{-itT}x\|^2 \, dt = 4\varepsilon^2 \int_{\mathbb{R}} \|SR(\lambda + i\varepsilon)R(\lambda - i\varepsilon)x\|^2 \, d\lambda \leq 4\varepsilon C \int_{\mathbb{R}} \|R(\lambda - i\varepsilon)x\|^2 \, d\lambda$$

and now use the Spectral Theorem 6.4.1 to observe

$$\|R(\lambda - i\varepsilon)x\|^2 = \langle R(\lambda + i\varepsilon)R(\lambda - i\varepsilon)x, x\rangle = \int_{\mathbb{R}} \frac{1}{|t-\lambda-i\varepsilon|^2}\, dE_{x,x}(t).$$

So we can rewrite the right hand side as

$$4\varepsilon C \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|t-\lambda-i\varepsilon|^2}\, dE_{x,x}(t)\, d\lambda = 4\varepsilon C \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|t-\lambda-i\varepsilon|^2}\, d\lambda\, dE_{x,x}(t)$$

(interchanging is valid since the integrand is positive), and the inner integral

$$\int_{\mathbb{R}} \frac{1}{|t-\lambda-i\varepsilon|^2}\, d\lambda = \int_{\mathbb{R}} \frac{1}{(t-\lambda)^2+\varepsilon^2}\, d\lambda = \frac{1}{\varepsilon}\arctan\Big(\frac{\lambda-t}{\varepsilon}\Big)\Big|_{\lambda=-\infty}^{\infty} = \frac{\pi}{\varepsilon}.$$

So we get

$$4\varepsilon C \int_{\mathbb{R}}\int_{\mathbb{R}} \frac{1}{|t-\lambda-i\varepsilon|^2}\, dE_{x,x}(t)\, d\lambda = 4\pi C \int_{\mathbb{R}} dE_{x,x}(t) = 4\pi C\|x\|^2$$

by the Spectral Theorem 6.4.1. So this leads to

$$2\pi \int_{\mathbb{R}} e^{-2\varepsilon|t|}\|Se^{-itT}x\|^2\, dt \le 4\pi C\|x\|^2, \qquad (3.4.2)$$

or $S$ is $T$-smooth. $\square$

The machinery of $T$-smooth operators and in particular Theorem 3.4.9 can be applied to the Schrödinger operator, but the proof is very technical and outside the scope of these lecture notes.

**Theorem 3.4.13.** *Assume $q \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, and let $L_0 = -\frac{d^2}{dx^2}$, $L = -\frac{d^2}{dx^2} + q$, then the wave operators $\Omega^{\pm}(L, L_0)$ are complete*

We put

$$a(x) = \begin{cases} \sqrt{|q(x)|}, & q(x) \neq 0, \\ e^{-x^2} & q(x) = 0 \end{cases}, \qquad b(x) = \frac{q(x)}{a(x)}.$$

Then we are in the situation of Theorem 3.4.9, but the space of absolute continuity has to brought into play. This is done by employing the spectral decomposition and assuming that there exists an open set $Z$ such that $E(Z)$ corresponds to the orthogonal projection on the absolutely continuous subspace. Next it turns out that even for $R$ being the resolvent of $L_0 = -\frac{d^2}{dx^2}$ one cannot prove the sufficient condition of Proposition 3.4.12 since there is no estimate uniformly in $\lambda \in \mathbb{R}$. One first shows that the condition can be relaxed to $\varepsilon\|AR(\lambda \pm i\varepsilon)\|^2 \le C_I$ independently of $\varepsilon > 0$, $\lambda \in I$ for any interval $I$ with compact closure in $Z$, where $E(Z)$ is $P_{ac}$.

For $R$ the resolvent of $L_0$ and $B$ multiplication by $b$ this is easily checked. Note that in the application indeed $b \in L^2(\mathbb{R})$.

**Lemma 3.4.14.** *With $R$ the resolvent of $L_0 = -\frac{d}{dx^2}$ and $B$ the multiplication operator by $b \in L^2(\mathbb{R})$ we have $\varepsilon\|BR(\lambda \pm i\varepsilon)\|^2 \leq C_I$ for all intervals $I$ with compact closure in $(0, \infty)$.*

Note that $BR(z)$, $\Im z \neq 0$, is a compact operator. Indeed, by Theorem 2.3.4 $B$ is $L_0$-compact, and if $\{f_n\}_{n=1}^{\infty}$ is a bounded sequence, say $\|f_n\| \leq M$, in $L^2(\mathbb{R})$ then we have

$$\begin{aligned} \|R(z)f_n\| + \|L_0 R(z) f_n\| &\leq M\|R(z)\| + \|(L_0 - z)R(z)f_n\| + \|zR(z)f_n\| \\ &\leq M\|R(z)\|(1 + |z|) + M, \end{aligned}$$

so that the sequence is bounded. Hence, $B$ being $L_0$-compact we see that $BR(z)f_n$ has a convergent subsequence, so that $BR(z)$ is a compact operator.

*Proof.* For this we need the resolvent of $L_0$, which we claim equals

$$\big(R(z)f\big)(x) = \frac{-1}{2\gamma i} \int_{\mathbb{R}} e^{i\gamma|x-y|} f(y)\, dy$$

where $z = \gamma^2 \in \mathbb{C}\backslash\mathbb{R}$ and $\Im\gamma > 0$, see Exercise 2.1.5.

Assuming this we see using the Cauchy-Schwarz inequality (6.1.1) in $L^2(\mathbb{R})$,

$$\begin{aligned} |b(x)\big(R(z)f\big)(x)|^2 &\leq \frac{|b(x)|^2}{4|\gamma|^2} \int_{\mathbb{R}} e^{-2\Im\gamma\,|x-y|}\, dy \int_{\mathbb{R}} |f(y)|^2\, dy = \frac{|b(x)|^2}{4|\gamma|^2} \int_{\mathbb{R}} e^{-2\Im\gamma\,|y|}\, dy\ \|f\|^2 \\ &= \|f\|^2 \frac{|b(x)|^2}{4|z|\,\Im\gamma} \Longrightarrow \|BR(z)f\|^2 \leq \frac{\|f\|^2\|a\|^2}{4|z|\,\Im\gamma} \end{aligned}$$

giving the required estimate. □

The analogous statement to Lemma 3.4.14 with $R$ the resolvent for the perturbed operator and the multiplication by $a \in L^2(\mathbb{R})$ is a much harder statement to prove. The idea is to rewrite the relation in Theorem 3.4.9 for the resolvent as

$$AR(z) = AR_0(z) + A\big(BR_0(\bar{z})\big)^* AR(z) \Longrightarrow \Big(1 - A\big(BR_0(\bar{z})\big)^*\Big)AR(z) = AR_0(z)$$

where we denote the resolvent for $L$ by $R$ and the resolvent for $L_0$ by $R_0$. If we now can show that $1 - A\big(BR_0(\bar{z})\big)^*$ is invertible and if we have sufficient control on its inverse we can use Lemma 3.4.14 once more to find the result. In particular one needs the inverse to be uniformly bounded in a neighbourhood of an interval $I$ (with $I$ as in Lemma 3.4.14). We will not go into this, but refer to Schechter [10, Ch. 9] and Reed and Simon [9, Ch. XIII].

# Chapter 4

# Schrödinger operators and scattering data

## 4.1 Jost solutions

The unperturbed Schrödinger operator $-\frac{d^2}{dx^2}$ has eigenvalues $\lambda = \gamma^2$ for the corresponding eigenfunctions $\exp(\pm i\gamma x)$. If the potential $q$ is of sufficient decay at $\pm\infty$ we can expect that eigenfunctions of the Schrödinger equation $-\frac{d^2}{dx^2} + q$ exist that behave as $\exp(\pm i\gamma x)$ for $x \to \pm\infty$. These solutions are known as the Jost[1] solutions.

The basic assumption in this chapter on the potential $q$ is that it is a real-valued function having sufficient decay. This is specified in each of the results.

**Definition 4.1.1.** *The Schrödinger integral equation at $\infty$ is the integral equation*

$$f(x) = e^{i\gamma x} - \int_x^\infty \frac{\sin(\gamma(x-y))}{\gamma}\, q(y)\, f(y)\, dy$$

*and the Schrödinger integral equation at $-\infty$ is the integral equation*

$$f(x) = e^{-i\gamma x} + \int_{-\infty}^x \frac{\sin(\gamma(x-y))}{\gamma}\, q(y)\, f(y)\, dy$$

For $f$ a solution to the Schrödinger integral equation at $\infty$ we can formally calculate

$$\begin{aligned}
f'(x) &= i\gamma e^{i\gamma x} + \frac{\sin(\gamma(x-x))}{\gamma}\, q(x)\, f(x) - \int_x^\infty \cos(\gamma(x-y))\, q(y)\, f(y)\, dy \\
&= i\gamma e^{i\gamma x} - \int_x^\infty \cos(\gamma(x-y))\, q(y)\, f(y)\, dy \Longrightarrow \\
f''(x) &= -\gamma^2 e^{i\gamma x} + \cos(\gamma(x-x))\, q(x)\, f(x) + \gamma \int_x^\infty \sin(\gamma(x-y))\, q(y)\, f(y)\, dy \\
&= -\gamma^2 f(x) + q(x)\, f(x),
\end{aligned}$$

[1] Res Jost, Swiss theoretical physicist.

so that it gives a solution to the Schrödinger eigenvalue equation $-f''+qf=\gamma^2 f$. The integral equation can be derived by viewing $f''+\gamma^2 f=u$, $u=q\,f$, as an inhomogeneous linear second-order differential equation and apply the method of variation of constants. Similarly, a solution of the Schrödinger integral equation at $-\infty$ gives rise to an eigenfunction of the Schrödinger operator for the eigenvalue $\gamma^2$. The Schrödinger integral equation can also be obtained using the method of variation of constants for $f''+\gamma^2 f=g$, and then take $g=qf$.

The three-dimensional analogues of the Schrödinger integral equations in quantum mechanics are known as the Lippmann-Schwinger equation.

**Theorem 4.1.2.** *Assume that the potential $q$ is a real-valued integrable function. Let $\gamma\in\mathbb{C}$, $\Im\gamma\geq 0$, $\gamma\neq 0$. Then the Schrödinger integral equation at $\infty$ has a unique solution $f_\gamma^+$ which is continuously differentiable and satisfies the estimates*

$$|f_\gamma^+(x)-e^{i\gamma x}|\leq e^{-x\Im\gamma}\,\Big|\exp(\frac{1}{|\gamma|}\int_x^\infty |q(y)|\,dy)-1\Big|$$
$$|\frac{df_\gamma^+}{dx}(x)-i\gamma\, e^{i\gamma x}|\leq |\gamma|\,e^{-x\Im\gamma}\,\Big|\exp(\frac{1}{|\gamma|}\int_x^\infty |q(y)|\,dy)-1\Big|.$$

*Moreover, the Schrödinger integral equation at $-\infty$ has a unique solution $f_\gamma^-$ which is continuously differentiable and satisfies the estimates*

$$|f_\gamma^-(x)-e^{-i\gamma x}|\leq e^{x\Im\gamma}\,\Big|\exp(\frac{1}{|\gamma|}\int_{-\infty}^x |q(y)|\,dy)-1\Big|,$$
$$|\frac{df_\gamma^-}{dx}(x)+i\gamma e^{i\gamma x}|\leq |\gamma|\,e^{x\Im\gamma}\,\Big|\exp(\frac{1}{|\gamma|}\int_{-\infty}^x |q(y)|\,dy)-1\Big|.$$

Using $e^x-1\leq xe^x$ we can estimate

$$\begin{aligned}|f_\gamma^+(x)-e^{i\gamma x}|&\leq e^{-x\Im\gamma}\,\frac{1}{|\gamma|}\int_x^\infty |q(y)|\,dy\ \exp(\frac{1}{|\gamma|}\int_x^\infty |q(y)|\,dy),\\ |\frac{df_\gamma^+}{dx}(x)-i\gamma\, e^{i\gamma x}|&\leq\ e^{-x\Im\gamma}\,\int_x^\infty |q(y)|\,dy\,\exp(\frac{1}{|\gamma|}\int_x^\infty |q(y)|\,dy),\end{aligned}\tag{4.1.1}$$

and a similar estimate for $f_\gamma^-$ and its derivative.

Since $q$ is real-valued it follows that for $x\in\mathbb{R}$ we have $\overline{f_\gamma^+(x)}=f_{-\bar\gamma}^+(x)$ and $\overline{f_\gamma^-(x)}=f_{-\bar\gamma}^-(x)$ as solutions to the Schrödinger integral equations. Since $q$ is an integrable function and $f_\gamma^+\in C^1(\mathbb{R})$ is bounded for $x\to\infty$, the differentiations in the calculations preceding Theorem 4.1.2 are justifiable using Lebesgue's Theorems 6.1.3 and 6.1.4 on differentiation and dominated convergence and hold almost everywhere. The solutions in Theorem 4.1.2 are known as Jost solutions.

*Proof.* The Schrödinger integral equations are Volterra[2] type integral equations, and a standard way to find a solution is by successive iteration. Put $f_0(x)=e^{-i\gamma x}$, and define

$$f_{n+1}(x)=-\int_x^\infty \frac{\sin(\gamma(x-y))}{\gamma}\,q(y)\,f_n(y)\,dy,\qquad n\geq 0.$$

[2]Vito Volterra (3 May 1860 — 11 October 1940), Italian mathematician.

Put $m_n(x) = e^{-i\gamma x} f_n(x)$, so that $m_n$ is defined inductively by $m_0(x) = 1$ and

$$\begin{aligned} m_{n+1}(x) &= -\int_x^\infty \frac{\sin(\gamma(x-y))}{\gamma}\, e^{i\gamma(y-x)}\, q(y)\, m_n(y)\, dy \\ &= \int_x^\infty \frac{1}{2i\gamma}\,(e^{2i\gamma(y-x)}-1)\, q(y)\, m_n(y)\, dy, \qquad n \geq 0. \end{aligned}$$

Now

$$\big|\sin(\gamma(x-y))\, e^{i\gamma(y-x)}\big| = \frac{1}{2}\big|1 - e^{2i\gamma(y-x)}\big| \leq \frac{1}{2}\big(1 + e^{-2(y-x)\Im\gamma}\big) \leq 1$$

for $y \geq x$ and $\Im\gamma \geq 0$. Hence, assuming $\Im\gamma \geq 0$ we find

$$\big|m_{n+1}(x)\big| \leq \frac{1}{|\gamma|}\int_x^\infty |q(y)|\,|m_n(y)|\, dy,$$

and then we have by induction on $n$ the estimate $|m_n(x)| \leq \dfrac{\big(R(x)\big)^n}{|\gamma|^n\, n!}$, where

$$R(x) = \int_x^\infty |q(y)|\, dy \leq \int_{\mathbb{R}} |q(y)|\, dy = \|q\|_1.$$

Note that $R$ is a continuous decreasing bounded function, which is almost everywhere differentiable by Lebesgue's differentation Theorem 6.1.4. Indeed, for $n = 0$ this inequality is valid since $m_0(x) = 1$, and

$$\big|m_{n+1}(x)\big| \leq \frac{1}{|\gamma|}\int_x^\infty |q(y)|\,\frac{\big(R(y)\big)^n}{|\gamma|^n\, n!}\, dy = \frac{1}{|\gamma|^{n+1}\, n!}\int_0^{R(x)} s^n\, ds = \frac{\big(R(x)\big)^{n+1}}{|\gamma|^{n+1}\,(n+1)!}$$

by putting $s = R(y)$, so $ds = -|q(y)|\, dy$ and the interval $[x,\infty)$ is mapped to $[0, R(x)]$, since $R$ is decreasing.

So the series $\sum_{n=0}^\infty m_n(x)$ converges uniformly, and so does the series $\sum_{n=0}^\infty f_n(x)$, for $\Im\gamma \geq 0$. It is straightforward to check that the series $\sum_{n=0}^\infty f_n(x)$ gives a solution to the Schrödinger equation at $\infty$, and this solution we denote by $f_\gamma^+$. Then

$$|f_\gamma^+(x) - e^{i\gamma x}| \leq \sum_{n=1}^\infty |f_n(x)| \leq e^{-x\Im\gamma}\sum_{n=1}^\infty |m_n(x)| \leq e^{-x\Im\gamma}|\exp(R(x)/|\gamma|) - 1| \to 0, \quad x \to \infty$$

for fixed $\gamma \in \mathbb{C}$ with $\gamma \neq 0$, $\Im\gamma \geq 0$.

Note that $m_0 \in C^\infty(\mathbb{R})$ for all $\gamma \in \mathbb{C}$, and since the integrals defining $m_n(x)$ in terms of $m_{n-1}$ converge absolutely for $\Im\gamma \geq 0$ we see that each $m_n$ is at least in $C^1(\mathbb{R})$. Consequently, $f_n \in C^1(\mathbb{R})$, and

$$\frac{df_{n+1}}{dx}(x) = -\int_x^\infty \cos(\gamma(x-y))\, q(y)\, f_n(y)\, dy = -\int_x^\infty \cos(\gamma(x-y))\, e^{i\gamma y}\, q(y)\, m_n(y)\, dy \quad (4.1.2)$$

and now using

$$\left|\cos(\gamma(x-y))\, e^{i\gamma y}\right| = |e^{i\gamma x}|\frac{1}{2}|1+e^{2i\gamma(y-x)}| \leq e^{-x\Im\gamma}$$

for $y \geq x$, $\Im\gamma \geq 0$. This gives

$$\left|\frac{df_{n+1}}{dx}(x)\right| = e^{-x\Im\gamma}\int_x^\infty |q(y)|\,|m_n(y)|\,dy \leq e^{-x\Im\gamma}\int_x^\infty |q(y)|\frac{\big(R(y)\big)^n}{|\gamma|^n\, n!}\,dy = \frac{e^{-x\Im\gamma}\big(R(x)\big)^{n+1}}{|\gamma|^n\,(n+1)!}.$$

It follows that the series $\sum_{n=0}^\infty \frac{df_n}{dx}(x)$ converges uniformly on compact subsets of $\mathbb{R}$, so this is a continuous function and $f_\gamma^+ \in C^1(\mathbb{R})$. We find for $\Im\gamma \geq 0$

$$\left|\frac{df_\gamma^+}{dx}(x) - i\gamma e^{i\gamma x}\right| \leq \sum_{n=1}^\infty \left|\frac{df_n}{dx}(x)\right| \leq \sum_{n=1}^\infty \frac{e^{-x\Im\gamma}\big(R(x)\big)^n}{|\gamma|^{n-1}\, n!} = |\gamma|\, e^{-x\Im\gamma}\left(\exp(R(x)/|\gamma|) - 1\right)$$

which tends to zero as $x \to \infty$.

In order to see that this solution is unique, let $f$ and $g$ be two $C^1$-solutions to the Schrödinger integral equation at $\infty$. Then $h(x) = e^{-i\gamma x}(f(x) - g(x))$ is a solution to

$$h(x) = -\int_x^\infty \frac{\sin(\gamma(x-y))}{\gamma}\, e^{i\gamma(y-x)}\, q(y)\, h(y)\, dy.$$

Let $x_0 \in \mathbb{R}$ be arbitrary, and put $L = \sup_{x \geq x_0}|h(x)| < \infty$, since $f$ and $g$ remain bounded as $x \to \infty$. So $|h(x)| \leq L$ for all $x \geq x_0$, and by induction, using the integral representation as before, we find $|h(x)| \leq L\frac{\left(R(x)\right)^n}{|\gamma|^n\, n!} \leq L\frac{\|q\|_1^n}{|\gamma|^n\, n!}$ for all $n \in \mathbb{N}$. Hence, $h(x) = 0$ for all $x \geq x_0$, and since $x_0 \in \mathbb{R}$ is arbitrary, $h = 0$ and uniqueness follows.

The statements for the Schrödinger integral equation at $-\infty$ are proved analogously, and are left as an exercise. □

**Exercise 4.1.3.** With the assumptions in Theorem 4.1.2 and assuming that $q$ is moreover an element of $C^k(\mathbb{R})$. Show that $f_\gamma^+, f_\gamma^- \in C^{k+2}$.

From the proof of Theorem 4.1.2 we obtain the following corollary, since a series of analytic functions is analytic if the convergence is uniformly on compact sets and each $f_n$ is analytic in $\gamma$ for $\Im\gamma > 0$.

**Corollary 4.1.4.** *$\gamma \mapsto f_\gamma^+(x)$, $\gamma \mapsto \frac{df_\gamma^+}{dx}$ and $\gamma \mapsto f_\gamma^-(x)$, $\gamma \mapsto \frac{df_\gamma^-}{dx}$ are analytic in $\gamma$ for $\Im\gamma > 0$ and continuous in $\gamma$ for $\Im\gamma \geq 0$, $\gamma \neq 0$.*

Note that in the proof of Theorem 4.1.2 we actually deal with $m_\gamma^+(x) = e^{-i\gamma x}f_\gamma^+(x)$ and $m_\gamma^-(x) = e^{i\gamma x}f_\gamma^-(x)$. These functions are solutions to the differential equation

$$m'' + 2i\gamma\, m' = q\, m \tag{4.1.3}$$

as follows by a straightforward calculation, and they are the solutions to an integral equation;

$$m(x) = 1 + \int_x^\infty \frac{e^{2i\gamma(y-x)} - 1}{2i\gamma}\, q(y)\, m(y)\, dy \tag{4.1.4}$$

for $m = m_\gamma^+$ and a similar one for $m_\gamma^-$.

The estimates in Theorem 4.1.2 can be improved by imposing more conditions on the potential $q$. We discuss two possible extensions. The first additional assumption also allows an extension to the case $\gamma = 0$.

**Theorem 4.1.5.** *Assume the potential $q$ is real-valued and $\int_{\mathbb{R}}(1+|x|)|q(x)|\,dx < \infty$. Then for $\gamma \in \mathbb{C}$ with $\Im\gamma \geq 0$,*

$$
\begin{aligned}
|f_\gamma^+(x) - e^{i\gamma x}| &\leq \frac{C\,e^{-x\Im\gamma}}{1+|\gamma|}(1+\max(-x,0))\int_x^\infty (1+|y|)|q(y)|\,dy \\
|\frac{df_\gamma^+}{dx}(x) - i\gamma\,e^{i\gamma x}| &\leq \frac{C\,e^{-x\Im\gamma}}{1+|\gamma|}\int_x^\infty (1+|y|)|q(y)|\,dy,
\end{aligned}
$$

*where $C$ is a constant only depending on the potential $q$. Moreover, the Schrödinger integral equation at $-\infty$ has a unique solution $f_\gamma^-$ which is continuously differentiable and satisfies the estimates*

$$
\begin{aligned}
|f_\gamma^-(x) - e^{-i\gamma x}| &\leq \frac{C\,e^{-x\Im\gamma}}{1+|\gamma|}(1+\max(x,0))\int_{-\infty}^x (1+|y|)|q(y)|\,dy \\
|\frac{df_\gamma^-}{dx}(x) + i\gamma e^{i\gamma x}| &\leq \frac{C\,e^{-x\Im\gamma}}{1+|\gamma|}\int_{-\infty}^x (1+|y|)|q(y)|\,dy.
\end{aligned}
$$

*Proof.* In particular, the potential $q$ satisfies the estimate of Theorem 4.1.2, and the estimates given there hold.

Use the estimate

$$
\Big|\frac{1}{2i\gamma}\,(e^{2i\gamma(y-x)} - 1)\Big| \leq (y-x)
$$

for $\gamma \in \mathbb{R}$, $y - x \geq 0$ and iterate to find

$$
\begin{aligned}
|m_n(x)| &\leq \iint\cdots\int_{x\leq y_1\leq y_2\cdots\leq y_n} (y_1-x)(y_2-y_1)\cdots(y_n-y_{n-1})|q(y_1)|\cdots|q(y_n)|\,dy_n\cdots dy_1 \\
&\leq \iint\cdots\int_{x\leq y_1\leq y_2\cdots\leq y_n} (y_1-x)(y_2-x)\cdots(y_n-x)|q(y_1)|\cdots|q(y_n)|\,dy_n\cdots dy_1.
\end{aligned}
$$

Note that the integrand is invariant with respect to permutations of $y_1$ up to $y_n$, but not the region. Taking all possible orderings gives, where $S_n$ is the group of permutations on $n$ elements,

$$
\begin{aligned}
& n!\,|m_n(x)| \\
&\leq \sum_{w\in S_n}\iint\cdots\int_{x\leq y_{w(1)}\leq y_{w(2)}\cdots\leq y_{w(n)}} (y_1-x)(y_2-x)\cdots(y_n-x)|q(y_1)|\cdots|q(y_n)|\,dy_n\cdots dy_1 \\
&= \int_x^\infty\int_x^\infty\cdots\int_x^\infty (y_1-x)(y_2-x)\cdots(y_n-x)|q(y_1)|\cdots|q(y_n)|\,dy_n\cdots dy_1 \\
&= \Big(\int_x^\infty (y-x)\,|q(y)|\,dy\Big)^n,
\end{aligned}
$$

so that, with $R(x) = \int_x^\infty (y-x)\,|q(y)|\,dy$, we get

$$|m_\gamma^+(x)| \leq \exp(R(x)) - 1 \leq R(x)\exp(R(x)).$$

Note that $R(x) \geq R(y)$ for $x \leq y$. Here we use again $e^x - 1 \leq xe^x$.

Next consider the estimate for $m_\gamma^+$ by

$$\begin{aligned}
|m_\gamma^+(x)| &\leq 1 + \int_x^\infty (y-x)|q(y)|\,|m_\gamma^+(y)|\,dy \\
&= 1 + \int_x^\infty y|q(y)|\,|m_\gamma^+(y)|\,dy + (-x)\int_x^\infty |q(y)|\,|m_\gamma^+(y)|\,dy \\
&\leq 1 + \int_0^\infty y|q(y)|\,|m_\gamma^+(y)|\,dy + (-x)\int_x^\infty |q(y)|\,|m_\gamma^+(y)|\,dy
\end{aligned}$$

and observe that this inequality holds for positive and negative $x \in \mathbb{R}$. We estimate the first term, which is independent of $x$, by

$$\begin{aligned}
&1 + \int_0^\infty y|q(y)|\,|m_\gamma^+(y)|\,dy \leq 1 + R(0)\exp(R(0)) \int_0^\infty y|q(y)|\,dy \\
&= 1 + \big(R(0)\big)^2 \exp(R(0)) = C_1 < \infty
\end{aligned}$$

where $C_1$ is a finite constant only depending on $R(0) = \int_0^\infty y|q(y)|\,dy$.

Now define $M(x) = \frac{m_\gamma^+(x)}{C_1(1+|x|)}$, $p(x) = (1+|x|)|q(x)|$, then we can rewrite the implicit estimate on $m_\gamma^+(x)$ in terms of $M(x)$ as follows;

$$\begin{aligned}
C_1(1+|x|)|M(x)| &\leq C_1 + (-x)\int_x^\infty C_1(1+|t|)\,|q(t)|\,|M(t)|\,dt \\
\Longrightarrow |M(x)| &\leq \frac{1}{1+|x|} + \frac{-x}{1+|x|}\int_x^\infty p(t)\,|M(t)|\,dt \qquad (4.1.5)\\
&\leq 1 + \int_x^\infty p(t)\,|M(t)|\,dt,
\end{aligned}$$

so that as before, cf. proof of Theorem 4.1.2, or using Gronwall's[3] Lemma, see Exercise 4.1.6, we get

$$|M(x)| \leq \exp\Big(\int_x^\infty p(y)\,dy\Big) \leq \exp\Big(\int_{\mathbb{R}} (1+|y|)\,|q(y)|\,dy\Big) = C_2 < \infty.$$

So $|m_\gamma^+(x)| \leq C_3(1+|x|)$ with $C_3 = C_1C_2$ only depending on properties of $q$. This estimate is now being used to estimate

$$\begin{aligned}
|m_\gamma^+(x) - 1| &\leq \int_0^\infty y|q(y)|\,|m_\gamma^+(y)|\,dy + (-x)\int_x^\infty |q(y)|\,|m_\gamma^+(y)|\,dy \\
&\leq R(0)\exp(R(0))\int_0^\infty y|q(y)|\,dy + (-x)C_3\int_x^\infty (1+|y|)\,|q(y)|\,dy
\end{aligned}$$

[3] Thomas Hakon Grönwall (16 January 1877 — 9 May 1932), Swedish-American mathematician, engineer, chemist.

and for $x \leq 0$ we can estimate this by

$$\begin{aligned}
&\leq R(0) \exp(R(0)) \int_x^\infty (1+|y|)\,|q(y)|\,dy + |x| C_3 \int_x^\infty (1+|y|)\,|q(y)|\,dy \\
&\leq C_4 (1+|x|) \int_x^\infty (1+|y|)\,|q(y)|\,dy
\end{aligned}$$

with $C_4 = \max\big(R(0)\exp(R(0)), C_3\big)$ only depending on properties of $q$. For $x \geq 0$ we already have the estimate

$$\begin{aligned}
|m_\gamma^+(x) - 1| \leq R(x)\exp(R(x)) \leq R(x)\exp(R(0)) &= \exp(R(0)) \int_x^\infty (y-x)\,|q(y)|\,dy \\
&\leq \exp(R(0)) \int_x^\infty y\,|q(y)|\,dy \leq \exp(R(0)) \int_x^\infty (1+|y|)\,|q(y)|\,dy.
\end{aligned}$$

Taking $C_5 = \max(C_4, \exp(R(0)))$ then gives

$$|m_\gamma^+(x) - 1| \leq C_5 (1 + \max(0,-x)) \int_x^\infty (1+|y|)\,|q(y)|\,dy,$$

which is an estimate uniform in $\gamma \in \mathbb{R}$. Combining this estimate in case $|\gamma| \leq 1$ with the estimate of Theorem 4.1.2 in case $|\gamma| \geq 1$ gives the result for $\gamma \in \mathbb{R}$. By Corollary 4.1.4 and Theorem 4.1.2 the result is extended to $\gamma \in \mathbb{C}$, $\Im\gamma \geq 0$.

Differentiating (4.1.4) gives

$$\frac{dm_\gamma^+}{dx}(x) = -\int_x^\infty e^{2i\gamma(y-x)} q(y)\, m_\gamma^+(y)\,dy,$$

so that

$$\Big|\frac{dm_\gamma^+}{dx}(x)\Big| \leq C \int_x^\infty |q(y)| \frac{(1+\max(0,-y))}{1+|\gamma|} dy,$$

which gives the result. The statements for $f_\gamma^-$ are proved analogously. $\square$

**Exercise 4.1.6.** The following is known as Gronwall's Lemma. Assume $f$, $p$ are positive continuous functions on $\mathbb{R}$ such that there exists $K \geq 0$ with $f(x) \leq K + \int_x^\infty f(t)p(t)\,dt$, then $f(x) \leq K \exp(\int_x^\infty p(t)\,dt)$. Prove this according to the following steps.

- Observe that
$$\frac{f(x)p(x)}{K + \int_x^\infty f(t)p(t)\,dt} \leq p(x)$$
and integrate both sides.
- Exponentiate the resulting inequality to get $K + \int_x^\infty f(t)p(t)\,dt \leq K\exp(\int_x^\infty p(t)\,dt)$, and deduce the result.

At what cost can we remove the continuity assumption on $f$ and $p$?

Recall the definition of the Hardy space in Section 6.3.

**Corollary 4.1.7.** *Under the assumptions of Theorem 4.1.5 $\gamma \mapsto e^{-i\gamma x} f^+_\gamma(x) - 1$ is an element of the Hardy class $H^+_2$ for each fixed $x \in \mathbb{R}$. Moreover, the $H^+_2$-norm can be estimated uniformly for $x \in [x_0, \infty)$.*

*Proof.* Put $\gamma = \alpha + i\beta$, with $\beta > 0$, and so $|\gamma| \geq |\alpha|$ and consider

$$\int_{\mathbb{R}} |e^{-i\gamma x} f^+_\gamma(x) - 1|^2 \, d\alpha \leq \Big( C(1 + \max(-x, 0)) \int_{\mathbb{R}} (1 + |y|) \, |q(y)| \, dy \Big)^2 \int_{\mathbb{R}} |\frac{1}{1+|\alpha|}|^2 \, d\alpha < \infty$$

independent of $\beta = \Im\gamma > 0$ by Theorem 4.1.5. □

The second extension of Theorem 4.1.2 deals with analytic extensions of the Jost function with respect to $\gamma$ under the assumption that the potential decays even faster.

**Theorem 4.1.8.** *Let $q$ be a real-valued potential. Assume that there exists $m > 0$ such that $\int_{\mathbb{R}} e^{2m|y|} |q(y)| \, dy < \infty$, then*

$$\begin{aligned} |f^+_\gamma(x) - e^{i\gamma x}| &\leq e^{-x\Im\gamma} \big| \exp\big( C(\gamma, m) e^{-2mx_0} \int_x^\infty e^{2my} |q(y)| \, dy \big) - 1 \big|, \\ |\frac{df^+_\gamma}{dx}(x) - i\gamma e^{i\gamma x}| &\leq \frac{e^{-x\Im\gamma}}{C(\gamma, m)} \big| \exp\big( C(\gamma, m) e^{-2mx_0} \int_x^\infty e^{2my} |q(y)| \, dy \big) - 1 \big|, \end{aligned}$$

*for $\Im\gamma > -m$, $x \geq x_0$, where*

$$C(\gamma, m) = \frac{1}{\varepsilon + 2|\Re\gamma|}$$

*with $\varepsilon = 2\min(m, m + \Im\gamma)$. In particular, $\gamma \mapsto f^+_\gamma(x)$ and $\gamma \mapsto \frac{df^+_\gamma}{dx}(x)$ are analytic for $\gamma \in \mathbb{C}$ with $\Im\gamma > -m$ for fixed $x \geq x_0$.*

Using $e^x - 1 \leq xe^x$ we see that

$$|f^+_\gamma(x) - e^{i\gamma x}| \leq e^{-x\Im\gamma} C(\gamma, m) e^{-2mx_0} \int_x^\infty e^{2my} |q(y)| \, dy \; \exp\big( C(\gamma, m) e^{-2mx_0} \int_x^\infty e^{2my} |q(y)| \, dy \big),$$

and similarly for its derivative, which is similar to the estimate in Theorem 4.1.5, but note that the $\gamma$-region where this estimate is valid is much larger.

*Proof.* Since the assumption implies that $q$ is integrable, Theorem 4.1.2 shows that there is a unique solution $f^+_\gamma$, and we only need to improve the estimates. Using the estimate $|\sin z| \leq \frac{2|z|}{1+|z|} \exp(|\Im z|)$ for $z \in \mathbb{C}$ (prove this estimate) we can now estimate, for $y \geq x \geq x_0$,

$$\begin{aligned} &\left| \frac{1}{\gamma} \sin(\gamma(x - y)) \, e^{i\gamma(y-x)} \right| \leq \frac{2|x - y|}{1 + |\gamma| \, |x - y|} e^{(y-x)|\Im\gamma|} e^{-(y-x)\Im\gamma} e^{-2m(y-x)} e^{2my} e^{-2mx} \\ &\leq \frac{2|x - y|}{1 + |\gamma| \, |x - y|} e^{(y-x)\big(|\Im\gamma| - \Im\gamma - 2m\big)} e^{-2mx_0} e^{2my} \leq C(\gamma, m) \, e^{-2mx_0} \, e^{2my} \end{aligned}$$

for $\Im\gamma > -m$. Here $C(\gamma, m)$ is a finite constant independent of $x$ and $y$, which we discuss later in the proof.

Under this assumption we now have for $x \geq x_0$

$$|m_{n+1}(x)| \leq C(\gamma, m) e^{-2mx_0} \int_x^\infty e^{2my} \, |q(y)| \, |m_n(y)| \, dy,$$

hence we obtain in a similar way the estimate

$$|m_n(x)| \leq \big(C(\gamma, m)\big)^n e^{-2mnx_0} \frac{\big(\int_x^\infty e^{2my}|q(y)| \, dy\big)^n}{n!}$$

for $x \geq x_0$, which gives the result.

It remains to discuss the constant $C(\gamma, m)$. Let $\varepsilon = 2(m + \Im\gamma) > 0$, in case $0 \geq \Im\gamma > -m$ and $\varepsilon = 2m$ in case $\Im\gamma \geq 0$, then we see that we can take for $C(\gamma, m)$ the maximum of the function

$$x \mapsto \frac{2x}{1 + |\gamma| x} e^{-\varepsilon x}, \qquad x \geq 0.$$

A calculation shows that the maximum is attained for $\frac{1}{2|\gamma|}(-1 + \sqrt{1 + \frac{4|\gamma|}{\varepsilon}}) = \frac{2}{\varepsilon(1+\sqrt{1+\frac{4|\gamma|}{\varepsilon}})}$. The maximum is

$$\frac{2\exp\big(-2/(1 + \sqrt{1 + \frac{4|\gamma|}{\varepsilon}})\big)}{\varepsilon(1 + \sqrt{1 + \frac{4|\gamma|}{\varepsilon}})^2} \leq \frac{1}{\varepsilon + 2|\gamma|} \leq \frac{1}{\varepsilon + 2|\Re\gamma|} = C(\gamma, m).$$

Next we use (4.1.2) and the estimate

$$|\cos(\gamma(x-y)) e^{i\gamma y}| \leq e^{-2mx_0} e^{-x\Im\gamma} e^{(y-x)\big(|\Im\gamma| - \Im\gamma - 2m\big)} e^{2my} \leq e^{-2mx_0} e^{-x\Im\gamma} e^{2my}$$

for $x \geq x_0$ and $\Im\gamma > -m$. This gives

$$\begin{aligned}
\left|\frac{df_{n+1}}{dx}(x)\right| &\leq e^{-2mx_0} e^{-x\Im\gamma} \int_x^\infty e^{2my} |q(y)| \, |m_n(y)| \, dy \\
&\leq e^{-2mx_0} e^{-x\Im\gamma} \big(C(\gamma, m)\big)^n e^{-2mnx_0} \frac{1}{n!} \int_x^\infty e^{2my} |q(y)| \left(\int_y^\infty e^{2mt} |q(t)| \, dt\right)^n dy \\
&= e^{-x\Im\gamma} \big(C(\gamma, m)\big)^n e^{-2m(n+1)x_0} \frac{1}{(n+1)!} \left(\int_x^\infty e^{2my} |q(y)| \, dy\right)^{n+1}
\end{aligned}$$

and this estimate gives the result as in Theorem 4.1.2. □

**Exercise 4.1.9.** Prove the corresponding statements for the Jost solution $f_\gamma^-$ under the assumptions on the potential $q$ in Theorem 4.1.8;

$$\begin{aligned}
|f_\gamma^-(x) - e^{-i\gamma x}| &\leq e^{x\Im\gamma} \big|\exp\big(C(\gamma, m) e^{2mx_0} \int_{-\infty}^x e^{-2my} |q(y)| \, dy\big) - 1\big|, \\
\big|\frac{df_\gamma^-}{dx}(x) + i\gamma e^{-i\gamma x}\big| &\leq \frac{e^{x\Im\gamma}}{C(\gamma, m)} \big|\exp\big(C(\gamma, m) e^{2mx_0} \int_{-\infty}^x e^{-2my} |q(y)| \, dy\big) - 1\big|,
\end{aligned}$$

for $\Im\gamma > -m$, $x \leq x_0$ with $(C\gamma, m)$ as in Theorem 4.1.8. Conclude $\gamma \mapsto f_\gamma^-(x)$ and $\gamma \mapsto \frac{df_\gamma^-}{dx}(x)$ are analytic for $\gamma \in \mathbb{C}$ with $\Im\gamma > -m$ for fixed $x \leq x_0$.

We also need some properties of the Jost solutions when differentiated with respect to $\gamma$.

**Proposition 4.1.10.** *Assume that $\int_{\mathbb{R}} |x|^k |q(x)|\, dx < \infty$ for $k = 0, 1, 2$, then $\frac{\partial m_\gamma^+}{\partial\gamma}(x)$ is a continously differentiable function, and it is the unique solution to the integral equation*

$$n(x) = M(x) + \int_x^\infty \frac{e^{2i\gamma x} - 1}{2i\gamma}\, q(y)\, n(y)\, dy,$$
$$M(x) = \int_x^\infty \left( \frac{y-x}{\gamma} e^{2i\gamma(y-x)} - \frac{e^{2i\gamma(y-x)} - 1}{2i\gamma^2} \right) q(y)\, m_\gamma^+(y)\, dy,$$

*with* $\lim_{x\to\infty} n(x) = 0$.

It follows from the proof below that we can also estimate $\frac{\partial m_\gamma^+}{\partial\gamma}(x)$ explicitly. Moreover, it is a solution to

$$n'' + 2i\gamma\, n' = q\, n - 2i\, m_\gamma^+,$$

i.e. the differential equation (4.1.3) differentiated with respect to $\gamma$. Switching back to the Jost solution $f_\gamma^+$, we see that we find a solution $\frac{\partial f_\gamma^+}{\partial\gamma}(x) = -ixe^{-i\gamma x} m_\gamma^+(x) + e^{-i\gamma x} \frac{\partial m_\gamma^+}{\partial\gamma}(x)$ to

$$-f'' + q\, f = \gamma^2\, f + 2\gamma\, f_\gamma^+.$$

*Proof.* Rewrite (4.1.4) with $m(x,\gamma) = m_\gamma^+(x)$,

$$m(x,\gamma) = 1 + \int_x^\infty D(y-x,\gamma)\, q(y)\, m(y,\gamma)\, dy, \qquad D(x,\gamma) = \frac{e^{2i\gamma x} - 1}{2i\gamma} = \int_0^x e^{2i\gamma t}\, dt.$$

Denoting $\dot{m}(x,\gamma) = \frac{\partial m}{\partial\gamma}(x,\gamma)$, we see that $\dot{m}$ satisfies the integral equation

$$\dot{m}(x,\gamma) = M(x,\gamma) + \int_x^\infty D(y-x,\gamma)\, q(y)\, \dot{m}(y,\gamma)\, dy,$$
$$M(x,\gamma) = \int_x^\infty \dot{D}(y-x,\gamma)\, q(y)\, m(y,\gamma)\, dy,$$

which we consider as an integral equation for $\dot{m}(x,\gamma)$ with known function $M$ and which want to solve in the same way by an iteration argument;

$$h_0(x) = M(x,\gamma), \qquad h_{n+1}(x) = \int_x^\infty D(y-x,\gamma)\, q(y)\, h_n(y)\, dy, \qquad \dot{m}(x,\gamma) = \sum_{n=0}^\infty h_n(x).$$

The iteration scheme is the same as in the proof of Theorem 4.1.2 except for the initial condition. So we investigate the initial function $M(x,\gamma)$. Note that

$$|\dot{D}(x,\gamma)| = |\int_0^x 2ite^{2i\gamma t}\, dt| = |\frac{x}{\gamma} e^{2i\gamma x} - \frac{1}{\gamma} D(x,\gamma)| \leq \frac{1}{|\gamma|^2}(1 + |\gamma| x)$$

for $x \geq 0$, $\Im\gamma \geq 0$, so that

$$|M(x,\gamma)| \leq \int_x^\infty \frac{1}{|\gamma|^2}(1+|\gamma|(y-x))|q(y)|\,|m_\gamma^+(y)|\,dy$$

By the estimate $|m_\gamma^+(y)| \leq C(1+|y|)$, cf. the proof of Theorem 4.1.5, we get

$$|M(x,\gamma)| \leq \frac{1}{|\gamma|^2}\int_x^\infty (1+|y|)\,|q(y)|\,dy + \frac{1}{|\gamma|}\int_x^\infty (y-x)|q(y)|\,(1+|y|)\,dy$$

and the first integral is bounded and tends to zero for $x \to \infty$, and for the second integral we use

$$\begin{aligned}\int_x^\infty (y-x)|q(y)|\,(1+|y|)\,dy &= \int_x^\infty y|q(y)|\,(1+|y|)\,dy + (-x)\int_x^\infty |q(y)|\,(1+|y|)\,dy \\ \leq \int_0^\infty |q(y)|\,(|y|+|y|^2)\,dy &+ (-x)\int_x^\infty |q(y)|\,(1+|y|)\,dy = K(x),\end{aligned}$$

cf. proof of Theorem 4.1.5. So $M(x)$ is bounded, and even tends to zero, for $x \to \infty$ since $\int_x^\infty (y-x)|q(y)|(1+|y|)\,dy \leq \int_x^\infty |q(y)|(|y|+|y|^2)\,dy \to 0$ and grows at most linearly for $x \to -\infty$,

$$|M(x,\gamma)| \leq \frac{C}{|\gamma|^2}\int_x^\infty (1+|y|)\,|q(y)|\,dy + \frac{C}{|\gamma|}K(x) = K_1(x)$$

Note that $K_1(x) \geq K_1(y)$ for $x \leq y$, and then we find

$$|h_n(x)| \leq \frac{K_1(x)}{|\gamma|^n n!}\left(\int_x^\infty |q(y)|\,dy\right)^n$$

and we find a solution to the integral equation. The remainder of the proof follows the lines of proofs of Theorems 4.1.2 and 4.1.5 and is left as an exercise. □

**Exercise 4.1.11.** Finish the proof of Proposition 4.1.10, and state and prove the corresponding proposition for $m_\gamma^-$.

## 4.2 Scattering data: transmission and reflection coefficients

We assume that the potential $q$ is a real-valued integrable function, so that Theorem 4.1.2 applies. We also assume the conditions of Theorems 2.3.4, so that the corresponding Schrödinger operator is self-adjoint with essential spectrum $[0,\infty)$. So we get several solutions of the eigenvalue equation for the operator $-\frac{d^2}{dx^2}+q$ for the eigenvalue $\lambda=\gamma^2$, $\gamma \in \mathbb{R}\setminus\{0\}$. In particular we get $f_\gamma^+$, $f_{-\gamma}^+$, $f_\gamma^-$, $f_{-\gamma}^-$ all as solutions of the eigenvalue equation, so there are relations amongst them since the solution space is 2-dimensional. In order to describe these we consider the Wronskian[4] $W(f,g)(x) = f(x)g'(x) - f'(x)g(x)$. The Wronskian of two solutions of the eigenvalue equation is non-zero if and only if the solutions are linearly independent.

[4] Josef Hoëné de Wronski (23 August 1778 — 8 August 1853), Polish-French mathematician.

**Proposition 4.2.1.** *Assume $q$ is a continuous real-valued integrable potential. For two solutions $f_1, f_2$ to $-f'' + qf = \lambda f$, the Wronskian $W(f_1, f_2)$ is constant, and in particular $W(f^+_\gamma, f^+_{-\gamma}) = -2i\gamma$ and $W(f^-_\gamma, f^-_{-\gamma}) = 2i\gamma$, $\gamma \in \mathbb{R}\backslash\{0\}$.*

*Proof.* Differentiating gives

$$\frac{d}{dx}[W(f,g)](x) = f(x)g''(x) - f''(x)g(x) = (q(x)-\lambda)f(x)g(x) - (q(x)-\lambda)f(x)g(x) = 0,$$

since $f$ and $g$ are solutions to the eigenvalue equation. In particular, in case $f = f^+_\gamma$, $g = f^+_{-\gamma}$ we can evaluate this constant by taking $x \to \infty$ and using the asymptotics of Theorem 4.1.2. Similarly for the Wronskian of $f^-_{\pm\gamma}$. □

**Exercise 4.2.2.** In case the function $q$ is not continuous, the derivative of the Wronskian has to be interpreted in the weak sense. Modify Proposition 4.2.1 and its proof accordingly.

Since we now have four solutions, two by two linearly independent for $\gamma \neq 0$, to the Schrödinger eigenvalue equation which has a two-dimensional solution space, for the eigenvalue $\lambda = \gamma^2$, $\gamma \in \mathbb{R}\backslash\{0\}$, we obtain $a^\pm_\gamma, b^\pm_\gamma$ for $\gamma \in \mathbb{R}\backslash\{0\}$ such that for all $x \in \mathbb{R}$,

$$\begin{aligned} f^-_\gamma(x) &= a^+_\gamma\, f^+_\gamma(x) + b^+_\gamma\, f^+_{-\gamma}(x), \\ f^+_\gamma(x) &= a^-_\gamma\, f^-_\gamma(x) + b^-_\gamma\, f^-_{-\gamma}(x). \end{aligned} \tag{4.2.1}$$

Note that for $\gamma \in \mathbb{R}\backslash\{0\}$ the relation $\overline{f^\pm_\gamma(x)} = f^\pm_{-\gamma}(x)$ implies $\overline{a^+_\gamma} = a^+_{-\gamma}$, $\overline{b^+_\gamma} = b^+_{-\gamma}$, $\overline{a^-_\gamma} = a^-_{-\gamma}$ and $\overline{b^-_\gamma} = b^-_{-\gamma}$. Now

$$\begin{aligned} 2i\gamma &= W(f^-_\gamma, f^-_{-\gamma}) = W(a^+_\gamma f^+_\gamma + b^+_\gamma f^+_{-\gamma}, a^+_{-\gamma} f^+_{-\gamma} + b^+_{-\gamma} f^+_\gamma) \\ &= a^+_\gamma a^+_{-\gamma} W(f^+_\gamma, f^+_{-\gamma}) + b^+_\gamma b^+_{-\gamma} W(f^+_{-\gamma}, f^+_\gamma) = -2i\gamma a^+_\gamma a^+_{-\gamma} + 2i\gamma b^+_\gamma b^+_{-\gamma}, \\ \Longrightarrow 1 &= |b^+_\gamma|^2 - |a^+_\gamma|^2 \end{aligned}$$

for $\gamma \in \mathbb{R}\backslash\{0\}$.

Taking Wronskians in (4.2.1) and using $W(f,f) = 0$ and Proposition 4.2.1 we obtain

$$\begin{aligned} a^+_\gamma\, W(f^+_\gamma, f^+_{-\gamma}) = W(f^-_\gamma, f^+_{-\gamma}) &\Longrightarrow a^+_\gamma = -\frac{1}{2i\gamma} W(f^-_\gamma, f^+_{-\gamma}), \\ b^+_\gamma\, W(f^+_{-\gamma}, f^+_\gamma) = W(f^-_\gamma, f^+_\gamma) &\Longrightarrow b^+_\gamma = \frac{1}{2i\gamma} W(f^-_\gamma, f^+_\gamma). \end{aligned}$$

Similarly, we find

$$a^-_\gamma = \frac{1}{2i\gamma} W(f^+_\gamma, f^-_{-\gamma}), \qquad b^-_\gamma = -\frac{1}{2i\gamma} W(f^+_\gamma, f^-_\gamma), \qquad 1 = |b^-_\gamma|^2 - |a^-_\gamma|^2.$$

It follows that $b^+_\gamma = b^-_\gamma$.

Using the Jost solutions we now define the solution $\psi_\gamma(x)$, $\gamma \in \mathbb{R}\backslash\{0\}$, by the boundary conditions at $\pm\infty$;

$$\psi_\gamma(x) \sim \begin{cases} T(\gamma)\, \exp(-i\gamma x), & x \to -\infty, \\ \exp(-i\gamma x) + R(\gamma)\, \exp(i\gamma x), & x \to \infty \end{cases}$$

Note that the first condition determines $\psi_\gamma$ up to a multiplicative constant, which is determined by the requirement that the coefficient of $\exp(-i\gamma x)$ is 1 as $x \to \infty$. The function $T(\gamma)$ is the transmission coefficient and $R(\gamma)$ is the reflection coefficient.

A potential $q$ satisfying the assumptions above is a reflectionless potential if $R(\gamma) = 0$ for $\gamma \in \mathbb{R}\backslash\{0\}$.

Using Theorem 4.1.2 it follows that

$$\psi_\gamma(x) = T(\gamma)\, f_\gamma^-(x) = f_{-\gamma}^+(x) + R(\gamma)\, f_\gamma^+(x).$$

It follows that

$$T(\gamma) = \frac{1}{b_\gamma^+} = \frac{1}{b_\gamma^-}, \qquad R(\gamma) = \frac{a_\gamma^+}{b_\gamma^+} = \frac{a_\gamma^+}{b_\gamma^-}.$$

This implies for $\gamma \in \mathbb{R}\backslash\{0\}$

$$\begin{aligned} &\overline{T(\gamma)} = T(-\gamma), \quad \overline{R(\gamma)} = R(-\gamma), \quad |T(\gamma)|^2 + |R(\gamma)|^2 = 1, \\ &T(\gamma) \;=\; \frac{2i\gamma}{W(f_\gamma^-, f_\gamma^+)}, \quad R(\gamma) \;=\; -\frac{W(f_\gamma^-, f_{-\gamma}^+)}{W(f_\gamma^-, f_\gamma^+)} \end{aligned} \tag{4.2.2}$$

Physically, $|T(\gamma)|^2 + |R(\gamma)|^2 = 1$ can be interpreted as conservation of energy for transmitted and reflected waves.

Note that the reflection coefficient is related to waves travelling from left to right, and we could also have (equivalently) studied the reflection coefficient $R_-(\gamma) = a_\gamma^-/b_\gamma^-$ for waves travelling from right to left. Note that the transmission coefficient does not change. Relabeling the reflection coefficient $R_+(\gamma) = R(\gamma)$, we define for $\gamma \in \mathbb{R}$ (or $\gamma \in \mathbb{R}\backslash\{0\}$ depending on the potential $q$) the scattering matrix

$$S(\gamma) = \begin{pmatrix} T(\gamma) & R_-(\gamma) \\ R_+(\gamma) & T(\gamma), \end{pmatrix} \in U(2), \tag{4.2.3}$$

i.e. $S(\gamma)$ is a $2 \times 2$-unitary matrix. To see this we note first that, as for $R(\gamma)$,

$$\frac{R_-(\gamma)}{T(\gamma)} = a_\gamma^- = \frac{1}{2i\gamma} W(f_\gamma^+, f_{-\gamma}^-), \quad R_-(-\gamma) = \overline{R_-(\gamma)}, \quad |T(\gamma)|^2 + |R_-(\gamma)|^2 = 1.$$

From the expressions in terms of Wronskians we find

$$\frac{R_+(\gamma)}{T(\gamma)} + \frac{R_-(-\gamma)}{T(-\gamma)} = 0 \Longrightarrow T(\gamma)R_-(-\gamma) + R_+(\gamma)T(-\gamma) = T(\gamma)\overline{R_-(\gamma)} + R_+(\gamma)\overline{T(\gamma)} = 0$$

which shows that the columns of $S(\gamma)$ are orthogonal vectors. Since we already established that each column vector has length 1, we obtain $S(\gamma) \in U(2)$.

**Exercise 4.2.3.** Work out the relation between the scattering matrix $S(\gamma)$ and the scattering operator $S$ as defined in Section 3.2 in the case $L_0 = -\frac{d^2}{dx^2}$, $L = -\frac{d^2}{dx^2} + q$ (with appropriate assumptions on the potential $q$). (Hint: use the Fourier transform to describe the spectral decomposition of $L_0$ in terms of a $\mathbb{C}^2$-vector-valued measure, and describe the action of the scattering operator in terms of this decomposition.)

**Proposition 4.2.4.** *Assuming the conditions of Theorem 4.1.2 we have*

$$\lim_{\gamma\to\pm\infty} T(\gamma) = 1, \qquad \lim_{\gamma\to\pm\infty} R(\gamma) = 0.$$

*Proof.* Write $f_\gamma^-(x) = e^{-i\gamma x} + R_0^-(x)$, $f_\gamma^+(x) = e^{i\gamma x} + R_0^+(x)$, $\frac{df_\gamma^-}{dx}(x) = -i\gamma e^{-i\gamma x} + R_1^-(x)$ $\frac{df_\gamma^+}{dx}(x) = i\gamma e^{i\gamma x} + R_1^+(x)$, where $R_i^\pm(x)$, $i = 0, 1$, also depend on $\gamma$, so that

$$\begin{aligned} W(f_\gamma^-, f_\gamma^+) &= \big(e^{-i\gamma x} + R_0^-(x)\big)\big(i\gamma e^{i\gamma x} + R_1^+(x)\big) - \big(-i\gamma e^{-i\gamma x} + R_1^-(x)\big)\big(e^{i\gamma x} + R_0^+(x)\big) \\ &= 2i\gamma + i\gamma e^{i\gamma x} R_0^-(x) + e^{-i\gamma x} R_1^+(x) + R_0^-(x) R_1^+(x) \\ &\qquad + i\gamma e^{-i\gamma x} R_0^+(x) - e^{i\gamma x} R_1^-(x) - R_0^+(x) R_1^-(x). \end{aligned}$$

Theorem 4.1.2 shows that for real $x$

$$|R_0^\pm| \le G(\gamma), \qquad |R_1^\pm| \le |\gamma| G(\gamma), \qquad G(\gamma) = \exp(\|q\|_1/|\gamma|) - 1 = \mathcal{O}\big(\frac{1}{|\gamma|}\big).$$

Hence for $\gamma \in \mathbb{R}\backslash\{0\}$

$$\left|\frac{W(f_\gamma^-, f_\gamma^+)}{2i\gamma} - 1\right| \le 2G(\gamma) + \big(G(\gamma)\big)^2 \to 0, \qquad |\gamma| \to \infty.$$

Using (4.2.2) this gives the limit for the transmission coefficient, and from this the limit for the reflection coefficient follows. □

The transmission and reflection can be written as integrals involving the potential function $q$, the solution $\psi_\gamma$, and the Jost solution.

**Proposition 4.2.5.** *Assume $q$ is continuous and satisfies the conditions of Theorem 4.1.2, then for $\gamma \in \mathbb{R}\backslash\{0\}$,*

$$\begin{aligned} R(\gamma) &= \frac{1}{2i\gamma} \int_{\mathbb{R}} q(x)\, \psi_\gamma(x)\, e^{-i\gamma x}\, dx, \\ T(\gamma) &= 1 + \frac{1}{2i\gamma} \int_{\mathbb{R}} q(x)\, \psi_\gamma(x)\, e^{i\gamma x}\, dx, \\ \frac{1}{T(\gamma)} &= 1 - \frac{1}{2i\gamma} \int_{\mathbb{R}} e^{-i\gamma x} q(x) f_\gamma^+(x)\, dx. \end{aligned}$$

In the three-dimensional analogue of Proposition 4.2.5, the last type of integrals is precisely what can be measured in experiments involving particle collission. Again, the continuity of $q$ is not essential, cf. Exercise 4.2.2.

*Proof.* Take $f$ any solution to $-f'' = \gamma^2 f$ and $g$ a solution to $-g''+qg = \gamma^2 g$. Proceeding as in the proof of Proposition 4.2.1 we see that $\frac{d}{dx}[W(f,g)](x) = q(x)f(x)g(x)$, so that integrating gives

$$W(f,g)(a) \; - \; W(f,g)(b) = \int_a^b q(x)\, f(x)\, g(x)\, dx.$$

Now use this result with $f(x) = e^{-i\gamma x}$, $g(x) = \psi_\gamma(x)$, and take the limit $a \to -\infty$ and $b \to \infty$. Using the explicit expression of $\psi_\gamma$ in terms of Jost solutions and Theorem 4.1.2, then gives

$$\begin{aligned}\int_{\mathbb{R}} q(x)\, \psi_\gamma(x)\, e^{-i\gamma x}\, dx &= \lim_{b\to\infty} W(e^{-i\gamma x}, \psi_\gamma)(b) - \lim_{a\to-\infty} W(e^{-i\gamma x}, \psi_\gamma)(a) \\ &= R(\gamma) W(e^{-i\gamma x}, e^{i\gamma x}) = 2i\gamma\, R(\gamma),\end{aligned}$$

which gives the result for the reflection coefficient. The limits of the Wronskian follow from Theorem 4.1.2, cf. proof of Proposition 4.2.4. The statement for the transmission coefficient follows similarly with $f(x) = e^{i\gamma x}$.

To find other integral representations of the reflection and transmission coefficients we write

$$\begin{aligned} m_\gamma^+(x) &= 1 + \int_x^\infty \frac{e^{2i\gamma(y-x)} - 1}{2i\gamma} q(y) m_\gamma^+(y)\, dy \\ &= \frac{e^{-2i\gamma x}}{2i\gamma} \int_x^\infty e^{2i\gamma y} q(y) m_\gamma^+(y)\, dy + \left(1 - \frac{1}{2i\gamma}\int_x^\infty q(y) m_\gamma^+(y)\, dy\right) \\ &= \frac{e^{-2i\gamma x}}{2i\gamma} \int_{\mathbb{R}} e^{2i\gamma y} q(y) m_\gamma^+(y)\, dy + \left(1 - \frac{1}{2i\gamma}\int_{\mathbb{R}} q(y) m_\gamma^+(y)\, dy\right) + o(1), \quad x \to -\infty. \end{aligned}$$

Note that the remainder terms

$$\int_{-\infty}^x e^{2i\gamma y} q(y) m_\gamma^+(y)\, dy, \qquad \int_{-\infty}^x q(y) m_\gamma^+(y)\, dy$$

are $o(1)$ as $x \to -\infty$, since, by Theorem 4.1.2, $m_\gamma^+$ is bounded for fixed $\gamma \in \mathbb{R}\backslash\{0\}$, and $q$ is integrable by assumption. So

$$f_\gamma^+(x) = \frac{e^{-i\gamma x}}{2i\gamma} \int_{\mathbb{R}} e^{i\gamma y} q(y) f_\gamma^+(y)\, dy + e^{i\gamma x}\left(1 - \frac{1}{2i\gamma}\int_{\mathbb{R}} e^{-i\gamma y} q(y) f_\gamma^+(y)\, dy\right) + o(1), \quad x \to -\infty,$$

so $b_\gamma^- = 1 - \frac{1}{2i\gamma}\int_{\mathbb{R}} e^{-i\gamma y} q(y) f_\gamma^+(y)\, dy$ and $a_\gamma^- = \frac{1}{2i\gamma}\int_{\mathbb{R}} e^{i\gamma y} q(y) f_\gamma^+(y)\, dy$. Since $T(\gamma) = 1/b_\gamma^-$ the result follows. □

Using Proposition 4.2.5 and its proof we can refine the asymptotic behaviour of the transmission coefficient. Corollary 4.2.6 and its proof also indicate how to obtain the asymptotic expansion of $\frac{1}{T(\gamma)}$ for $\gamma \to \pm\infty$.

**Corollary 4.2.6.** *With the assumptions as in Proposition 4.2.5, then for* $\Im\gamma \geq 0$,

$$\frac{1}{T(\gamma)} = 1 - \frac{1}{2i\gamma}\int_{\mathbb{R}} q(y)\, dy + \mathcal{O}(\frac{1}{|\gamma|^2}).$$

*Proof.* Using $e^{-i\gamma x} f^+_\gamma(x) = m^+_\gamma(x) = 1 + \sum_{n=1}^\infty m_n(x)$ with $m_n(x) = \mathcal{O}(\frac{1}{|\gamma|^n})$ for $\gamma \to \pm\infty$, see proof of Theorem 4.1.2, in the last integral equation of Proposition 4.2.5 gives the result. □

Recall that a function is meromorphic in an open domain of $\mathbb{C}$ if it is holomorphic except at a set without accumulation points where the function has poles. Such a function can always be written as a quotient of two holomorphic functions.

**Theorem 4.2.7.** *Assume that $q$ satisfies the assumptions of Theorems 4.1.5, 2.3.4 and Proposition 4.1.10 and assume moreover $q \in L^\infty(\mathbb{R})$. The transmission coefficient $T$ is meromorphic in the the open upper half plane $\Im\gamma > 0$ with a finite number of simple poles at $ip_n$, $p_n > 0$, $1 \le n \le N$. Moreover, $T$ is continuous in $\Im\gamma \ge 0$ except for $\gamma = 0$, $\gamma = ip_n$, $1 \le n \le N$. Then $-p_n^2$, $1 \le n \le N$, are the simple eigenvalues of the corresponding Schrödinger operator with eigenfunction $f_n = f^+_{ip_n}$. Put $C_n = \lim_{x\to\infty} e^{p_n x} f^-_{ip_n}$, then*

$$\operatorname{Res}_{\gamma=ip_n} T = \frac{i}{C_n} \frac{1}{\|f_n\|^2} = i\frac{\rho_n}{C_n}. \tag{4.2.4}$$

*Proof.* By Corollary 4.1.4 we see that $W(f^-_\gamma, f^+_\gamma)$ is analytic in $\gamma$ for $\Im\gamma > 0$. By (4.2.2) $T$ is an analytic function in the open upper half plane except for poles that can only occur at zeros of $\gamma \mapsto W(f^-_\gamma, f^+_\gamma)$, $\Im\gamma > 0$.

Next using the integral representation

$$\frac{1}{T(\gamma)} = 1 - \frac{1}{2i\gamma} \int_\mathbb{R} q(x)\, m^+_\gamma(x)\, dx$$

as in Proposition 4.2.5 and the estimate $|m^+_\gamma(x)| \le C(1 + |x|)$, see Theorem 4.1.5 and its proof, we get that $\frac{1}{T(\gamma)}$ is continuous in $\Im\gamma \ge 0$, $\gamma \ne 0$, since $m^+_\gamma$ is continuous in $\Im\gamma \ge 0$. By (4.2.2) we have $|T(\gamma)|^{-1} \ge 1$ for $\gamma \in \mathbb{R}\backslash\{0\}$, so that $T(\gamma) = \frac{1}{T(\gamma)^{-1}}$ is continuous near $\Im\gamma = 0$, $\gamma \ne 0$.

For $\gamma \in \mathbb{C}$, $\Im\gamma > 0$, we put $\gamma = \alpha + i\beta$, $\beta > 0$, and consider, using Proposition 4.2.5,

$$\begin{aligned} m^+_\gamma(x) &= 1 + \int_x^\infty \frac{e^{2i\gamma(y-x)} - 1}{2i\gamma} q(y)\, m^+_\gamma(y)\, dy \\ &= \frac{1}{T(\gamma)} + \frac{1}{2i\gamma} \int_{-\infty}^x q(y)\, m^+_\gamma(y)\, dy + \int_x^\infty \frac{e^{2i\gamma(y-x)}}{2i\gamma} q(y)\, m^+_\gamma(y)\, dy. \end{aligned}$$

We want to use this expression to establish the behaviour of $m^+_\gamma(x)$ as $x \to -\infty$, so we assume $x < 0$. By Theorem 4.1.2 we see that

$$\left| \frac{1}{2i\gamma} \int_{-\infty}^x q(y)\, m^+_\gamma(y)\, dy \right| \le C \int_{-\infty}^x |q(y)|\, dy = o(1), \quad x \to -\infty,$$

with $C$ depending on $q$ and $\gamma$, since $q$ is integrable. Next, with $C$ depending on $q$ and $\gamma$,

$$\begin{aligned} \left| \int_x^\infty \frac{e^{2i\gamma(y-x)}}{2i\gamma} q(y)\, m^+_\gamma(y)\, dy \right| &\le C \int_x^{x/2} e^{-2\beta(y-x)}\, |q(y)|\, dy + C \int_{x/2}^\infty e^{-2\beta(y-x)}\, |q(y)|\, dy \\ &\le C \int_x^{x/2} |q(y)|\, dy + Ce^{\beta x} \int_\mathbb{R} |q(y)|\, dy \end{aligned}$$

by Theorem 4.1.2. The first term is $o(1)$ as $x \to -\infty$, since $q$ is integrable, and the second term $\mathcal{O}(e^{x\beta})$, $x \to -\infty$. So we obtain for $\gamma$, $\Im\gamma > 0$, the asymptotic behaviour

$$m^+_\gamma(x) = \frac{1}{T(\gamma)} + o(1), \qquad x \to -\infty.$$

Similarly, one shows $m^-_\gamma(x) = (T(\gamma))^{-1} + o(1)$, $x \to \infty$, for $\gamma$ in the open upper half plane.

Suppose that $\gamma_0$, $\Im\gamma_0 > 0$, is not a pole of $T$, so $\frac{1}{T(\gamma_0)} \neq 0$. Then $f^+_{\gamma_0}$ and $f^-_{\gamma_0}$ are linearly independent solutions and hence span the solution space, since the Wronskian is non-zero. By the above result we have

$$f^+_{\gamma_0}(x) = e^{i\gamma_0 x} m^+_{\gamma_0}(x) = \frac{e^{i\gamma_0 x}}{T(\gamma_0)} + o(e^{-x\Im\gamma_0}), \quad x \to -\infty \implies f^+_{\gamma_0} \notin L^2(\mathbb{R})$$

Similarly, $f^-_{\gamma_0} \notin L^2(\mathbb{R})$, and since $f^+_{\gamma_0}$ and $f^-_{\gamma_0}$ span the solution space, there is no square integrable solution, hence $\gamma_0^2$ is not an eigenvalue of the corresponding Schrödinger operator.

Assume next that $T^{-1}$ has a zero at $\gamma_0$ with $\Im\gamma_0 > 0$, so that $f^-_{\gamma_0}$ is a multiple of $f^+_{\gamma_0}$. By Theorem 4.1.2 it follows that $f^+_{\gamma_0}$, respectively $f^-_{\gamma_0}$, is a square integrable function for $x \to \infty$, respectively for $x \to -\infty$. Since $f^-_{\gamma_0}$ is a multiple of $f^+_{\gamma_0}$, it follows that $f^+_{\gamma_0} \in L^2(\mathbb{R})$. Theorem 4.1.2 then also gives $\frac{df^+_{\gamma_0}}{dx} = \frac{df^-_{\gamma_0}}{dx} \in L^2(\mathbb{R})$, and since $(f^\pm_{\gamma_0})''(x) = -\gamma_0^2 f^\pm_{\gamma_0}(x) + q(x) f^\pm_{\gamma_0}(x) \in L^2(\mathbb{R})$ since we assume $q \in L^\infty(\mathbb{R})$. This then gives that the eigenfunction is actually in the domain $W^2(\mathbb{R})$. Hence $f^+_{\gamma_0}$ is an eigenfunction for the corresponding Schrödinger equation for the eigenvalue $\gamma_0^2$. Since the Schrödinger operator is self-adjoint by Corollary 2.2.7, we have $\gamma_0^2 \in \mathbb{R}$ and so $\gamma_0 \in i\mathbb{R}_{>0}$.

So the poles of $T$ are on the positive imaginary axis, and such a point, say $ip$, $p > 0$, corresponds to an eigenvalue $-p^2$ of the corresponding Schrödinger operator. Since $q \in L^\infty(\mathbb{R})$ we have that the spectrum is contained in $[-\|q\|_\infty, \infty)$, and by Theorems 2.3.4 and 2.3.2 its essential spectrum is $[0, \infty)$. By Theorem 6.5.5 it follows that the intersection of the spectrum with $[-\|q\|_\infty, 0)$ can only have a finite number of points which all correspond to the point spectrum.

So we can label the zeros of the Wronskian on the positive imaginary axis as $ip_n$, $p_n > 0$, $n \in \{1, 2, \cdots, N\}$, and then $f_n(x) = f^+_{ip_n}(x)$ is a square integrable eigenfunction of the Schrödinger operator. We put

$$\frac{1}{\rho_n} = \int_{\mathbb{R}} |f_n(x)|^2 \, dx, \qquad \|f_n\| = \frac{1}{\sqrt{\rho_n}}.$$

It remains to show that the residue of $T$ at $ip_n$ is expressible in terms of $\rho_n$. Start with $2i\gamma\big(T(\gamma)\big)^{-1} = W(f^+_\gamma, f^-_\gamma)$, which is an equality for analytic functions in the open upper half plane. Differentiating with respect to $\gamma$ gives

$$\frac{2i}{T(\gamma)} + 2i\gamma \frac{dT^{-1}}{d\gamma}(\gamma) = W(\frac{\partial f^+_\gamma}{\partial\gamma}, f^-_\gamma)(x) + W(f^+_\gamma, \frac{\partial f^-_\gamma}{\partial\gamma})(x),$$

where we have emphasized the $x$-dependence in the Wronskian. In particular, for $\gamma = \gamma_0$ a pole of $T$, we get

$$2i\gamma_0 \frac{dT^{-1}}{d\gamma}(\gamma_0) = W(\frac{\partial f^+_\gamma}{\partial \gamma}|_{\gamma=\gamma_0}, f^-_{\gamma_0})(x) + W(f^+_{\gamma_0}, \frac{\partial f^-_\gamma}{\partial \gamma}|_{\gamma=\gamma_0})(x).$$

Since $f^+_\gamma$ is a solution to $-f'' + q\,f = \gamma^2 f$ and $\frac{\partial f^-_\gamma}{\partial \gamma}$ is a solution to $-f'' + q\,f = \gamma^2 f + 2\gamma\, f^-_\gamma$, cf. Proposition 4.1.10, we find, cf. the proof of Proposition 4.2.1,

$$\frac{d}{dx}\big(W(f^+_\gamma, \frac{\partial f^-_\gamma}{\partial \gamma})\big)(x) = f^+_\gamma(x) \frac{d^2}{dx^2}\frac{\partial f^-_\gamma}{\partial \gamma}(x) - \frac{d^2 f^+_\gamma}{dx^2}(x) \frac{\partial f^-_\gamma}{\partial \gamma}(x) = 2\gamma f^+_\gamma(x)\, f^-_\gamma(x),$$

so that

$$2\gamma \int_a^x f^+_\gamma(y)\, f^-_\gamma(y)\, dy = W(f^+_\gamma, \frac{\partial f^-_\gamma}{\partial \gamma})(x) - W(f^+_\gamma, \frac{\partial f^-_\gamma}{\partial \gamma})(a)$$

and this we want to consider more closely for $\gamma = \gamma_0$ a pole of the transmission coefficient $T$. Since we already have established that poles lie on the positive imaginary axis we can take $\gamma_0 = ip_n$, $p_n > 0$. Then $f_n(x) = f^+_{ip_n}(x)$ is a multiple of $f^-_{ip_n}(x)$ and Theorem 4.1.2 implies that $f_n(x)$ and its derivate $f'_n(x)$ behave like $e^{p_n x}$ as $x \to -\infty$. Combined with Proposition 4.1.10, we see that we can take the limit $a \to -\infty$ to get

$$2ip_n \int_{-\infty}^x f_n(y)\, f^-_{ip_n}(y)\, dy = W(f^+_{ip_n}, \frac{\partial f^-_\gamma}{\partial \gamma}|_{\gamma=-ip_n})(x).$$

In a similar way we get

$$2ip_n \int_x^\infty f_n(y)\, f^-_{ip_n}(y)\, dy = W(\frac{\partial f^+_\gamma}{\partial \gamma}|_{\gamma=ip_n}, f^-_{ip_n})(x)$$

so that we obtain

$$-2\, p_n \frac{dT^{-1}}{d\gamma}(ip_n) = 2ip_n \int_{\mathbb{R}} f_n(y)\, f^-_{ip_n}(y)\, dy.$$

Since $f^\pm_{ip_n}$ are real-valued, cf. remark following Theorem 4.1.2, non-zero and multiples of each other we see that $f^-_{ip_n} = C_n f^+_{ip_n}(x) = C_n f_n(x)$ for some real non-zero constant $C_n$, so that

$$\frac{dT^{-1}}{d\gamma}(ip_n) = \frac{C_n}{i} \int_{\mathbb{R}} |f_n(y)|^2\, dy \neq 0.$$

Note that $C_n = \lim_{x\to\infty} C_n e^{p_n x} f^+_{ip_n}(x) = \lim_{x\to\infty} e^{p_n x} f^-_{ip_n}$. It follows that the zero of $\frac{1}{T}$ at $ip_n$ is simple, so that $T$ has a simple pole at $ip_n$ with residue $\frac{i}{C_n}\Big(\int_{\mathbb{R}} |f_n(y)|^2\, dy\Big)^{-1}$. □

**Exercise 4.2.8.** The statement on the simplicity of the eigenvalues in Theorem 4.2.7 has not been proved. Show this.

**Definition 4.2.9.** *Assume the conditions as in Theorem 4.2.7, then the transmission coefficient $T$, the reflection coefficient $R$ together with the poles on the positive imaginary axis with the corresponding square norms; $\{(p_n, \rho_n) \mid p_n > 0, 1 \leq n \leq N\}$ constitute the scattering data.*

Given the potential $q$, the direct scattering problem constitutes of determining $T$, $R$ and $\{(p_n, \rho_n)\}$.

**Remark 4.2.10.** It can be shown that it suffices to take the reflection coefficient $R$ together with $\{(p_n, \rho_n) \mid p_n > 0, 1 \leq n \leq N\}$ as the scattering data, since the transmission coefficient can be completely recovered from this. Indeed, the norm of $T$ follows from $|T(\gamma)| = \sqrt{1 - |R(\gamma)|^2}$, see 4.2.2, and the transmission coefficient can be completely reconstructed using complex function techniques and Hardy spaces.

**Exercise 4.2.11.** Work out the scattering data for the $\cosh^{-2}$-potential using the results as in Section 2.5.2. What can you say about the scattering data for the other two examples in Sections 2.5.1, 2.5.3?

## 4.3 Fourier transform properties of the Jost solutions

We assume that the potential $q$ satisfies the conditions of Theorem 4.1.5. By Corollary 4.1.7 we see that $\gamma \mapsto m^+_\gamma(x) - 1$ is in the Hardy class $H^+_2$ for each $x \in \mathbb{R}$, see Section 6.3. So by the Paley-Wiener Theorem 6.3.2 it is the inverse Fourier transform of an $L^2(0, \infty)$ function;

$$m^+_\gamma(x) = 1 + \int_0^\infty B(x, y)\, e^{2i\gamma y}\, dy,$$

where we have switched to $2y$ instead of $y$ in order to have nicer looking formulas in the sequel. Note that for the Jost solution we have

$$f^+_\gamma(x) = e^{i\gamma x} + \int_x^\infty A(x, y)\, e^{i\gamma y}\, dy, \qquad A(x, y) = \frac{1}{2} B(x, \frac{1}{2}(y - x)).$$

So the Paley-Wiener Theorem 6.3.2 gives $B(x, \cdot) \in L^2(0, \infty)$ for each $x \in \mathbb{R}$, but the kernel $B$ satisfies many more properties. Let us consider the kernel $B$ more closely. Recall the proof of Theorem 4.1.2 and (4.1.4), and write

$$m^+_\gamma(x) - 1 = \int_x^\infty \frac{1}{2i\gamma}(e^{2i\gamma(y-x)} - 1) q(y)\, dy + \sum_{n=2}^\infty m_n(x; \gamma),$$

where we have emphasized $m_n(x; \gamma) = m_n(x)$ to express the dependence of $m_n$ on $\gamma$. Then $y \mapsto \frac{1}{2} B(x, \frac{1}{2} y)$ is the inverse Fourier transform of $m^+_\gamma(x) - 1$ with respect to $\gamma$. By the estimates in the proof of Theorem 4.1.2 it follows that each $m_n(x; \gamma)$, $n \geq 2$, is of order $\mathcal{O}(\frac{1}{|\gamma|^2})$, so we see that $\sum_{n=2}^\infty m_n(x; \gamma)$ is in $L^1(\mathbb{R})$ as function of $\gamma$, so its Fourier transform, say $\frac{1}{2}B_1(x,\frac{1}{2}y)$, is in $C_0(\mathbb{R})$ by the Riemann-Lebesgue Lemma. So it remains to take the Fourier transform of the integral. First recall, cf. proof of Theorem 4.1.5, that the integrand is majorized by $(y-x)|q(y)|$ which is assumed to be integrable on $[x,\infty)$ and the integral is of order $\mathcal{O}(\frac{1}{|\gamma|})$, so that it is in $L^2(\mathbb{R})$ with respect to $\gamma$. Write

$$\int_x^\infty \frac{1}{2i\gamma}(e^{2i\gamma(y-x)}-1)q(y)\,dy = -\frac{1}{2i\gamma}(e^{2i\gamma(y-x)}-1)w(y)\Big|_{y=x}^{\infty} + \int_x^\infty w(y)\,e^{2i\gamma(y-x)}\,dy$$
$$= \int_0^\infty w(x+y)\,e^{2i\gamma y}\,dy = \frac{1}{2}\int_0^\infty w(x+\frac{1}{2}y)\,e^{i\gamma y}\,dy$$

where we put $w(x)=\int_x^\infty q(y)\,dy$, so that $\lim_{x\to\infty} w(x)=0$. So we have written the integral as the inverse Fourier transform of $\frac{1}{2}H(y)w(x+\frac{1}{2}y)$, where $H$ is the Heaviside function $H(x)=1$ for $x\geq 0$ and $H(x)=0$ for $x<0$. So we obtain

$$B(x,y) = H(y)w(x+y) + B_1(x,y), \qquad B_1(x,\cdot)\in C_0(\mathbb{R}).$$

In particular, $B(x,0)=w(x)=\int_x^\infty q(t)\,dt$.

Since $m_\gamma^+(x)$ is a solution to $m''+2i\gamma\,m' = qm$, we see that $m_\gamma^+(x)-1$ is a solution to $m''+2i\gamma\,m' = qm+q$. Since $\lim_{x\to\infty} m_\gamma^+(x)-1=0$ and $\lim_{x\to\infty}\frac{dm_\gamma^+}{dx}(x)=0$, we can integrate this over the interval $[x,\infty)$ to find the integral equation for $m_\gamma^+$;

$$-m'(x) - 2i\gamma m(x) = \int_x^\infty q(y)\,m(y)\,dy + \int_x^\infty q(y)\,dy.$$

**Theorem 4.3.1.** *Assume $q$ satisfies the conditions of Theorem 4.1.5. The integral equation*

$$B(x,y) = \int_{x+y}^\infty q(t)\,dt + \int_0^y\int_{x+y-z}^\infty q(t)\,B(t,z)\,dt\,dz, \qquad y\geq 0,$$

*has a unique real-valued solution $B(x,y)$ satisfying*

$$|B(x,y)| \leq \int_{x+y}^\infty |q(t)|\,dt\ \exp\big(\int_x^\infty (t-x)\,|q(t)|\,dt\big).$$

*So in particular, $B(x,\cdot)\in L^\infty(0,\infty)\cap L^1(0,\infty)\subset L^p(0,\infty)$, $1\leq p\leq\infty$, with*

$$\|B(x,\cdot)\|_\infty \leq \int_x^\infty |q(t)|\,dt\ \exp\big(\int_x^\infty (t-x)\,|q(t)|\,dt\big),$$
$$\|B(x,\cdot)\|_1 \leq \int_x^\infty (t-x)|q(t)|\,dt\ \exp\big(\int_x^\infty (t-x)\,|q(t)|\,dt\big).$$

*Moreover, $B$ is a solution to*

$$\frac{\partial}{\partial x}\big(B_x(x,y)-B_y(x,y)\big) = q(x)B(x,y)$$

*with boundary conditions $B(x,0)=\int_x^\infty q(t)\,dt$ and $\lim_{x\to\infty}\|B(x,\cdot)\|_\infty = 0$.*

*Moreover, defining $m(x;\gamma)=1+\int_0^\infty B(x,y)\,e^{2i\gamma y}\,dy$, then the function $e^{-i\gamma x}m(x;\gamma)$ is the Jost solution $f_\gamma^+$ for the corresponding Schrödinger operator.*

The partial differential equation is a hyperbolic boundary value problem known as a Goursat partial differential equation.

*Proof.* We solve the integral equation by an iteration as before. Put $B(x,y) = \sum_{n=0}^\infty K_n(x,y)$ with $K_n(x,y)$ defined recursively

$$K_0(x,y) = \int_{x+y}^\infty q(t)\,dt, \qquad K_{n+1}(x,y) = \int_0^y \int_{x+y-z}^\infty q(t)\,K_n(t,z)\,dt\,dz.$$

It is then clear that $B(x,y)$ solves the integral equation provided the series converges. We claim that

$$|K_n(x,y)| \leq \frac{\big(R(x)\big)^n}{n!}\,S(x+y), \qquad R(x) = \int_x^\infty (t-x)|q(t)|\,dt, \quad S(x) = \int_x^\infty |q(t)|\,dt. \tag{4.3.1}$$

Note that $\int_0^\infty S(x+y)\,dy = R(x)$. Let us first assume the claim is true. Then the series converges uniformly on compact sets in $\mathbb{R}^2$ and the required estimate follows. It is then also clear that $K_n(x,y) \in \mathbb{R}$ for all $n$ since $q$ is real-valued, so that $B$ is real-valued. We leave uniqueness as an exercise, cf. the uniqueness proof in the proof of Theorem 4.1.2.

Observe that $S(x+y) \leq S(x)$ for $y \geq 0$, so that estimate on the $L^\infty(0,\infty)$-norm of $B(x,\cdot)$ follows immediately, and this estimate also gives $\lim_{x\to\infty} \|B(x,\cdot)\|_\infty = 0$, since $S(x) \to 0$ as $x \to \infty$. For the $L^1(0,\infty)$-norm we calculate

$$\int_0^\infty |B(x,y)|\,dy \leq \exp\big(R(x)\big) \int_0^\infty S(x+y)\,dy = \exp\big(R(x)\big)\,R(x)$$

Differentiating with respect to $x$ and $y$ gives

$$\begin{aligned}
\frac{\partial B}{\partial x}(x,y) &= -q(x+y) - \int_0^y q(x+y-z)\,B(x+y-z,z)\,dz, \\
\frac{\partial B}{\partial y}(x,y) &= -q(x+y) + \int_x^\infty q(t)\,B(t,y)\,dt - \int_0^y q(x+y-z)\,B(x+y-z,z)\,dz.
\end{aligned}$$

Here we use Lebesgue's Differentiation Theorem 6.1.4, so the resulting identities hold almost everywhere. Unless we impose differentiability conditions on $q$, we cannot state anything about the higher order partial derivatives, but $B_x(x,y) - B_y(x,y) = \int_x^\infty q(t)\,B(t,y)\,dt$ can be differentiated with respect to $x$, and this gives the required partial differential equation. We also obtain

$$\begin{aligned}
&\Big|\frac{\partial B}{\partial x}(x,y) + q(x+y)\Big| \leq \int_0^y |q(x+y-z)\,B(x+y-z,z)|\,dz, \\
&\leq \int_0^y |q(x+y-z)|\,\exp(R(x+y-z))\,S(x+y)\,dz \\
&\leq S(x+y)\,\exp(R(x)) \int_x^{x+y} |q(t)|\,dt \;\leq\; S(x+y)\,\exp(R(x))\,S(x)
\end{aligned} \tag{4.3.2}$$

since $R$ is decreasing. The one but last estimate can also be used to observe that

$$\Big|\frac{\partial B}{\partial x}(x,y)+q(x+y)\Big| \leq S(x)\,\exp(R(x))\int_x^{x+y}|q(t)|\,dt\to 0, \qquad y\downarrow 0,$$

since $S(x+y)\leq S(x)$ and $q$ is integrable. This gives the other boundary condition for the partial differential equation. Similarly,

$$\begin{aligned}
\Big|\frac{\partial B}{\partial y}(x,y)+q(x+y)\Big| &\leq \int_0^y |q(x+y-z)\,B(x+y-z,z)|\,dz+\int_x^\infty |q(t)\,B(t,y)|\,dt,\\
\leq &\int_0^y |q(x+y-z)|\,\exp(R(x+y-z))\,S(x+y)\,dz+\int_x^\infty |q(t)|\,\exp(R(t))\,S(t+y)\,dt\\
\leq &\, S(x+y)\,\exp(R(x))\int_x^{x+y}|q(t)|\,dt\,+S(x+y)\,\exp(R(x))\int_x^\infty |q(t)|\,dt\\
\leq &\, 2\,S(x+y)\,\exp(R(x))\,S(x).
\end{aligned}$$

Define $n(x;\gamma)=\int_0^\infty B(x,y)\,e^{2i\gamma y}\,dy$, then by (4.3.2) we find $|\frac{\partial B}{\partial x}(x,y)|\leq |q(x+y)|+S(x+y)S(x)\exp(R(x))$ and the right hand side is integrable with respect to $y\in[0,\infty)$. So we can differentiate with respect to $x$ in the integrand to get

$$\begin{aligned}
n'(x,\gamma) &= \int_0^\infty B_x(x,y)\,e^{2i\gamma y}\,dy=\int_0^\infty \Big(B_x(x,y)-B_y(x,y)\Big)\,e^{2i\gamma y}\,dy+\int_0^\infty B_y(x,y)\,e^{2i\gamma y}\,dy\\
&= -\int_0^\infty\int_x^\infty q(t)\,B(t,y)\,dt\,e^{2i\gamma y}\,dy+B(x,y)e^{2i\gamma y}\Big|_{y=0}^\infty-2i\gamma\int_0^\infty B(x,y)\,e^{2i\gamma y}\,dy\\
&= -\int_0^\infty\int_x^\infty q(t)\,B(t,y)\,dt\,e^{2i\gamma y}\,dy-B(x,0)-2i\gamma\int_0^\infty B(x,y)\,e^{2i\gamma y}\,dy\\
&= \int_x^\infty q(t)\int_0^\infty B(t,y)\,e^{2i\gamma y}\,dydt-B(x,0)-2i\gamma\int_0^\infty B(x,y)\,e^{2i\gamma y}\,dy\\
&= -\int_x^\infty q(t)\,n(t;\gamma)\,dt-\int_x^\infty q(t)\,dt-2i\gamma\,n(x;\gamma)
\end{aligned}$$

since $\lim_{y\to\infty}B(x,y)=0$ by $\lim_{y\to\infty}S(x+y)=0$, and where Fubini's theorem is applied and $B(x,0)=\int_x^\infty q(t)\,dt$. So $n(x;\gamma)$ satisfies the integrated version of the differential equation $m''+2i\gamma m'=qm+q$. Since $|n(x;\gamma)|\leq \|B(x,\cdot)\|_1\to 0$ as $x\to\infty$, it follows that $n(\gamma;x)=m_\gamma^+(x)-1$ and the result follows.

It remains to prove the estimate in (4.3.1). This is proved by induction on $n$. The case $n=0$ is trivially satisfied by definition of $S(x+y)$. For the induction step, we obtain by the induction hypothesis and the monotonicity of $S$ the estimate

$$\begin{aligned}
|K_{n+1}(x,y)| &\leq \int_0^y\int_{x+y-z}^\infty |q(t)|\,S(t+z)\frac{(R(t))^n}{n!}\,dt\,dz\\
&\leq S(x+y)\int_0^y\int_{x+y-z}^\infty |q(t)|\,\frac{(R(t))^n}{n!}\,dt\,dz
\end{aligned}$$

and it remains to estimate the double integral. Interchanging the order of integration, the integral equals

$$
\begin{aligned}
&\int_x^{x+y} |q(t)| \frac{(R(t))^n}{n!} \int_{x+y-t}^{y} dz\,dt + \int_{x+y}^{\infty} |q(t)| \frac{(R(t))^n}{n!} \int_0^y dz\,dt \\
= &\int_x^{x+y} (t-x)|q(t)| \frac{(R(t))^n}{n!}\,dt + \int_{x+y}^{\infty} y|q(t)| \frac{(R(t))^n}{n!}\,dt \\
\le &\int_x^{\infty} (t-x)|q(t)| \frac{(R(t))^n}{n!}\,dt = \int_x^{\infty} (t-x)|q(t)| \frac{1}{n!} \left(\int_t^{\infty} (u-t)|q(u)|\,du\right)^n dt \\
\le &\int_x^{\infty} (t-x)|q(t)| \frac{1}{n!} \left(\int_t^{\infty} (u-x)|q(u)|\,du\right)^n dt = \frac{(R(x))^{n+1}}{(n+1)!}
\end{aligned}
$$

using $y \le t-x$ in the first inequality and $u-t \le u-x$ for $x \ge t$ in the second inequality. This proves the induction step. $\square$

**Exercise 4.3.2.** Work out the kernel $B$ for the $\cosh^{-2}$-potential using the results as in Section 2.5.2, see also Section 4.5. What can you say about the kernel $B$ for the other two examples in Sections 2.5.1, 2.5.3?

Note that in the above considerations for the Jost solution $\gamma \in \mathbb{R}$, but it is possible to extend the results to $\gamma$ in the closed upper half plane, $\Im\gamma \ge 0$.

**Proposition 4.3.3.** *Assume that $q$ satisfies the assumptions of Theorem 4.1.5. The relations*

$$
m^+_\gamma(x) = 1 + \int_0^\infty B(x,y)\, e^{2i\gamma y}\,dy, \qquad f^+_\gamma(x) = e^{i\gamma x} + \int_x^\infty A(x,y)\, e^{i\gamma y}\,dy
$$

*remain valid for $\Im\gamma \ge 0$.*

*Proof.* Fix $x \in \mathbb{R}$ and consider $F(\gamma) = m^+_\gamma(x) - 1 - \int_0^\infty B(x,y)e^{2i\gamma y}\,dy$, then we know that $F$ is analytic in the open upper half plane $\Im\gamma > 0$ and continuous on $\Im\gamma \ge 0$. Moreover, $F(\gamma) = 0$ for $\gamma \in \mathbb{R}$. We now use for fixed $\gamma$ in the open upperhalf plane $F(\gamma) = \frac{1}{2\pi i}\int_{\mathcal{C}} \frac{F(z)}{z-\gamma}\,dz$ for a suitable contour $\mathcal{C}$ in the open upper half plane. We take $\mathcal{C}$ to be a semicircle of sufficiently large radius $R$ just above the real axis at $\Im z = \varepsilon < \Im\gamma$. This gives the estimate

$$
\begin{aligned}
|F(\gamma)| &\le \frac{1}{2\pi} \int_{|z|=R,\Im z>0} \frac{|F(z)|}{|z-\gamma|}\,dz + \frac{1}{2\pi} \int_{-R+i\varepsilon}^{R+i\varepsilon} \frac{|F(z)|}{|z-\gamma|}\,dz \\
&\le \frac{1}{2\pi} \frac{R}{\operatorname{dist}(\gamma, |z|=R)} \int_0^\pi |F(Re^{i\theta})|\,d\theta + \frac{1}{2\pi} \int_{-R}^{R} \frac{|F(t+i\varepsilon)|}{|t+i\varepsilon-\gamma|}\,dt.
\end{aligned}
$$

For $\gamma$ in the open upper half plane we can take $\varepsilon \downarrow 0$ in the second integral by dominated convergence, which then gives zero. The factor in front of the first integral is bounded as $R \to \infty$ for $\gamma$ fixed in the upper half plane, so the result follows from the claim

$$
\lim_{R\to\infty} \int_0^\pi |F(Re^{i\theta})|\,d\theta = 0.
$$

To prove this first observe that $\int_0^\pi |m^+_{Re^{i\theta}} - 1|\, d\theta \to 0$ as $R \to \infty$, since the integrand is $\mathcal{O}(\frac{1}{R})$ by Theorem 4.1.2. So it remains to estimate

$$\int_0^\pi \int_0^\infty |B(x,y)e^{2iRe^{i\theta}y}|\, dy\, d\theta = \int_0^\pi \int_0^\infty |B(x,y)|e^{-2Ry\sin\theta}\, dy\, d\theta$$
$$= \left( \int_0^{\varepsilon(R)} + \int_{\varepsilon(R)}^{\pi-\varepsilon(R)} + \int_{\pi-\varepsilon(R)}^{\pi} \right) \int_0^\infty |B(x,y)|e^{-2Ry\sin\theta}\, dy\, d\theta,$$

where $\varepsilon(R) \in (0, \frac{1}{2}\pi)$ is choosen such that $\sin\theta \geq \frac{1}{\sqrt{R}}$ for all $\theta \in (\varepsilon(R), \pi - \varepsilon(R))$. We have $\sin\varepsilon(R) = \frac{1}{\sqrt{R}}$ and $\varepsilon(R) \sim \frac{1}{\sqrt{R}}$ as $R \to \infty$. Now the integral can be estimated by

$$2\varepsilon(R) \int_0^\infty |B(x,y)|\, dy + \pi \int_0^\infty e^{-2y\sqrt{R}}|B(x,y)|\, dy = 2\varepsilon(R)\|B(x,\cdot)\|_1 + \frac{\pi}{2\sqrt[4]{R}}\|B(x,\cdot)\|_2 \to 0$$

as $R \to \infty$. □

**Exercise 4.3.4.** Work out the proof of the second statement of Proposition 4.3.3.

.

## 4.4 Gelfand-Levitan-Marchenko integral equation

In this section we consider the inverse scattering problem, namely how to construct the potential from the scattering data. From Theorem 4.3.1 we see that the potential $q$ can be recovered from the kernel $B$ for the Jost solution $f^+_\gamma$. So if we can characterize the kernel $B$ in terms of scattering data we are done, and this is described by the Gelfand[5]-Levitan[6]-Marchenko[7] integral equation. To see how this comes about we first start with a formal calculation. We assume that $T$ has no poles in the open upper half plane, i.e. the corresponding Schrödinger operator has no discrete spectrum. Assume that the reflection coefficient $R(\gamma)$ has a Fourier transform $R(\gamma) = \int_{\mathbb{R}} r(y)e^{i\gamma y}\, dy$, where we absorb the factor $\frac{1}{\sqrt{2\pi}}$ in $r$, then using the results in Section 4.3 give

$$T(\gamma)\, f^-_\gamma(x) = f^+_{-\gamma}(x) + R(\gamma)\, f^+_\gamma(x)$$
$$= e^{-i\gamma x} + \int_x^\infty A(x,y)e^{-i\gamma y}\, dy + \int_{\mathbb{R}} r(y)e^{i\gamma(x+y)}\, dy + \int_{\mathbb{R}} r(z)e^{i\gamma z}\, dz \int_x^\infty A(x,y)e^{-i\gamma y}\, dy$$

and this is rewritten as

$$\int_{-\infty}^{-x} A(x,-y)e^{i\gamma y}\, dy + \int_{\mathbb{R}} r(y-x)e^{i\gamma y}\, dy + \int_{\mathbb{R}} \Big( \int_x^\infty A(x,z)\, r(y-z)\, dz \Big) e^{i\gamma y} dy$$
$$= T(\gamma)\, f^-_\gamma(x) - e^{-i\gamma x}.$$

[5]Israil Moiseevic Gelfand (2 September 1913 — ), Russian mathematician, one of the greatest mathematicians of the 20th century.

[6]Boris Levitan (1915 — 4 April 2004), Russian mathematician.

[7]Vladimir Aleksandrovich Marchenko, (7 July 1922 — ), Ukrainian mathematician.

Now as in Section 4.3 we have that $m^-_\gamma(x) - 1$ is in the Hardy class $H^+_2$, so we similarly get $f^-_\gamma(x) = e^{-i\gamma x} + \int_{-x}^\infty A_-(x,y)e^{i\gamma y}\, dy$, hence the right hand side equals

$$T(\gamma)\, f^-_\gamma(x) - e^{-i\gamma x} \;=\; \bigl(T(\gamma) - 1\bigr)e^{-i\gamma x} + T(\gamma)\,\bigl(m^-_\gamma(x) - 1\bigr)\, e^{-i\gamma x}.$$

Now if $\gamma \mapsto T(\gamma) - 1$ and $\gamma \mapsto T(\gamma)\,\bigl(m^-_\gamma(x) - 1\bigr)$ are of Hardy class $H^+_2$, which can be shown by using that $\gamma \mapsto m^-_\gamma(x) - 1$ is in $H^+_2$ and by refining the estimates on $T$ in Proposition 4.2.4, it follows from the Paley-Wiener Theorem 6.3.2 and shifting by $x$ that Fourier transform of the right hand side is supported on $[-x, \infty)$. But the left hand side is a Fourier transform, so that

$$A(x,-y) + r(y-x) + \int_x^\infty A(x,z)\, r(y-z)\, dz = 0, \qquad y < -x. \tag{4.4.1}$$

So assuming the reflection coefficient, hence its Fourier transform, is known the kernel $A$, satisfies (4.4.1). Assuming that the integral equation can be uniquely solved, the potential $q$ then follows from $B$ by a formula as in Theorem 4.3.1. The integral equation (4.4.1) is known as the Gelfand-Levitan-Marchenko equation. We see that the Gelfand-Levitan-Marchenko equation is essentially expressing a fact on the Fourier transform of the fundamental relation $T(\gamma)\, f^-_\gamma(x) = f^+_{-\gamma}(x) + R(\gamma)\, f^+_\gamma(x)$ between Jost solutions.

In case the Schrödinger operator has point spectrum, the transmission coefficient has poles. In this case the Fourier transform is not identically zero for $y < -x$, but there are non-zero contributions. The idea is to find these non-zero contributions by shifting the path in $\int_\mathbb{R} T(\gamma) f^-_\gamma(x) e^{-i\gamma x}\, d\gamma$ to $\Im\gamma$ is a large enough constant, and by picking residues at $ip_n$, $1 \le n \le N$, with notation and residues as in Theorem 4.2.7. This idea shows that the above approach can be adapted by adding a finite sum to the kernel $r$ in (4.4.1).

In order to make the above approach rigorous we need to investigate the reflection coefficient more closely. Instead of dealing with the kernel $A$ we deal with the kernel $B$ as considered in Theorem 4.3.1.

**Proposition 4.4.1.** *Assume the potential $q$ satisfies the conditions of Theorem 4.1.2, then the reflection coefficient $R \in L^2(\mathbb{R})$, so that its inverse Fourier transform, up to scaling and linear transformation of the argument, $K_c \colon y \mapsto \frac{1}{\pi}\int_\mathbb{R} R(\gamma) e^{2i\gamma y}\, dy$ is defined as an element in $L^2(\mathbb{R})$.*

So $K_c(x) = \frac{1}{\pi}\int_\mathbb{R} R(\gamma)\, e^{2i\gamma x}\, d\gamma$ is considered as an element of $L^2(\mathbb{R})$. Since $\overline{R(\gamma)} = R(-\gamma)$ we see that $\overline{K_c(x)} = \frac{1}{\pi}\int_\mathbb{R} R(-\gamma)\, e^{-2i\gamma x}\, d\gamma = K_c(x)$ or $K_c$ is real-valued.

*Proof.* First observe that the reflection coefficient is bounded on $\mathbb{R}$ by (4.2.2). From the proof of Proposition 4.2.4 it follows that $\frac{1}{T(\gamma)} - 1 = \mathcal{O}(\frac{1}{|\gamma|})$ as $\gamma \to \pm\infty$. So $T(\gamma) = 1 + \mathcal{O}(\frac{1}{|\gamma|})$ and so is $|R(\gamma)| = \sqrt{1 - |T(\gamma)|^2} = \mathcal{O}(\frac{1}{|\gamma|})$. So $|R(\gamma)|^2 = \mathcal{O}(\frac{1}{|\gamma|^2})$, and $R \in L^2(\mathbb{R})$. $\square$

Assuming the conditions of Theorem 4.2.7, we can consider the discrete spectrum of the corresponding Schrödinger operator. With the notation of Theorem 4.2.7 we define

$$K_d(x) = 2\sum_{n=1}^N \rho_n e^{-2p_n x}$$

and $K_d(x) = 0$ if the transmission coefficient has no poles, i.e. the Schrödinger operator has no discrete eigenvalues. So we let $K_c$, respectively $K_d$, correspond to the continuous, respectively discrete, spectrum of the Schrödinger operator. Now define, $K = K_c + K_d$ as the sum of two square integrable functions on the interval $[a, \infty)$ for any fixed $a \in \mathbb{R}$.

**Theorem 4.4.2.** *Assume the potential $q$ satisfies the conditions of Theorem 4.2.7. Then the kernel $B$ satisfies the integral equation*

$$K(x+y) + \int_0^\infty B(x,z)\, K(x+y+z)\, dz + B(x,y) = 0,$$

*for allmost all $y \geq 0$ which for each fixed $x \in \mathbb{R}$ is an equation that holds for $B(x,\cdot) \in L^2(0,\infty)$. Moreover, the integral equation has a unique solution $B(x,\cdot) \in L^2(0,\infty)$.*

The integral equation is the Gelfand-Levitan-Marchenko equation, and we see that the kernel $B$, hence by Theorem 4.3.1 the potential $q$, is completely determined by the scattering data. So in this way the inverse scattering problem is solved. In particular, the transmission coefficient $T$ is not needed, cf. Remark 4.2.10, and hence is determined by the remainder of the scattering data.

*Proof.* So consider $T(\gamma)\, f^-_\gamma(x) = f^+_{-\gamma}(x) + R(\gamma)\, f^+_\gamma(x)$ and rewrite this in terms of $m^\pm_{\pm\gamma}(x)$ to find for $\gamma \in \mathbb{R}\backslash\{0\}$

$$\begin{aligned} T(\gamma)\, m^-_\gamma(x) &= m^+_{-\gamma}(x) \;+\; R(\gamma)\, e^{2i\gamma x}\, m^+_\gamma(x) \\ &= 1 + \int_0^\infty B(x,y)\, e^{-2i\gamma y}\, dy + R(\gamma) e^{2i\gamma x}\Big(1 + \int_0^\infty B(x,y)\, e^{2i\gamma y}\, dy\Big) \\ \Longrightarrow\; T(\gamma)\, m^-_\gamma(x) - 1 &= \int_0^\infty B(x,y)\, e^{-2i\gamma y}\, dy + R(\gamma)e^{2i\gamma x} + R(\gamma)e^{2i\gamma x}\int_0^\infty B(x,y)\, e^{2i\gamma y}\, dy \end{aligned}$$

using Theorem 4.3.1. As functions of $\gamma$, the first term on the right hand side is an element of $L^2(\mathbb{R})$ by Theorem 4.3.1, and similarly for the last term on the right hand side using that $R(\gamma)$ is bounded by 1, see (4.2.2). Proposition 4.4.1 gives that the middle term on the right hand side is an element of $L^2(\mathbb{R})$. So we see that the function on the left hand side is an element of $L^2(\mathbb{R})$, which we can also obtain directly from $T(\gamma)\, m^-_\gamma(x) - 1 = T(\gamma)\big(m^-_\gamma(x) - 1\big) + \big(T(\gamma) - 1\big)$. By Corollary 4.1.7 and the boundedness of $T$, the first term is even in the Hardy class $H^+_2$ and the second term is in $L^2(\mathbb{R})$ by the estimates in the proof of Proposition 4.2.4.

So we take the inverse Fourier transform of this identity for elements of $L^2(\mathbb{R})$. Since we have switched to other arguments we use the Fourier transform in the following form, cf. Section 6.3;

$$g(\lambda) = \int_{\mathbb{R}} f(y)\, e^{-2i\lambda y}\, dy, \qquad f(y) = (\mathcal{G}g)(y) = \frac{1}{\pi}\int_{\mathbb{R}} g(\lambda)\, e^{2i\lambda y}\, d\lambda,$$

where $\mathcal{G}$ is a bounded invertible operator on $L^2(\mathbb{R})$. So applying $\mathcal{G}$ we get an identity in $L^2(\mathbb{R})$ for each fixed $x$;

$$\begin{aligned} \mathcal{G}\big(\gamma \mapsto T(\gamma)\, m^-_\gamma(x) - 1\big) = {} & B(x,\cdot) + \mathcal{G}\big(\gamma \mapsto R(\gamma) e^{2i\gamma x}\big) \\ & + \mathcal{G}\Big(\gamma \mapsto R(\gamma)e^{2i\gamma x}\int_0^\infty B(x,z)\, e^{2i\gamma z}\, dz\Big). \end{aligned}$$

It remains to calculate the three $\mathcal{G}$-transforms explicitly. Since the identity is not in $L^2(\mathbb{R})$ we have to employ approximations.

We first calculate $\mathcal{G}\big(\gamma \mapsto R(\gamma)e^{2i\gamma x}\big)$. Put $R_\varepsilon(\gamma) = \exp(-\varepsilon\gamma^2)\, R(\gamma)$, so that $R_\varepsilon \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, and note that

$$\int_{\mathbb{R}} |R_\varepsilon(\gamma)e^{2i\gamma x} - R(\gamma)e^{2i\gamma x}|^2\, d\gamma = \int_{\mathbb{R}} |R(\gamma)|^2 |1 - e^{-\varepsilon\gamma^2}|^2\, d\gamma \to 0, \qquad \varepsilon \downarrow 0,$$

by the Dominated Convergence Theorem 6.1.3. By continuity of $\mathcal{G}$ on $L^2(\mathbb{R})$ we then have

$$\lim_{\varepsilon\downarrow 0} \mathcal{G}\big(\gamma \mapsto R_\varepsilon(\gamma)e^{2i\gamma x}\big) = \mathcal{G}\big(\gamma \mapsto R(\gamma)e^{2i\gamma x}\big) \text{ in } L^2(\mathbb{R}).$$

Now

$$\mathcal{G}\big(\gamma \mapsto R_\varepsilon(\gamma)e^{2i\gamma x}\big)(y) = \frac{1}{\pi}\int_{\mathbb{R}} R(\gamma)\, e^{-\varepsilon\gamma^2} e^{2i\gamma(x+y)}\, dy = \mathcal{G}\big(\gamma \mapsto R_\varepsilon(\gamma)\big)(x+y)$$

and this tends to $y \mapsto K_c(x+y)$ as an element of $L^2(\mathbb{R})$ as $\varepsilon \downarrow 0$.

Similarly we consider the other $\mathcal{G}$ transform on the right hand side;

$$\frac{1}{\pi}\int_{\mathbb{R}} \Big(R_\varepsilon(\gamma)e^{2i\gamma x}\int_0^\infty B(x,z)e^{2i\gamma z}\, dz\Big)e^{2i\gamma y}\, d\gamma = \int_0^\infty B(x,z)\Big(\frac{1}{\pi}\int_{\mathbb{R}} R_\varepsilon(\gamma)e^{2i\gamma(x+y+z)}\, d\gamma\Big)\, dz,$$

since the integrals converge absolutely by $|R_\varepsilon(\gamma)| \le e^{-\varepsilon\gamma^2}$ and $B(x,\cdot) \in L^1(\mathbb{R})$ by Theorem 4.3.1. The inner integral converges to $K_c(x+y+z)$ as $\varepsilon \downarrow 0$ in $L^2(\mathbb{R})$, and since $B(x,\cdot) \in L^2(0,\infty)$ by Theorem 4.3.1 the Cauchy-Schwarz inequality (6.1.1) for $L^2(0,\infty)$ shows that the integral converges to $\int_0^\infty B(x,z)K_c(x+y+z)\, dz$ as $\varepsilon \downarrow 0$.

It remains to calculate the $\mathcal{G}$-transform of the left hand side, and this is where the poles of the transmission coefficient play a role. By Theorem 4.2.7 the function $\gamma \mapsto T(\gamma)m^-_\gamma(x) - 1$ is meromorphic in $\Im\gamma > 0$ for fixed $x$ and continuous in $\Im\gamma \ge 0$. Moreover, it has simple poles at $ip_n$, $1 \le n \le N$, so we want to employ Cauchy's Theorem. We first multiply by $\frac{1}{1-i\varepsilon\gamma}$, $\varepsilon > 0$, which has a pole at $\gamma = 1/i\varepsilon = -i/\varepsilon$ in the open lower half plane. (Note that $\exp(-\varepsilon\gamma^2)$ is not a good modification, because we want to consider the function in the upper half plane.) Then, for $\varepsilon > 0$,

$$\mathcal{I}_\varepsilon(x,y) = \frac{1}{\pi}\int_{\mathbb{R}} \frac{1}{1-i\varepsilon\gamma}(T(\gamma)m^-_\gamma(x) - 1)e^{2i\gamma y}\, d\gamma$$

has an integrable integrand meromorphic in $\Im\gamma > 0$ and continuous in $\Im\gamma \ge 0$. We only consider this integral for $y \ge 0$. We claim that

$$\mathcal{I}_\varepsilon(x,y) = \lim_{M\to\infty} \frac{1}{\pi}\int_{\mathcal{C}_M} \frac{1}{1-i\varepsilon\gamma}(T(\gamma)m^-_\gamma(x) - 1)e^{2i\gamma y}\, d\gamma,$$

where $\mathcal{C}_M$ is the closed contour in the complex plane consisting of the interval $[-M, M]$ on the real axis and the half circle $z = Me^{i\theta}$, $0 \le \theta \le \pi$. (Note that we first observe this for $\mathcal{C}^\delta_M$

where the interval is taken $[-M+i\delta, M+i\delta]$ for some $\delta>0$ and next let $\delta \searrow 0$.) This is a consequence of

$$T(\gamma)m^-_\gamma(x) - 1 = \mathcal{O}(\frac{1}{|\gamma|}), \qquad \Im\gamma \geq 0,$$

so that the integrand is $\mathcal{O}(\frac{1}{|\gamma|^2})$ and the integrand over the half circle tends to zero.

Now the contour integral can be evaluated, cf. proof of Proposition 4.3.3, by Cauchy's Theorem;

$$\begin{aligned}\mathcal{I}_\varepsilon(x,y) &= \frac{2\pi i}{\pi}\sum_{n=1}^N \mathrm{Res}_{\gamma=ip_n}\frac{1}{1-i\varepsilon\gamma}(T(\gamma)m^-_\gamma(x)-1)e^{2i\gamma y}\\ &= 2i\sum_{n=1}^N \frac{1}{1+\varepsilon p_n}\bigl(\mathrm{Res}_{\gamma=ip_n}T(\gamma)\bigr)m^-_{ip_n}(x)e^{-2p_n y}.\end{aligned}$$

Since $f^-_{ip_n}(x) = C_n\, f^+_{ip_n}(x) = C_n\, f_n(x)$, cf. proof of Theorem 4.2.7, we find $m^-_{ip_n}(x) = e^{-2p_n x}C_n m^+_{ip_n}(x)$. With the value of the residue in Theorem 4.2.7, we find

$$\begin{aligned}\lim_{\varepsilon\downarrow 0}\mathcal{I}_\varepsilon(x,y) &= -2\sum_{n=1}^N \frac{1}{\|f_n\|^2}m^+_{ip_n}(x)e^{-2p_n(x+y)}\\ &= -2\sum_{n=1}^N \frac{1}{\|f_n\|^2}e^{-2p_n(x+y)} - 2\sum_{n=1}^N\frac{1}{\|f_n\|^2}\int_0^\infty B(x,z)e^{-2p_n z}\,dz\, e^{-2p_n(x+y)}\\ &= -K_d(x+y) - \int_0^\infty B(x,z)\,K_d(x+y+z)\,dz.\end{aligned}$$

Combining the ingredients gives the required Gelfand-Levitan-Marchenko integral equation for $B$.

In order to prove the uniqueness of the solution, we consider the operator $f\mapsto K^{(x)}f$ with

$$K^{(x)}f(y) = \int_0^\infty K(x+y+z)\,f(z)\,dz,$$

then $K^{(x)}\colon L^2(0,\infty)\to L^2(0,\infty)$ is a bounded operator as we show below. For uniqueness we need to show that $K^{(x)}f+f=0$ only has the trivial solution $f=0$ in $L^2(\mathbb{R})$.

First, to show that $K^{(x)}$ is bounded on $L^2(0,\infty)$ we consider for $f,g \in L^2(0,\infty)\cap L^1(0,\infty)$,

$$\begin{aligned}\langle K^{(x)}f,g\rangle &= \int_0^\infty \Big(\int_0^\infty K(x+y+z)\,f(z)\,dz\Big)\overline{g(y)}\,dy \\ &= 2\sum_{n=1}^N \int_0^\infty \int_0^\infty \rho_n e^{-2p_n(x+y+z)} f(z)\,g(y)\,dz\,dy \\ &\qquad + \frac{1}{\pi}\int_0^\infty \int_0^\infty \int_{\mathbb{R}} f(z)\overline{g(y)}R(\gamma)e^{2i\gamma(x+y+z)}\,d\gamma\,dy\,dz \\ &= \sum_{n=1}^N \langle f,e_n\rangle\langle e_n,g\rangle + 2\int_{\mathbb{R}} \big(\mathcal{F}^{-1}f\big)(2\gamma)\big(\mathcal{F}^{-1}\bar{g}\big)(2\gamma)\,R(\gamma)\,e^{2i\gamma x}\,d\gamma \\ &= \sum_{n=1}^N \langle f,e_n\rangle\langle e_n,g\rangle + \int_{\mathbb{R}} \big(\mathcal{F}^{-1}f\big)(\gamma)\big(\mathcal{F}^{-1}\bar{g}\big)(\gamma)\,R(\tfrac{1}{2}\gamma)\,e^{i\gamma x}\,d\gamma\end{aligned}$$

where $e_n(y)=\sqrt{2\rho_n}e^{-2p_ny-p_nx}$ is an element of $L^2(0,\infty)$ and $\langle\cdot,\cdot\rangle$ denotes the inner product of the Hilbert space $L^2(0,\infty)$, which we consider as a subspace of $L^2(\mathbb{R})$ in the obvious way. Note that interchanging of the integrals is justified because all integrals converge for $f,g\in L^1(0,\infty)$. Next we estimate the right hand side in terms of the $L^2(0,\infty)$-norm of $g$ by

$$\begin{aligned}&\|g\|_{L^2(0,\infty)}\,\|f\|_{L^2(0,\infty)}\sum_{n=1}^N \|e_n\|^2_{L^2(0,\infty)} + \|\mathcal{F}^{-1}f\|_{L^2(\mathbb{R})}\|\mathcal{F}^{-1}\bar{g}\|_{L^2(\mathbb{R})} \\ \le\ &\|g\|_{L^2(0,\infty)}\,\|f\|_{L^2(0,\infty)}\Big(\sum_{n=1}^N \|e_n\|^2_{L^2(0,\infty)}+1\Big),\end{aligned}$$

since $|R(\gamma)\,e^{2i\gamma x}|\le 1$ and, recall $L^2(0,\infty)\subset L^2(\mathbb{R})$, the Fourier transform being an isometry. So $K^{(x)}$ is a bounded operator, and the above expression for $\langle K^{(x)}f,g\rangle$ remains valid for arbitrary $f,g\in L^2(0,\infty)$.

So for a real-valued $f\in L^2(0,\infty)$

$$\langle f+K^{(x)}f,f\rangle = \|f\|^2_{L^2(0,\infty)} + \sum_{n=1}^N |\langle f,e_n\rangle|^2 + \int_{\mathbb{R}} |\big(\mathcal{F}^{-1}f\big)(\gamma)|^2\,R(\tfrac{1}{2}\gamma)\,e^{i\gamma x}\,d\gamma$$

so for real-valued $f\in L^2(0,\infty)$ with $K^{(x)}f+f=0$ we get

$$\int_{\mathbb{R}} |\big(\mathcal{F}^{-1}f\big)(\gamma)|^2\,(1+R(\tfrac{1}{2}\gamma)\,e^{i\gamma x})\,d\gamma = -\sum_{n=1}^N |\langle f,e_n\rangle|^2 \le 0$$

using $\|f\|^2_{L^2(0,\infty)} = \int_{\mathbb{R}} |\big(\mathcal{F}^{-1}f\big)(\gamma)|^2\,d\gamma$. Since $f$ is real-valued, $x,\gamma\in\mathbb{R}$, we have

$$\overline{|\big(\mathcal{F}^{-1}f\big)(\gamma)|^2\,(1+R(\tfrac{1}{2}\gamma)\,e^{i\gamma x})} = |\big(\mathcal{F}^{-1}f\big)(-\gamma)|^2\,(1+R(-\tfrac{1}{2}\gamma)\,e^{-i\gamma x})$$

by (4.2.2), so

$$2\int_0^\infty |(\mathcal{F}^{-1}f)(\gamma)|^2\,\Re\bigl(1+R(\frac{1}{2}\gamma)\,e^{i\gamma x}\bigr)\,d\gamma = 2\Re\int_0^\infty |(\mathcal{F}^{-1}f)(\gamma)|^2\,(1+R(\frac{1}{2}\gamma)\,e^{i\gamma x})\,d\gamma \le 0.$$

Since $|R(\gamma)| \le 1$ by (4.2.2) it follows that $\Re\bigl(1+R(\frac{1}{2}\gamma)\,e^{i\gamma x}\bigr) \ge 0$, so that the integral is non-negative and hence it has to be zero and since the integrand is non-negative it has to be zero almost everywhere. Note that a zero of $\Re\bigl(1+R(\frac{1}{2}\gamma)\,e^{i\gamma x}\bigr)$ can only occur if $|R(\frac{1}{2}\gamma)|=1$, its maximal value. The transmission coefficient is zero, $T(\gamma)=0$, by (4.2.2) and hence $f^+_{-\gamma}(x)+R(\gamma)\,f^+_\gamma(x)=0$, or $f^+_{-\gamma}$ and $f^+_\gamma$ are linearly dependent solutions, i.e. $W(f^+_\gamma, f^+_{-\gamma})=0$. By Proposition 4.2.1 this implies $\gamma=0$. We conclude that $\mathcal{F}^{-1}f$ is zero almost everywhere, hence $f$ is zero almost everywhere, or $f=0\in L^2(0,\infty)$.

So any real-valued $f\in L^2(0,\infty)$ satisfying $f+K^{(x)}f=0$ equals $f=0\in L^2(0,\infty)$. Since the kernel $K$ is real-valued, for any $f\in L^2(0,\infty)$ with $f+K^{(x)}f=0$ we have $\Re f+K^{(x)}\Re f=0$ and $\Im f+K^{(x)}\Im f=0$, so then $f=0\in L^2(0,\infty)$. This proves uniqueness of the solution. □

**Remark 4.4.3.** The Gelfand-Levitan-Marchenko integral equation of Theorem 4.4.2 presents us with an algorithm to reconstruct uniquely the potential $q$ from the scattering data, and actually we can even do this just knowing the reflection coefficient and the bound states, i.e. the eigenvalues plus the corresponding norms. This is actually the only part of information related to the transmission coefficient that is needed, cf. Theorem 4.2.7, and Remark 4.2.10. Note moreover that, given the scattering data, the Gelfand-Levitan-Marchenko integral equation is a linear problem for $B$.

We do not address the characterisation problem, i.e. given a matrix $S(\gamma)$ as in (4.2.3), under which conditions on its matrix elements is $S(\gamma)$ the scattering matrix corresponding to a potential $q$? The characterisation problem depends on the class of potentials that is taken into account. We refer to the paper [3] of Deift and Trubowitz for these results.

**Remark 4.4.4.** We briefly sketch another approach to recover the potential function from the scattering data, which is known as the Fokas-Its Riemann-Hilbert approach. We assume that the transmission coefficient $T$ has no poles in the upper half plane, but the line of reasoning can be easily adapted to this case. We write

$$T(\gamma)e^{i\gamma x}f^-_\gamma(x) - e^{i\gamma x}f^+_{-\gamma}(x) = R(\gamma)f^+_\gamma(x)e^{i\gamma x}, \qquad \gamma\in\mathbb{R}.$$

Note that $T(\gamma)e^{i\gamma x}f^-_\gamma(x)$ is analytic in the open upper half plane $\Im\gamma>0$ and that $e^{i\gamma x}f^+_{-\gamma}(x)$ is analytic in the open lower half plane $\Im\gamma<0$, and both have continuous extensions to the real axis. Such a problem is a Riemann-Hilbert type problem, and this was solved by Plemelj in 1908. Taking into account the behaviour of the functions as $\gamma\to\pm\infty$, the Plemelj solution to such a Riemann-Hilbert problem is given by

$$e^{i\gamma x}f^+_{-\gamma}(x) = 1+\frac{1}{2\pi i}\int_{\mathbb{R}}\frac{R(\lambda)f^+_\lambda(x)e^{i\lambda x}}{\lambda-\gamma}\,d\lambda.$$

Relabelling gives an integral equation for the Jost solution;

$$f^+_\gamma(x) = e^{i\gamma x} + \frac{1}{2\pi i}\int_{\mathbb{R}} \frac{R(\lambda) f^+_\lambda(x) e^{i(\lambda+\gamma)x}}{\lambda+\gamma}\, d\lambda$$

and this determines the Jost solution from the scattering data.

Now the Jost solution $f^+_\gamma$ determines the potential $q$, as can be seen as follows. Write $f^+_\gamma(x) = e^{i\gamma x + u(x;\gamma)}$ with $u(x;\gamma) \to 0$ as $x \to \infty$, $\Im\gamma \geq 0$ and $u(x;\gamma) \to 0$ as $\gamma \to \pm\infty$, $\Im\gamma \geq 0$. Then the Schrödinger equation for $f^+_\gamma$ translates into the differential equation $-2i\gamma u_x = u_{xx} + u_x^2 - q$, which is a first order equation for $u_x$. Because of its behaviour as $\gamma \to \pm\infty$ we expand $u_x(x;\gamma) = \sum_{n=1}^\infty \frac{v_n(x)}{(2i\gamma)^n}$ and this gives $v_1(x) = q(x)$ and recursively defined $v_n$'s. So in particular, $u_x(x;\gamma) = \frac{1}{2i\gamma} q(x)$ as $\gamma \to \pm\infty$. Moreover, $f^+_\gamma(x)e^{-i\gamma x} = e^{u(x;\gamma)} \sim 1 + u(x;\gamma)$, so that we formally obtain

$$q(x) = \lim_{\gamma\to\infty,\, \Im\gamma\geq 0} 2i\gamma \frac{d}{dx}\Big( f^+_\gamma(x)e^{-i\gamma x} - 1\Big).$$

So in this way, one can also recover the potential $q$ from the scattering data.

## 4.5 Reflectionless potentials

We now consider the situation of a reflectionless potential, $R(\gamma) = 0$, $\gamma \in \mathbb{R}$. This is a very special case, and the Gelfand-Levitan-Marchenko equation essentially is a matrix equation. Of course, we need to assume that the corresponding Schrödinger equation has at least one eigenvalue, otherwise the kernel $K$ is identically equal to zero, so that $B$ is identically equal to zero and hence the potential is trivial, and we get the Schrödinger equation $-\frac{d^2}{dx^2}$.

We first consider the easiest non-trival case, $N = 1$. So that $K(x) = K_d(x) = 2\rho e^{-2px}$, $\rho = \rho_1$, $p = p_1$, and the Gelfand-Levitan-Marchenko equation becomes

$$2\rho e^{-2p(x+y)} + \int_0^\infty B(x,z) 2\rho e^{-2p(x+y+z)}\, dz + B(x,y) = 0, \qquad y \geq 0.$$
$$\Longrightarrow B(x,y) = -2\rho e^{-2p(x+y)} - 2\rho e^{-2p(x+y)} \int_0^\infty B(x,z) e^{-2pz}\, dz,$$

so that the $y$-dependence of $B(x,y)$ is $2\rho e^{-2py}$. Substitute $B(x,y) = -2\rho e^{-2py}\, w(x)$, so that

$$w(x) = e^{-2xp} + e^{-2px} w(x) \int_0^\infty -2\rho e^{-4pz}\, dz = e^{-2px} + w(x) e^{-2px} \frac{-\rho}{2p}$$

so that $w(x) = e^{-2px}/(1 + \frac{\rho}{2p}e^{-2px})$ and we get

$$B(x,y) = \frac{-2\rho e^{-2p(x+y)}}{1 + \frac{\rho}{2p}e^{-2px}} \implies B(x,0) = \frac{-2\rho e^{-2px}}{1 + \frac{\rho}{2p}e^{-2px}}.$$

Deriving this expression and multiplying by $-1$ gives the potential by Theorem 4.3.1;

$$q(x) \;=\; -\frac{4p\rho e^{-2px}}{(1+\frac{\rho}{2p}e^{-2px})^2} = \frac{-2p^2}{\cosh^2(px+\frac{1}{2}\ln(2p/\rho))}, \tag{4.5.1}$$

which is, up to a affine scaling of the variable, the potential considered in Section 2.5.2.

So the potential $-2p^2\cosh^{-2}(px)$ is reflectionless, and we can ask whether there are more values for $a$ such that the potential $a\cosh^{-2}(px)$ is reflectionless. By Exercise 2.5.6 it suffices to consider the case $p=1$. We can elaborate on the discussion in Section 2.5.2 by observing

$$\begin{aligned}
f^+_\gamma(x) \;&=\; 2^{i\gamma}\big(\cosh(x)\big)^{i\gamma}\,{}_2F_1\left(\begin{matrix}\frac12-i\gamma+\sqrt{\frac14-a},\frac12-i\gamma-\sqrt{\frac14-a}\\ 1-i\gamma\end{matrix};\frac{1}{1+e^{2x}}\right),\\
f^-_\gamma(x) \;&=\; 2^{i\gamma}\big(\cosh(x)\big)^{i\gamma}\,{}_2F_1\left(\begin{matrix}\frac12-i\gamma+\sqrt{\frac14-a},\frac12-i\gamma-\sqrt{\frac14-a}\\ 1-i\gamma\end{matrix};\frac{e^{2x}}{1+e^{2x}}\right),\\
f^+_{-\gamma}(x) \;&=\; e^{-ix\gamma}\,{}_2F_1\left(\begin{matrix}\frac12+\sqrt{\frac14-a},\frac12-\sqrt{\frac14-a}\\ 1+i\gamma\end{matrix};\frac{1}{1+e^{2x}}\right),
\end{aligned}$$

so $f^+_\gamma$ corresponds to the solution ${}_2F_1(a,b;c,z)$ of the corresponding hypergeometric differential equation (2.5.1), $f^-_\gamma$ corresponds to ${}_2F_1(a,b;a+b+1-c;1-z)$, and $f^+_{-\gamma}$ corresponds to $z^{1-c}\,{}_2F_1(a-c+1,b-c+1;2-c;z)$ with the values $(a,b,c)$ given by $(\frac12-i\gamma\pm\sqrt{\frac14-a},1-i\gamma)$ as in Section 2.5.2. Note that $1+a+b-c=c$ in this case. So the transmission and reflection coefficient defined by $T(\gamma)f^-_\gamma(x)=f^+_{-\gamma}(x)+R(\gamma)f^+_\gamma(x)$ follow from the relation (2.5.4) for hypergeometric functions; $T(\gamma)$ is $1/B$ and $R(\gamma)$ equals $A/B$. Plugging in the values of $A$ and $B$ from (2.5.4) with the values of $(a,b,c)$ in terms of $a$ and $\gamma$ gives an explicit expression for the transmission and reflection coefficient;

$$\begin{aligned}
T(\gamma) \;&=\; \frac{\Gamma(\frac12-i\gamma+\sqrt{\frac14-a})\Gamma(\frac12-i\gamma-\sqrt{\frac14-a})}{\Gamma(1-i\gamma)\Gamma(-i\gamma)},\\
R(\gamma) \;&=\; \cos\big(\pi\sqrt{\frac14-a}\big)\Gamma(\frac12-i\gamma+\sqrt{\frac14-a})\Gamma(\frac12-i\gamma-\sqrt{\frac14-a})\frac{\Gamma(i\gamma)}{\pi\Gamma(-i\gamma)}.
\end{aligned}$$

So $R(\gamma)=0$ can only occur if the cosine vanishes, so we need $\pi\sqrt{\frac14-a}=\frac12\pi+l\pi$, $l\in\mathbb{Z}$, and this implies $a=-l(l+1)$, and in this case

$$T(\gamma)=\frac{\Gamma(1-i\gamma+l)\Gamma(-i\gamma-l)}{\Gamma(1-i\gamma)\Gamma(-i\gamma)}=\frac{(1-i\gamma)_l}{(-i\gamma-l)_l}=(-1)^l\frac{(1-i\gamma)_l}{(1+i\gamma)_l}.$$

So $T$ is rational in $\gamma$, and we can read off the poles on the positive imaginary axis. There are $l$ simple poles at $ik$, $k\in\{1,\cdots,l\}$.

**Proposition 4.5.1.** *The potential $q(x) = -l(l+1)\cosh^{-2}(x)$ is a reflectionless potential. The corresponding self-adjoint Schrödinger operator has essential spectrum $[0,\infty)$ and discrete spectrum $-l^2, -(l-1)^2, \cdots, -1$. The eigenfunction for the eigenvalue $-k^2$ is given by*

$$f_k(x) = f^+_{ik}(x) = \frac{1}{(2\cosh(x))^k}\, {}_2F_1\left(\begin{matrix} k-l, 1+k+l \\ 1+k \end{matrix}; \frac{1}{1+e^{2x}}\right)$$

*with $L^2(\mathbb{R})$-norm given by $\|f_k\|^2 = \binom{l}{k}\frac{1}{(k-1)!}$.*

Note that the ${}_2F_1$-series in the eigenfunction is a terminating series, since $k-l \in -\mathbb{N}$ and $(-n)_m = 0$ for $m > n$.

*Proof.* The statements about the spectrum and the precise form of the eigenvalues and eigenfunctions follow from Theorem 4.2.7 and the previous considerations. It remains to calculate the squared norm, for which we use Theorem 4.2.7. First we calculate

$$\begin{aligned} C_k &= \lim_{x\to\infty} e^{kx} f^-_{ik}(x) = \lim_{x\to\infty} \frac{e^{kx}}{(e^x+e^{-x})^k}\, {}_2F_1\left(\begin{matrix} k-l, 1+k+l \\ 1+k \end{matrix}; \frac{e^{2x}}{1+e^{2x}}\right) \\ &= {}_2F_1\left(\begin{matrix} k-l, 1+k+l \\ 1+k \end{matrix}; 1\right) = \frac{(-l)_{l-k}}{(1+k)_{l-k}} = (-1)^{l-k}, \end{aligned}$$

where we use ${}_2F_1(-n, b; c; 1) = (c-b)_n/(b)_n$ for $n \in \mathbb{N}$, which is known as the Chu-Vandermonde summation formula. In order to apply Theorem 4.2.7 we also need to calculate the residue of the transmission coefficient at $\gamma = ik$;

$$\begin{aligned} \mathrm{Res}_{\gamma=ik} T(\gamma) &= \mathrm{Res}_{\gamma=ik}(-1)^l \frac{(1-i\gamma)_l}{(1+i\gamma)_l} = \lim_{\gamma\to ik}(\gamma - ik)(-1)^l \frac{(1-i\gamma)_l}{(1+i\gamma)_l} \\ &= \frac{-i\,(-1)^l(1+k)_l}{(-1)^{k-1}(k-1)!\,(l-k)!} = i\,(-1)^{l-k}\frac{1}{(k-1)!}\binom{l}{k}, \end{aligned}$$

so that Theorem 4.2.7 gives the required result. □

**Exercise 4.5.2.** Calculate $\int_{\mathbb{R}} |f_k(x)|^2\, dx$ directly using the substitution $z = 1/(1+e^{2x})$, to see that this integral equals

$$\frac{1}{2}\int_0^1 |\, {}_2F_1\left(\begin{matrix} k-l, l+k+1 \\ 1+k \end{matrix}; z\right)|^2\, z^{k-1}(1-z)^{k-1}\, dz.$$

Expand the terminating ${}_2F_1$-series, and use the beta-integral $\int_0^1 z^{\alpha-1}(1-z)^{\beta-1}\, dz = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}$, to rewrite this as a double series. Rephrase the result of Proposition 4.5.1 as a double summation formula.

Now that we have established the existence of reflectionless potentials, we can try to solve the Gelfand-Levitan-Marchenko equation for a reflectionless potential with an arbitrary, but finite, number of discrete eigenvalues (or bound states). So we have now $K(x) = K_c(x) = 2\sum_{n=1}^{N} \rho_n e^{-2p_n x}$ and we have to solve $B(x,y)$ from

$$2\sum_{n=1}^{N} \rho_n e^{-2p_n(x+y)} + \int_0^\infty B(x,z)\, 2\sum_{n=1}^{N} \rho_n e^{-2p_n(x+y+z)}\, dz + B(x,y) = 0,$$

and this shows that we can expand $B(x,y)$ as a linear combination of $e^{-2p_n y}$ when considered as function of $y$. We put —the form choosen makes the matrix involved of the form $I$ plus a positive definite matrix—

$$B(x,y) = \sum_{n=1}^{N} \sqrt{\rho_n} e^{-p_n(x+2y)} w_n(x),$$

and we need to determine $w_n(x)$ from the Gelfand-Levitan-Marchenko equation in this case. Plugging this expression into the integral equation we see that we get an identity, when considered as function in $y$, is a linear combination of $e^{-2p_n y}$. Since the $p_n$'s are different, each coefficient of $e^{-2p_n y}$ has to be zero. This gives, after dividing by $\sqrt{\rho_n} e^{-p_n x}$,

$$2\sqrt{\rho_n} e^{-p_n x} + \sum_{m=1}^{N} 2\sqrt{\rho_m \rho_n} w_m(x) e^{-(p_n+p_m)x} \int_0^\infty e^{-2(p_n+p_m)z}\, dz + w_n(x) = 0$$

for $n = 1, \cdots, N$. Put $\mathbf{w}(x) = (w_1(x), \cdots, w_N(x))^t$ and $\mathbf{v}(x) = 2(\sqrt{\rho_1} e^{-p_1 x}, \cdots, \sqrt{\rho_n} e^{-p_n x})^t$ we can rewrite this as $(I + S(x))\mathbf{w}(x) + \mathbf{v}(x) = 0$, where $I$ is the identity $N \times N$-matrix and $S(x)_{nm} = \sqrt{\rho_n \rho_m} e^{-(p_n+p_m)x}/(p_n + p_m)$, which is also a symmetric matrix. In order to see that $S(x)$ is also positive definite we take an arbitrary vector $\xi \in \mathbb{C}^N$,

$$\begin{aligned}
\langle S(x)\xi, \xi\rangle &= \sum_{i,j=1}^{N} S(x)_{ij} \xi_j \overline{\xi_i} = \sum_{i,j=1}^{N} \int_0^\infty \sqrt{\rho_j} e^{-p_j x} \xi_j e^{-p_j t} \overline{\sqrt{\rho_i} e^{-p_i x} \xi_i e^{-p_i t}}\, dt \\
&= \int_0^\infty |f(x,t)|^2\, dt \geq 0,
\end{aligned}$$

with $f(x,t) = \sum_{i=1}^{N} \sqrt{\rho_i} \xi_i e^{-p_i(x+t)}$. It follows that $I + S(x)$ is invertible, as predicted by Theorem 4.4.2, so that we can solve for $\mathbf{w}(x) = -\big(I + S(x)\big)^{-1} \mathbf{v}(x)$. So

$$\begin{aligned}
B(x,y) &= \sum_{n=1}^{N} w_n(x) \sqrt{\rho_n} e^{-p_n(x+2y)} = -\langle \big(I + S(x)\big)^{-1} \mathbf{v}(x), \frac{1}{2}\mathbf{v}(x+2y)\rangle \\
\Longrightarrow\ B(x,0) &= -\frac{1}{2}\langle \big(I + S(x)\big)^{-1} \mathbf{v}(x), \mathbf{v}(x)\rangle = -\frac{1}{2}\sum_{n,m=1}^{N} \big(I + S(x)\big)^{-1}_{n,m} \mathbf{v}_m(x) \mathbf{v}_n(x) \\
&= 2\sum_{n,m=1}^{N} \big(I + S(x)\big)^{-1}_{n,m} \frac{d}{dx}\big(I + S(x)\big)_{m,n} = 2\,\mathrm{tr}\Big(\big(I + S(x)\big)^{-1} \frac{d}{dx}\big(I + S(x)\big)\Big)
\end{aligned}$$

observing that

$$\frac{d}{dx}\big(I+S(x)\big)_{n,m} = -\sqrt{\rho_n\rho_m}e^{-(p_n+p_m)x} = -\frac{1}{4}\mathbf{v}_n(x)\mathbf{v}_m(x).$$

In order to rewrite $B(x,0)$ in an even more compact way, note that for a $N\times N$-matrix $A(x)$ depending on a variable $x$, we can calculate

$$\begin{aligned}
&\frac{d}{dx}\det(A(x)) \\
&= \det\begin{pmatrix} a'_{11}(x) & a_{12}(x) & \cdots & a_{1N}(x) \\ a'_{21}(x) & a_{22}(x) & \dots & a_{2N}(x) \\ \vdots & & \ddots & \vdots \\ a'_{N1}(x) & a_{N2}(x) & \cdots & a_{NN}(x)\end{pmatrix} + \cdots + \det\begin{pmatrix} a_{11}(x) & a_{12}(x) & \cdots & a'_{1N}(x) \\ a_{21}(x) & a_{22}(x) & \cdots & a'_{2N}(x) \\ \vdots & & \ddots & \vdots \\ a_{N1}(x) & a_{N2}(x) & \cdots & a'_{NN}(x)\end{pmatrix} \\
&= \sum_{j=1}^{N} a'_{1j}(x)A_{1j}(x) + \cdots + \sum_{j=1}^{M} a'_{Nj}(x)A_{Nj}(x) = \sum_{i,j=1}^{N} a'_{ij}(x)A_{ij}(x) \\
&= \det(A(x))\sum_{i,j=1}^{N} a'_{ij}(x)A^{-1}_{ji}(x) = \det(A(x))\,\mathrm{tr}\big(\frac{dA}{dx}(x)A^{-1}(x)\big)
\end{aligned}$$

by developing according to the columns that have been differentiated, denoting the signed principal minors by $A_{ij}(x)$, so that $A^{-1}(x)_{ij} = \det(A(x))^{-1}A_{ji}(x)$.

This observation finally gives

$$B(x,0) = 2\frac{d}{dx}\big(\ln\det(I+S(x))\big), \qquad q(x) = -2\frac{d^2}{dx^2}\big(\ln\det(I+S(x))\big),$$

by Theorem 4.3.1. We formalise this result.

**Proposition 4.5.3.** *If $q$ is a reflectionless potential with scattering data $R(\gamma)=0$, $\{(p_n,\rho_n) \mid p_n>0, 1\leq n\leq N\}$, then*

$$q(x) = -2\frac{d^2}{dx^2}\big(\ln\det(I+S(x))\big),$$

*with $S(x)$ the $N\times N$-matrix given by*

$$S(x)_{n,m} = \sqrt{\rho_n\rho_m}e^{-(p_n+p_m)x}/(p_n+p_m).$$

In Section 5.5 we consider the case $N=2$ with an additional time $t$-dependence of Proposition 4.5.3. In case $N = 2$ we can make Proposition 4.5.3 somewhat more explicit;

$$
\begin{aligned}
\det(I + S(x)) &= \det \begin{pmatrix} 1 + \frac{\rho_1}{2p_1} e^{-2p_1 x} & \frac{\sqrt{\rho_1\rho_2}}{p_1+p_2} e^{-(p_1+p_2)x} \\ \frac{\sqrt{\rho_1\rho_2}}{p_1+p_2} e^{-(p_1+p_2)x} & 1 + \frac{\rho_2}{2p_2} e^{-2p_2 x} \end{pmatrix} \\
&= 1 + \frac{\rho_1}{2p_1} e^{-2p_1 x} + \frac{\rho_2}{2p_2} e^{-2p_2 x} + \Big( \frac{1}{4p_1p_2} - \frac{1}{(p_1+p_2)^2} \Big) \rho_1\rho_2 e^{-2(p_1+p_2)x} \\
&= 1 + \frac{\rho_1}{2p_1} e^{-2p_1 x} + \frac{\rho_2}{2p_2} e^{-2p_2 x} + \frac{\rho_1\rho_2}{4p_1p_2} \frac{(p_2-p_1)^2}{(p_1+p_2)^2} e^{-2(p_1+p_2)x} \\
&= \frac{\sqrt{\rho_1\rho_2}}{2\sqrt{p_1p_2}} e^{-(p_1+p_2)x} \Big\{ \frac{p_2-p_1}{p_1+p_2} \Big( \frac{p_1+p_2}{p_2-p_1} \frac{2\sqrt{p_1p_2}}{\sqrt{\rho_1\rho_2}} e^{(p_1+p_2)x} + \frac{p_2-p_1}{p_1+p_2} \frac{\sqrt{\rho_1\rho_2}}{2\sqrt{p_1p_2}} e^{-(p_1+p_2)x} \Big) \\
&\qquad\qquad + \Big( \frac{\sqrt{\rho_1 p_2}}{\sqrt{p_1\rho_2}} e^{(p_2-p_1)x} + \frac{\sqrt{p_1\rho_2}}{\sqrt{\rho_1 p_2}} e^{(p_1-p_2)x} \Big) \Big\} \\
&= \frac{p_2-p_1}{p_1+p_2} \frac{\sqrt{\rho_1\rho_2}}{\sqrt{p_1p_2}} e^{-(p_1+p_2)x} \Big\{ \cosh\big( (p_1+p_2)x + \ln( \frac{p_1+p_2}{p_2-p_1} \frac{2\sqrt{p_1p_2}}{\sqrt{\rho_1\rho_2}} ) \big) \\
&\qquad\qquad + \frac{p_1+p_2}{p_2-p_1} \cosh\big( (p_2-p_1)x + \ln( \frac{\sqrt{\rho_1 p_2}}{\sqrt{p_1\rho_2}} ) \big) \Big\}.
\end{aligned}
$$

This expression is used in Section 5.5.

# Chapter 5

# Inverse scattering method and the Korteweg-de Vries equation

## 5.1 The Korteweg-de Vries equation and some solutions

The Korteweg[1]-de Vries[2], or KdV, equation is the following partial differential equation

$$q_t(x,t) - 6\,q(x,t)\,q_x(x,t) + q_{xxx}(x,t) = 0 \quad \text{or} \quad q_t - 6qq_x + q_{xxx} = 0, \tag{5.1.1}$$

where $q$ is a function of two variables $x$, space, and $t$, time, with $x, t \in \mathbb{R}$. Here $q_t(x,t) = \frac{\partial q}{\partial t}(x,t)$, etc. This equation can be viewed as a non-linear evolution equation by writing it as $q_t = S(q)$ with $S$ a non-linear map on a suitable function space defined by $S(f) = 6f\,f_x - f_{xxx}$.

We also consider the Korteweg-de Vries equation together with an initial condition;

$$q_t(x,t) - 6\,q(x,t)\,q_x(x,t) + q_{xxx}(x,t) = 0, \qquad q(x,0) = q_0(x), \quad x \in \mathbb{R},\, t > 0. \tag{5.1.2}$$

We first discuss some straightforward properties of the KdV-equation (5.1.1), also in relation to some other types of (partial) differential equations in the following exercises.

**Exercise 5.1.1.** Show that with $q$ a solution to the Korteweg-de Vries equation (5.1.1) also $\tilde{q}(x,t) = q(x - 6Ct, t) - C$ is a solution. This is known as Galilean invariance.

**Exercise 5.1.2.** Show that by a change of variables the Korteweg-de Vries equation can be transformed into $q_t + aqq_x + bq_x + cq_{xxx} = 0$ for arbitrary real constants $a, b, c$.

**Exercise 5.1.3.** The Burgers[3] equation $q_t = q_{xx} + 2qq_x$ looks similar to the KdV-equation. Show that the Burgers equation can be transformed into a linear equation $u_t = u_{xx}$ by the Hopf-Cole transformation $q = (\ln u)_x$.

[1] Diederik Johannes Korteweg (31 March 1848 — 10 May 1941), professor of mathematics at the University of Amsterdam and supervisor of de Vries's 1894 thesis "Bijdrage tot de kennis der lange golven".

[2] Gustav de Vries (22 January 1866 — 16 December 1934), mainly worked as a high school teacher.

[3] Johannes Martinus Burgers (13 January 1895 — 7 June 1981), is one of the founding fathers of research in fluid dynamics in the Netherlands.

**Exercise 5.1.4.** The modified KdV-equation, or mKdV-equation, is $u_t + u_{xxx} - 6u^2u_x = 0$. Show that for a solution $u$ of the mKdV-equation, the relation $q = u_x + u^2$ gives a solution $q$ to the KdV-equation. This transformation is known as the Miura transformation. Hint: Show that $q_t + q_{xxx} - 6qq_x$ can be written as a first order differential applied to $u_t + u_{xxx} - 6u^2u_x$.

With writing down this initial value problem, the question arises on the existence and uniqueness of solutions. This is an intricate questions and the answer depends, of course, on smoothness and decay properties of $q_0$. We do not go into this, but formulate two results which we will not prove. Our main concern is to establish a method in order to construct solutions explicitly.

**Theorem 5.1.5.** *Assume $q_0 \in C^4(\mathbb{R})$ and $\frac{d^k q_0}{dx^k}(x) = \mathcal{O}(|x|^{-M})$, $M > 10$, for $k \in \{0,1,2,3,4\}$. Then the Korteweg-de Vries initial value problem* (5.1.2) *has a real-valued unique solution (in the classical sense).*

**Exercise 5.1.6.** In this exercise we sketch a proof of the unicity statement. Assume $q$ and $u$ are solutions to (5.1.2), and put $w = u - q$.

- Show that $w_t = 6uw_x + 6q_xw - w_{xxx}$ using the KdV-equation.
- Multiply by $w$ and integrate to conclude
$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\int_{\mathbb{R}} w^2(x,t)\,dx = 6\int_{\mathbb{R}} u(x,t)w(x,t)w_x(x,t)\,dx + 6\int_{\mathbb{R}} q_x(x,t)w^2(x,t)\,dx\\ - \int_{\mathbb{R}} w(x,t)w_{xxx}(x,t)\,dx\end{aligned}$$
and argue that the last integral vanishes.
- Integrate by parts in the first integral to obtain
$$\frac{d}{dt}\int_{\mathbb{R}} w^2(x,t)\,dx = 12\int_{\mathbb{R}} \left(q_x(x,t) - \frac{1}{2}u_x(x,t)\right) w^2(x,t)dx.$$
- Use $|q_x(x,t) - \frac{1}{2}u_x(x,t)| \leq C$ to conclude $\frac{d}{dt}\int_{\mathbb{R}} w^2(x,t)\,dx \leq 12C\int_{\mathbb{R}} w^2(x,t)\,dx$ and conclude $\int_{\mathbb{R}} w^2(x,t)\,dx \leq e^{12Ct}\int_{\mathbb{R}} w^2(x,0)\,dx = 0$. Hence $w(x,t) = 0$.

Theorem 5.1.5 is proved using the Inverse Spectral Method, a method that we discuss later, and it should be noted that even a $C^\infty(\mathbb{R})$-condition of the initial value $q_0$ is not sufficient to guarantee a continuous global solution to (5.1.2). Methods from evolution equations have led to the following existence result.

**Theorem 5.1.7.** *Assume the initial value $q_0$ is an element of the Sobolev space $W^s(\mathbb{R})$ for $s \geq 2$. Then the Korteweg-de Vries initial value problem* (5.1.2) *has a solution $q$ such that $t \mapsto q(\cdot,t)$ is a continuous map from $\mathbb{R}_{\geq 0}$ into $W^s(\mathbb{R})$ and a $C^1$-map from $\mathbb{R}_{\geq 0}$ into $L^2(\mathbb{R})$.*

The last statement means that $\lim_{h\to 0} \|\frac{1}{h}\big(q(\cdot, t+h) - q(\cdot, t)\big) - q_t(\cdot, t)\| = 0$ in $L^2(\mathbb{R})$, and moreover that $t \mapsto q_t(\cdot, t)$ is a continuous map from $\mathbb{R}_{\geq 0}$ to $L^2(\mathbb{R})$.

Solutions to the KdV-equation (5.1.1) have many nice properties, such as a large number of invariants. Let us show that $\int_{\mathbb{R}} q(x,t)\, dx$ is an invariant, i.e. independent of time $t$. Write

$$0 = q_t - 6qq_x + q_{xxx} = q_t + \big(-3q^2 + q_{xx}\big)_x.$$

Assuming that we can differentiate under the integral sign and that $q$ and $q_{xx}$ decay sufficiently fast we get

$$\frac{d}{dt}\int_{\mathbb{R}} q(x,t)\, dx = \int_{\mathbb{R}} q_t(x,t)\, dx = \int_{\mathbb{R}} (3q^2(x,t) - q_{xx}(x,t))_x\, dx = 0.$$

In physical applications this is considered as conservation of mass. More generally, whenever we have a relation of the form $T_t + X_x = 0$, where $T$ and $X$ are depending on the solution $q$ of the KdV-equation and its derivatives with respect to $x$, we have $\int_{\mathbb{R}} T\, dx$ as a (possible) invariant. In the above example we have $T = q$ and $X = -3q^2 + q_{xx}$.

**Exercise 5.1.8.** Show also that under suitable conditions $\int_{\mathbb{R}} q^2(x,t)\, dx$ is an invariant by considering $q(q_t - 6qq_x + q_{xxx}) = 0$ and writing this in the form $(q^2)_t$ equals a derviative with respect to $x$. This is considered as conservation of momentum. What are $T$ and $X$?

In fact there is an infinite number of conserved quantities for the KdV-equation, and this point of view is exploited in integrable systems.

We now give a class of solutions to (5.1.1) of the form $q(x,t) = f(x - ct)$ for some $c \in \mathbb{R}$. This method is already worked out in the 1895-paper of Korteweg and de Vries. So the KdV equation gives an ordinary partial differential equation for $f$;

$$-cf' - 6ff' + f''' = 0 \implies -cf - 3f^2 + f'' = a,$$

where $a$ is some integration constant. Multiplying by $f'$ shows that we can integrate again, and

$$-cff' - 3f^2f' + f''f' = af' \implies -\frac{c}{2}f^2 - f^3 + \frac{1}{2}(f')^2 = af + b$$

for some integration constant $b$. This is a non-linear first order (ordinary) differential equation

$$(f')^2 = F(f), \quad F(x) = 2x^3 + cx^2 + ax + b,$$

after rescaling the integrating constants. Since the left hand side is a square, the regions where the cubic polynomial $F$ is positive are of importance. So the zeros of the $F$ play a role in the analysis.

**Remark 5.1.9.** In general the equation $y^2 = F(x)$, with $F$ a cubic polynomial, is an elliptic curve, so that we can expect elliptic functions involved in the solution. The elliptic curve is non-singular (i.e. no cusps or self-intersections) if and only if the polynomial $F$ has three distinct roots.

The analysis now has to be split up according to the following cases;

1. $F$ has three distinct real roots;
2. $F$ has two real roots, of which one necessarily is of order two, and we have two cases: the double root is smaller or larger than the simple root;
3. $F$ has one simple root;
4. $F$ has one root of order three.

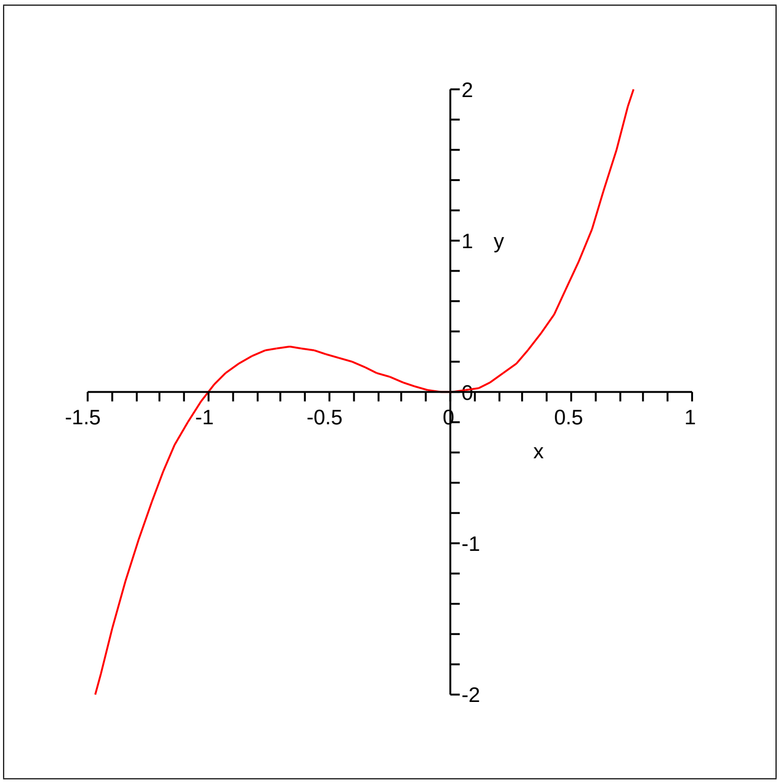


Figure 5.1: The cubic polynomial $F$ in case 2 with double zero larger than the simple zero.

Case 1 can be completely solved in terms of elliptic functions. For our purposes case 2 is the most interesting, since the corresponding solution is related to the so-called soliton solution of the KdV equation (5.1.1) The case 2 is of interest in case the simple root, say $\alpha$, is smaller than the double root, say $\beta$, so $F(x) = 2(x-\alpha)(x-\beta)^2$ as in the situation of Figure 5.1 with $\alpha = -1$ and $\beta = 0$.

If one considers the differential equation $(f')^2 = F(f)$ in this case then we find that a solution $f$ with initial value $\alpha < f(x_0) < \beta$ satisfies $\alpha < f(x) < \beta$ for all $x$. So we can expect bounded solutions in this case.

Taking square roots and noting that the differential equation is separable gives

$$\int_\alpha^f \frac{d\xi}{(\xi-\beta)\sqrt{\xi-\alpha}} = \pm\sqrt{2}x + C,$$

where $C$ denotes a general arbitrary constant. In the integral we substitute $\xi = \alpha + (\beta - \alpha)\sin^2\nu$, so $d\xi = (\beta-\alpha)2\sin\nu\cos\nu\, d\nu$ and the integration runs over $[0,\phi]$ with $\sin\phi = \sqrt{\frac{f-\alpha}{\beta-\alpha}}$. So the integral equals $\frac{-2}{\sqrt{\beta-\alpha}}\int_0^\phi \frac{1}{\cos\nu} d\nu$, and now using that $\frac{d}{d\nu}\ln|\tan(\frac{\nu}{2})| = \frac{1}{\sin\nu}$ by an elementary computation we find

$$\frac{-2}{\sqrt{\beta-\alpha}}\ln|\tan(\frac{\phi}{2}+\frac{\pi}{4})| = \pm\sqrt{2}x + C,$$

and using the addition formula for tan or for sin and cos we can rewrite this as

$$\ln\Big|\frac{1+\tan(\frac{\phi}{2})}{1-\tan(\frac{\phi}{2})}\Big| = \pm\sqrt{\frac{\beta-\alpha}{2}}(x-C).$$

Denoting the right hand side by $y$, we get $\frac{1+\tan(\frac{\phi}{2})}{1-\tan(\frac{\phi}{2})} = e^y$ which gives $\tan(\frac{\phi}{2}) = \tanh(\frac{y}{2})$. Now we can determine $f$ as a function of $x$

$$\begin{aligned} f(x) &= \alpha + (\beta-\alpha)\,\sin^2\phi \;=\; \alpha + 4(\beta-\alpha)\,\sin^2(\frac{\phi}{2})\cos^2(\frac{\phi}{2}) \\ &= \alpha + 4(\beta-\alpha)\,\tan^2(\frac{\phi}{2})\cos^4(\frac{\phi}{2}) \\ &= \alpha + 4(\beta-\alpha)\,\frac{\tan^2(\frac{\phi}{2})}{\big(1+\tan^2(\frac{\phi}{2})\big)^2} \\ &= \alpha + 4(\beta-\alpha)\,\frac{\tanh^2(\frac{y}{2})}{\big(1+\tanh^2(\frac{y}{2})\big)^2} \\ &= \alpha + (\beta-\alpha)\,\tanh^2(y) \;=\; \beta + \frac{\alpha-\beta}{\cosh^2(y)} \\ &= \beta + \frac{\alpha-\beta}{\cosh^2(\sqrt{\frac{\beta-\alpha}{2}}(x-C))} \end{aligned}$$

using $\cos^2\phi = 1/(1+\tan^2\phi)$ and $\frac{1}{2}\big(1+\tanh^2(\frac{y}{2})\big)\tanh y = \tanh(\frac{y}{2})$ and using that cosh is an even function. In this solution the zeros of $F$ are related to $c$ by $c = -2\alpha - 4\beta$ by comparing the coefficients of $x^2$ in the cubic polynomial $F$. We see that $\lim_{|x|\to\infty} f(x) = 0$ can only be achieved by choosing $\beta = 0$, so that $\alpha < 0$ and $c = -\alpha > 0$, then $f$ is essentially a $\cosh^{-2}$-function, see Figure 2.1 for the case $c = 4$. So we have proved the following proposition.

**Proposition 5.1.10.** *For $c>0$, the function*

$$q(x,t) = \frac{-c}{2\cosh^2(\frac{1}{2}\sqrt{c}(x-ct+C))}$$

*is a solution to the KdV-equation* (5.1.1) *for any real constant $C$.*

Note that $q(x,t)$ is negative and its minimum occurs for $x=ct$, so we can view this as a solitary wave (directed downwards) of height $\frac{1}{2}c$ travelling to the right at a speed $c$. Note that the height and speed are related!

**Exercise 5.1.11.** Assume now that $F$ has one root of order three. Show that this root is $-\frac{1}{6}c$, and that the corresponding solution is $f(x) = -\frac{1}{6}c + \frac{2}{(x-C)^2}$.

**Exercise 5.1.12.** Give a qualitative analysis of possible growth/decay behaviour of the solutions to $(f')^2 = F(f)$ for the other listed cases for the cubic polynomial $F$.

**Exercise 5.1.13.** Assume now that $F$ has three distinct real roots, then one can proceed in the same way, except that now we get the integral of the form $\int_0^\phi \frac{1}{\sqrt{1-k^2\sin^2\nu}}d\nu$ instead of $\int_0^\phi \frac{1}{\cos\nu}d\nu$. Use the Jacobian elliptic function cn defined by

$$v = \int_0^\phi \frac{1}{\sqrt{1-k^2\sin^2\nu}}d\nu \qquad \cos\phi = \mathrm{cn}(v;k).$$

The corresponding solutions to the KdV-equation (5.1.1) are known as *cnoidal* waves, and were already obtained by Korteweg and de Vries in their 1895 paper.

In the course of history the KdV-equation (5.1.1) has been linked to other well-known ordinary differential equations by other suitable substitutions, and two of them are discussed in the following exercises.

**Exercise 5.1.14.** Put $q(x,t) = t + f(x+3t^2)$, and show that $q$ satisfies the KdV-equation (5.1.1) if and only if $f$ satisfies $1 - 6ff' + f''' = 0$, or by integrating $C + z - 3f^2 + f'' = 0$. This equation is essentially the Painlevé I equation $g''(x) = 6g^2(x) + x$, which is the simplest equation in the Painlevé[4] equations consisting of 6 equations. The Painlevé equations are essentially the second order differential equations of the form $y''(t) = R(t,y,y')$ with $R$ a polynomial in $y$, $y'$ with meromorphic coefficients in $t$ together with the Painlevé property meaning that there are no movable branch points and no movable essential singularities exluding linear and integrable differential equations.

**Exercise 5.1.15.** Put $q(x,t) = -(3t)^{-2/3} f\big(\frac{x}{(3t)^{1/3}}\big)$, and show that $q$ is a solution to the KdV-equation (5.1.1) if and only if $f$ satisfies $f''' + (6f-z)f' - 2f = 0$. This is related to the Painlevé II equation.

[4]Paul Painlevé (5 December 1863 — 29 October 1933), French mathematician and politician. Painlevé was Minister in several French Cabinets, as well as Prime-Minister of France.

## 5.2 The KdV equation related to the Schrödinger operator

This section is of a motivational and historical nature, and no proofs are given, only heuristical derivations.

The link between the Korteweg-de Vries equation and the Schrödinger operator has been pointed out in a three-page paper by Gardner, Greene, Kruskal and Miura of the Plasma Physics Laboratory of Princeton University in the Physical Review Letters in 1967. This paper[5] has turned out to be a starting point for a whole line of research for solving certain non-linear partial differential equations. We give a short description of their line of reasoning, which apparently was strongly motivated by numerical experiments. The approach has been generalised enormously, and we consider the approach by Lax in Section 5.3 in more detail.

Consider the Schrödinger equation with time-dependent potential,

$$-f_{xx}(x,t) + q(x,t)f(x,t) = \lambda(t)f(x,t),$$

where the eigenfunctions and eigenvalues will also depend on $t$. Expressing $q$ in terms of $f$ and $\lambda$ and plugging this into the KdV-equation (5.1.1) gives a huge equation, that upon multiplying by $f^2$, can be written as

$$\lambda_t f^2 + \big(f\,u_x - f_x\,u\big)_x = 0, \qquad u(x,t) = f_t(x,t) + f_{xxx}(x,t) - 3\big(q(x,t)+\lambda(t)\big)f_x(x,t). \quad (5.2.1)$$

This is a tedious verification and one of the main steps, assuming that all partial derivatives exist and $f_{txx} = f_{xxt}$. Note that the second term in (5.2.1) is a derivative of a Wronskian. Later it has been pointed out that the KdV-equation can be interpreted as a compatibility condition $f_{txx} = f_{xxt}$ for solutions of systems of partial differential equations. This approach has also led to several other generalisations.

Integrating relation (5.2.1) over $\mathbb{R}$, and assuming that $f \in L^2(\mathbb{R})$, so that $\lambda$ corresponds to the discrete spectrum of the Schrödinger operator, we get

$$\lambda_t \|f\|^2 = -\lim_{a\to\infty} f(x,t)\,u_x(x,t) - f_x(x,t)u_x(x,t)\Big|_{-a}^{a}$$

and the right hand side gives zero, so that the (discrete) spectrum is constant. So the important observation is that the KdV-equation is a description of an isospectral family of Schrödinger operators. Hence, we can proceed as follows to find a solution to an initial value problem (5.1.2) for the KdV-equation:

1. Describe the spectral data of the Schrödinger operator with potential $q_0$; this is described in Section 4.2.

2. Solve the evolution of the spectral data when the potential evolves according to the KdV-equation; this is yet unclear.

[5]Gardner, Greene, Kruskal and Miura have received the 2006 AMS Leroy P. Steele Prize for a Seminal Contribution to Research for one of their follow-up papers.

3. Determine the potential $q(x,t)$ from the spectral data of the Schrödinger operator at time $t$; this can be done essentially using the Gelfand-Levitan-Marchenko integral equation of Theorem 4.4.2 and Theorem 4.3.1.

We shortly derive heuristically that the evolution in step 2 is linear, and since the Gelfand-Levitan-Marchenko integral equation is also linear, this procedure gives a mainly linear method to solve the KdV-inital value problem (5.1.2). Note however that in explicit cases it is hard to solve the Gelfand-Levitan-Marchenko equation explicitly, except for the reflectionless potentials as discussed in Section 4.5. This method is now known as the Inverse Scattering Method (ISM), or inverse spectral method, or inverse scattering transformation. The inverse scattering method can be considered as an analogue of the Fourier transform used to solve linear differential equations.

Now that we have established $\lambda_t = 0$ for an eigenvalue $\lambda$ in the discrete spectrum, we use this in (5.2.1) and carrying out the differentiation gives

$$0 = (f\, u_x - f_x\, u)_x = f\, u_{xx} - f_{xx}\, u = f\,\big(u_{xx} - (q-\lambda)u\big),$$

or $u$ is also a solution to the Schrödinger equation. Hence, $u = C\,f + D\,g$, with $C, D \in \mathbb{C}$ and $g$ a linearly independent solution, i.e.

$$f_t + f_{xxx} - 3(q+\lambda)\, f_x \;=\; C\,f + D\,g. \tag{5.2.2}$$

Assume $\lambda = \lambda_n = -p_n^2$ a discrete eigenvalue using the notation as in Theorem 4.2.7, so that $f(x,t) = f_n(x,t) \sim e^{-p_n x}$ for $x \to \infty$. So in the region where the potential vanishes, in particular for $x \to \infty$, we see that left hand side has exponential decay, and since $g$ doesn't have exponential decay, it follows that $D = 0$.

Now fixing $n$, normalise $\psi(x,t) = c(t) f_n(x,t)$, so that $\|\psi(\cdot,t)\| = 1$ for all $t$, and since in the above considerations $f$ was an arbitrary solution to the Schrödinger equation we get

$$\psi_t + \psi_{xxx} - 3(q+\lambda)\psi_x = C\psi.$$

We claim that $C = 0$, and in order to see this we multiply this equation by $\psi$ and integrate over $\mathbb{R}$ with respect to $x$. Then the left hand side equals $C$. Now recall $\int_{\mathbb{R}} \psi_t(x,t)\psi(x,t)\,dx = \frac{1}{2}\big(\langle \psi_t(\cdot,t), \psi(\cdot,t)\rangle + \langle \psi(\cdot,t), \psi_t(\cdot,t)\rangle\big) = \frac{1}{2}\frac{d}{dt}\|\psi(\cdot,t)\|^2 = 0$, since its norm is constant 1. Also $\int_{\mathbb{R}} \lambda_n \psi_x(x,t)\psi(x,t)\,dx = \lambda_n \frac{1}{2}\psi(x,t)^2|_{-\infty}^{\infty} = 0$, since the eigenfunction decays exponentially fast. Similarly, $\int_{\mathbb{R}} \psi_{xxx}(x,t)\psi(x,t)\,dx = -\int_{\mathbb{R}} \psi_{xx}(x,t)\psi_x(x,t)\,dx = -\frac{1}{2}\big(\psi_x(x,t)\big)^2|_{-\infty}^{\infty} = 0$, since the derivative of the eigenfunction decays exponentially. $\int_{\mathbb{R}} q(x,t)\psi_x(x,t)\psi(x,t)\,dx = \int_R \lambda_n \psi_x(x,t)\psi(x,t)\,dx + \int_{\mathbb{R}} \psi_x(x,t)\psi_{xx}(x,t)\,dx = 0$, as before. So for the normalised eigenfunction $\psi(\cdot,t)$ for the constant eigenvalue $\lambda_n$ we find

$$\psi_t + \psi_{xxx} - 3(q+\lambda)\psi_x = 0.$$

Now use $\psi(x,t) \sim c(t)e^{-p_n x}$ as $x \to \infty$, and since we assume that the potential decays sufficiently fast we get a linear first order differential equation for $c(t)$;

$$\frac{dc}{dt}(t) + (-p_n)^3 c(t) - 3(-p_n^2)(-p_n)c(t) = 0 \Longrightarrow\; c(t) = e^{4p_n^3 t}c(0).$$

Now that we have determined the evolution of the discrete part of the spectral data, we consider next the evolution of the continuous part of the spectrum. Let $\lambda = \gamma^2$, and consider (5.2.2) for $\psi(x,t) = \psi_\gamma(x,t)$ with $\psi_\gamma$ as in Section 4.2, where we now assume that the transmission and reflection coefficient also depend on $t$; $R(\gamma,t)$, $T(\gamma,t)$. Again using that the potential $q$ vanishes for large enough $x$, we see that

$$\begin{aligned}
\psi_t(x,t) + \psi_{xxx}(x,t) - 3(q(x,t)+\lambda)\psi_x(x,t) &\sim \big(T_t(\gamma,t) + 4i\gamma^3 T(\gamma,t)\big)e^{-i\gamma x}, \qquad x \to -\infty,\\
\psi_t(x,t) + \psi_{xxx}(x,t) - 3(q(x,t)+\lambda)\psi_x(x,t) &\sim 4i\gamma^3 e^{-i\gamma x} + \big(R_t(\gamma,t) - 4i\gamma^3\big)e^{i\gamma x}, \qquad x \to \infty.
\end{aligned}$$

We conclude that $\psi_t + \psi_{xxx} - 3(q+\lambda)\psi_x$ is a constant multiple of $\psi$, and this constant is $4i\gamma^3$ as follows by looking at the coefficient of $e^{-i\gamma x}$ for $x \to \infty$. Equating gives two linear first order differential equations for the transmission and reflection coefficients;

$$\begin{aligned}
T_t(\gamma,t) + 4i\gamma^3 T(\gamma,t) &= 4i\gamma^3 T(\gamma,t) \implies T(\gamma,t) = T(\gamma,0),\\
R_t(\gamma,t) - 4i\gamma^3 R(\gamma,t) &= 4i\gamma^3 R(\gamma,t) \implies R(\gamma,t) = R(\gamma,0)e^{8i\gamma^3 t}.
\end{aligned}$$

Note that this also implies that starting with a reflectionless potential $q_0$, we stay within the class of reflectionless potentials.

**Exercise 5.2.1.** Assume that the solution scheme for the Korteweg-de Vries equation with initial value $q_0(x) = -\frac{c}{2}\cosh^{-2}(\frac{1}{2}\sqrt{c}x)$ of this section is valid. Use the results of Section 4.5 to derive the solution $q(x,t)$ of Proposition 5.1.10. in this way. This solution is known as the pure 1-soliton solution, see Section 5.5.

## 5.3 Lax pairs

The method of Lax[6] pairs is a more general method to find isospectral time evolutions. In the general setup, we have a family of operators $L(t)$, $t \in I$ with $I \subset \mathbb{R}$ some interval, acting on a Hilbert space $\mathcal{H}$. We assume that the domains do not vary with $t$, so $D(L(t)) = D(L)$ for all $t$ and that $D(L)$ is dense. We say that the family is strongly continuous if for each $x \in D(L) = D(L(t))$ the map $t \mapsto L(t)x$, $I \to \mathcal{H}$, is continuous. The family $L(t)$ is isospectral if the spectrum of $L(t)$ is independent of $t$.

The basic example is the Schrödinger operator with time-dependent potential

$$L(t) = -\frac{d^2}{dx^2} + q(\cdot,t), \qquad D(L(t)) = W^2(\mathbb{R}),$$

assuming the potential $q(\cdot,t)$ satisfies the conditions of Corollary 2.2.7 for all $t$.

**Definition 5.3.1.** *The derivative $\frac{dL}{dt}(t) = L_t(t)$, $t \in I$, of a strongly continuous family $L(t)$ is defined with respect to the strong operator topology, i.e. $D(L_t(t))$ consists of those $x \in D(L) \subset \mathcal{H}$ such that*

$$\lim_{h\to 0} \frac{L(t+h)x - L(t)x}{h}$$

*converges in $\mathcal{H}$ to, say, $y \in \mathcal{H}$, and then $L_t(t)x = y$.*

[6]Peter D. Lax (1 May 1926 — ), Hungarian-American mathematician, winner of the 2005 Abelprize.

Definition 5.3.1 should be compared with Stone's Theorem 6.4.2.

Assuming that $D(L_t(t))$ is independent of $t$ and dense in $\mathcal{H}$, then again $L_t(t)$ gives a family of operators on $\mathcal{H}$. If this family is again strongly continuous, then we say that $L(t)$ is a strongly $C^1$-family of operators.

Return to the example of a family of Schrödinger operators, then for any $f \in W^2(\mathbb{R})$, we have as elements in $L^2(\mathbb{R})$

$$\frac{1}{h}\Big(-f'' + q(\cdot, t+h)f + f'' - q(\cdot,t)f\Big) = f\,\frac{q(\cdot,t+h) - q(\cdot,t)}{h}.$$

Assuming that the partial derivative with respect to $t$ of $q$ exists we obtain

$$\|\frac{1}{h}\big(L(t+h)f - L(t)f\big) - q_t(\cdot,t)f\|^2 = \int_{\mathbb{R}}\Big|\frac{q(x,t+h)-q(x,t)}{h} - q_t(x,t)\Big|^2\, |f(x)|^2\, dx.$$

If we assume moreover that $q_t(\cdot, t) \in L^\infty(\mathbb{R})$ with locally bounded $L^\infty$-norm we can apply Dominated Convergence Theorem 6.1.3 to see that the right hand tends to zero as $h \to 0$ even for arbitrary $f \in L^2(\mathbb{R})$. So in this case we have established $L_t(t)$ as multiplication operator by $q_t(\cdot,t)$ with domain $D(L) = W^2(\mathbb{R})$.

Let us assume that we also have a strongly continuous family of bounded operators $V(t) \in B(\mathcal{H})$. As an application we derive a product rule, which is the same as for functions except that we have to keep track of domains. Note that $D(V(t)L(t)) = D(L(t)) = D(L)$ is independent of $t$, and write for $x \in D(L_t(t))$

$$\begin{aligned}
&\frac{1}{h}\Big(V(t+h)L(t+h)x - V(t)L(t)x\Big)\\
=&\frac{1}{h}\Big(V(t+h)L(t+h)x - V(t+h)L(t)x\Big) + \frac{1}{h}\Big(V(t+h)L(t)x - V(t)L(t)x\Big)\\
=&V(t+h)\frac{1}{h}\Big(L(t+h)x - L(t)x\Big) + \frac{1}{h}\Big(V(t+h)L(t)x - V(t)L(t)x\Big)
\end{aligned}$$

and the first term tends to $V(t)L_t(t)x$ as follows from

$$\begin{aligned}
&\Big\|V(t+h)\frac{1}{h}\Big(L(t+h)x - L(t)x\Big) - V(t)L_t(t)x\Big\|\\
\leq &\Big\|V(t+h)\frac{1}{h}\Big(L(t+h)x - L(t)x\Big) - V(t+h)L_t(t)x\Big\| + \Big\|V(t+h)L_t(t)x - V(t)L_t(t)x\Big\|\\
\leq &\|V(t+h)\|\,\Big\|\frac{1}{h}\Big(L(t+h)x - L(t)x\Big) - L_t(t)x\Big\| + \Big\|V(t+h)L_t(t)x - V(t)L_t(t)x\Big\|
\end{aligned}$$

and the first term tends to $0$ as $h \to 0$ by definition of the derived operator assuming that $\|V(t)\|$ is locally bounded and the second tends to zero since $V$ is strongly continuous. Moreover, the second term tends to $V_t(t)L(t)x$ if we assume that $L(t)x \in D(V_t(t))$. So we have proved Lemma 5.3.2.

**Lemma 5.3.2.** (i) *Let $L(t)$ be a strongly continuous family of operators on a Hilbert space $\mathcal{H}$ with constant domain $D(L) = D(L(t))$ and let $V(t)$ be a strongly continuous family of locally bounded operators on $\mathcal{H}$ which is locally bounded in the operator norm. If $x \in D(L_t(t))$ and $L(t)x \in D(V_t(t))$, then $x \in D\big((VL)_t(t)\big)$ and*

$$\frac{d(VL)}{dt}(t)x = V_t(t)L(t)x + V(t)L_t(t)x.$$

(ii) *Let $V(t)$ be as in (i), then $\frac{dV^*}{dt}(t) = \big(V_t(t)\big)^*$.*

**Exercise 5.3.3.** Prove the remaining statement of Lemma 5.3.2. What happens if we try to differentiate $L(t)V(t)$ with respect to $t$?

For any two (possibly) unbounded operators $(A, D(A))$, and $(B, D(B))$ the commutator $[A, B]$ is defined as the operator $[A, B] = AB - BA$ with $D([A, B]) = D(AB) \cap D(BA) = \{x \in D(A) \cap D(B) \mid Bx \in D(A) \text{ and } Ax \in D(B)\}$. A (possibly unbounded) operator $B$ is anti-selfadjoint if $iB$ is a self-adjoint operator. So $B^* = -B$, and in particular $D(B) = D(B^*)$.

**Theorem 5.3.4** (Lax)**.** *Let $L(t)$, $t \geq 0$, be a family of self-adjoint operators on a Hilbert space with $D(L(t)) = D(L)$ independent of $t$ which is strongly continuously differentiable. Assume that there exists a family of anti-selfadjoint operators $B(t)$, with constant domain $D(B(t)) = D(B)$, depending continuously on $t$ such that*

- *$L_t = [B, L]$, i.e. $L_t(t) = [B(t), L(t)]$ for all $t \geq 0$,*
- *there exists a strongly continuous family $V(t) \in B(\mathcal{H})$ satisfying $V_t(t) = B(t)V(t)$, $V(0) = 1 \in B(\mathcal{H})$,*
- *$L(t)V(t)$ is differentiable with respect to $t$.*

*Then $L(t)$ is unitarily equivalent to $L(0)$ and in particular, the spectrum of $L(t)$ is independent of $t$.*

Such pairs $L$, $B$ are called Lax pairs, and this idea has been fruitful in e.g. integrable systems, see Exercise 5.3.9 for an easy example.

Note that in case $B = B(t)$ is independent of $t$, then we can take $V(t) = \exp(tB)$. In particular, this is a family of unitary operators, since $B$ is anti-selfadjoint and so the second requirement is automatically fulfilled. This remains true in the general time dependent case under suitable conditions on $B(t)$, but there is not such an easy description of the solution. This is outside the scope of these notes, but in the case of the KdV-equation as in the sequel $V_t(t) = B(t)V(t)$, $V(0) = 1$ has a unitary solution in case $q(\cdot, 0) \in W^3(\mathbb{R})$.

*Sketch of proof.* We first claim that $V(t)$ is actually unitary for each $t$. To see this, take $w(t) = V(t)w$, $v(t) = V(t)v$ and so $\frac{dw}{dt}(t) = B(t)w(t)$ and $\frac{dv}{dt}(t) = B(t)v(t)$, so that

$$\begin{aligned}\frac{d}{dt}\langle w(t), v(t)\rangle &= \langle \frac{d}{dt}w(t), v(t)\rangle + \langle w(t), \frac{d}{dt}v(t)\rangle = \langle B(t)w(t), v(t)\rangle + \langle w(t), B(t)v(t)\rangle \\ &= \langle B(t)w(t), v(t)\rangle - \langle B(t)w(t), v(t)\rangle = 0.\end{aligned}$$

Or $\langle V(t)w, V(t)v\rangle = \langle w, v\rangle$, and $V(t)$ is an isometry, and since we also get from this $\langle w, v\rangle = \langle V(t)^*V(t)w, v\rangle$ for arbitrary $v$ it follows $V(t)^*V(t) = 1$. Note that $W(t) = V(t)V(t)^*$ satisfies $W_t = BVV^* + VV^*B^* = BW - WB = [B, W]$ with initial condition $W(0) = 1$. Since $W(t) = 1$ is a solution, we find $W(t) = V(t)V(t)^* = 1$, or $V(t)$ is unitary, and the claim follows.

By Lemma 5.3.2 we see that $V(t)^*$ is also differentiable, and so is $\tilde{L}(t) = V(t)^*L(t)V(t)$. We want to show that $\tilde{L}(t)$ is independent of $t$. Assuming this for the moment, it follows that $V(t)^*L(t)V(t) = L(0)$, since $V(0) = 1$, and hence $L(t)$ is unitarily equivalent to $L(0)$ by $L(t) = V(t)L(0)V(t)^*$.

To prove the claim we differentiate with respect to $t$ the relation $L(t)V(t) = V(t)\tilde{L}(t)$;

$$
\begin{aligned}
&\frac{dL}{dt}(t)\,V(t) + L(t)\,\frac{dV}{dt}(t) = \frac{dV}{dt}(t)\,\tilde{L}(t) + V(t)\,\frac{d\tilde{L}}{dt}(t) \\
\Longrightarrow\ &\frac{dL}{dt}(t)\,V(t) + L(t)\,B(t)\,V(t) = B(t)\,V(t)\,\tilde{L}(t) + V(t)\,\frac{d\tilde{L}}{dt}(t) \\
\Longrightarrow\ &\frac{dL}{dt}(t)\,V(t) + L(t)\,B(t)\,V(t) = B(t)\,V(t)\,V(t)^*\,L(t)\,V(t) + V(t)\,\frac{d\tilde{L}}{dt}(t) \\
\Longrightarrow\ &V(t)\,\frac{d\tilde{L}}{dt}(t) = \Big(\frac{dL}{dt}(t) + L(t)\,B(t) - B(t)\,L(t)\Big)V(t) = 0
\end{aligned}
$$

using the product rule of Lemma 5.3.2, the differential equation for the unitary family $V(t)$. Since $V(t)$ is unitary we get $\frac{d\tilde{L}}{dt}(t) = 0$. □

**Exercise 5.3.5.** Show formally that a self-adjoint operator of the form $L = L_0 + M_q$, where $L_0$ is a fixed self-adjoint operator and $M_q$ is multiplication by a $t$-dependent function $q$, and assuming there exists a anti-selfadjoint $B$ such that $BL - LB = M_{K(q)}$, then $L$ is isospectral if $q$ satisfies the equation $q_t = K(q)$.

Lax's Theorem 5.3.4 dates from 1968, shortly after the the discovery of Gardner, Greene, Kruskal and Miura of the isospectral relation of the Schrödinger operator and the KdV-equation. In order to see how the KdV-equation arises in the context of Lax pairs, we take $L(t)$ as before as the Schrödinger operator with time-dependent potential $q(\cdot, t)$. We look for $B(t)$ in the form of a differential operator, and since it has to be anti-self-adjoint we only allow for odd-order derivatives, i.e. we try for integer $m$ and yet undetermined functions $b_j$, $j = 0, \cdots, m-1$,

$$
B_m(t) = \frac{d^{2m+1}}{dx^{2m+1}} + \sum_{j=0}^{m-1}\Big(M_j(t)\frac{d^{2j+1}}{dx^{2j+1}} + \frac{d^{2j+1}}{dx^{2j+1}}M_j(t)\Big), \qquad \big(M_j(t)f\big)(x) = b_j(x,t)f(x),
$$

considered as operator on $L^2(\mathbb{R})$ with domain $W^{2m+1}(\mathbb{R})$ for suitable functions $b_j$.

In case $m = 0$ we have $B_0(t)$ is $\frac{d}{dx}$ independent of $t$, and $[B, L] = q_x$, i.e. the multiplication operator on $L^2(\mathbb{R})$ by multiplying by $q_x$. So then the condition $L_t = [B, L]$ is related to the partial differential equation $q_t = q_x$.

**Exercise 5.3.6.** Solve $q_t = q_x$, and derive directly the isospectral property of the corresponding Schrödinger operator $L(t)$.

In case $m = 1$ we set $B_1 = \partial^3 + b\partial + \partial b$, where $\partial$ denotes derivative with respect to $x$ and where $b = b(x,t)$, $B_1 = B_1(t)$, then

$$\begin{aligned} [B_1(t), L(t)] &= \big(\partial^3 + b\partial + \partial b\big)\big(-\partial^2 + q\big) - \big(-\partial^2 + q\big)\big(\partial^3 + b\partial + \partial b\big) \\ &= [\partial^3, q] - [\partial^3, b] + [\partial, \partial b\partial] + [b\partial, q] + [\partial b, q] \end{aligned}$$

and using the general commutation $[\partial, f] = f_x$ repeatedly we see $[\partial^3, q] = 3\partial q_x \partial + q_{xxx}$, $[\partial, \partial b\partial] = \partial b_x \partial$, $[b\partial, q] = bq_x$, $[\partial b, q] = bq_x$, so that we obtain

$$[B_1(t), L(t)] = \partial(3q_x - 2b_x)\partial + q_{xxx} - b_{xxx} + 2bq_x,$$

and in order to make this a multiplication operator we need $3q_x - 2b_x = 0$, or $b_x = \frac{3}{2}q_x$. Choosing $b = \frac{3}{2}q$ we see that we require the relation

$$-\frac{1}{2}q_{xxx} + 3qq_x = [B_1(t), L(t)] = L_t(t) = q_t,$$

which is the KdV-equation up to a change of variables, see Exercise 5.1.2.

**Exercise 5.3.7.** Check that taking $B(t) = -4\frac{d^3}{dx^3} + 6q(x,t)\frac{d}{dx} + 3q_x(x,t)$ gives $[B(t), L(t)] = -q_{xxx}(\cdot,t) + 6q_x(\cdot,t)q(\cdot,t)$ corresponding to the KdV-equation (5.1.1).

**Exercise 5.3.8.** Consider the case $m = 2$ and derive the corresponding 5-th order partial differential equation for $q$. Proceeding in this way, one obtains a family of Korteweg-de Vries equations.

**Exercise 5.3.9.** Assume that we have a Lax pair as in Theorem 5.3.4 in the case of a finite dimensional Hilbert space, e.g. $\mathcal{H} = \mathbb{C}^2$. Then we can view $L_t = [B, L]$ as a system of $N = \dim \mathcal{H}$ first order coupled differential equations. Show that $\mathrm{tr}\big(L(t)\big)^n$ then gives invariants for this system. Show also that $(L^k)_t = [B, L^k]$ for $k \in \mathbb{N}$. Work this out for the example of the harmonic oscillator; $\ddot{q} + \omega^2 q = 0$, where dot denotes derivative with respect to time $t$, by checking that $L = \begin{pmatrix} p & \omega q \\ \omega q & -p \end{pmatrix}$, $B$ is the constant matrix $\begin{pmatrix} 0 & -\frac{1}{2}\omega \\ \frac{1}{2}\omega & 0 \end{pmatrix}$ and $\dot{q} = p$ gives a Lax pair.

The idea of Lax pairs has turned out to be very fruitful in many other occassions; similar approaches can be used for other nonlinear partial differential equations, such as the sine-Gordon equation, the nonlinear Schrödinger equations, see Exercise 5.3.5. These equations have many properties in common, e.g. an infinite number of conserved quantities, so-called Bäcklund transformations to combine solutions into new solutions –despite the nonlinearity. We refer to [2], [6] for more information.

## 5.4 Time evolution of the spectral data

Assume that we have a Lax pair as in Section 5.3, and assume that $L(0)$ has $\mu$ as a discrete eigenvalue with eigenvector $w \in \mathcal{H}$. By Theorem 5.3.4, it follows that $\mu$ is an eigenvalue of $L(t)$, and since $L(t) = V(t)L(0)V(t)^*$ it follows that $L(t)V(t)w = V(t)L(0)w = \mu V(t)w$, or $w(t) = V(t)w$ is the eigenvector of $L(t)$ for the eigenvalue $\mu$. So we have an explicit evolution of the eigenvector for the constant eigenvalue $\mu$. This eigenfunction also satisfies a first order differential equation, since

$$\frac{d}{dt}w(t) = V_t(t)w = B(t)V(t)w = B(t)w(t).$$

**Exercise 5.4.1.** Check directly for the case $m = 0$, cf. Exercise 5.3.6, that the eigenfunction for a discrete eigenvalue $\mu$ satisfies the appropriate differential equation at arbitrary time $t$.

Assume now that $q(\cdot, t)$ satisfies the conditions of Theorem 4.2.7 for all $t$, and assume that the Schrödinger operator at time $t = 0$ has bound states. Then it follows that it has the same eigenvalues at all times $t$. It follows that $\psi_n(x, 0) = N_n(0)f_n(x, 0)$, $N_n(0) = \sqrt{\rho_n(0)}$, is an eigenfunction of the Schrödinger operator at $t = 0$ of length 1. Hence $V(t)\psi_n(\cdot, 0) = \psi_n(\cdot, t)$ is an eigenfunction of the Schrödinger operator at $t$ of length 1, since $V(t)$ is unitary. Moreover, $\psi_n(\cdot, t)$ is a multiple of $f_n(x, t)$, the solution of the Schrödinger integral equation at time $t$. So $\psi_n(x, t) = N_n(t)f_n(x, t)$, $N_n(t) = \sqrt{\rho_n(t)}$ with the notation as in Theorem 4.2.7 with time dependency explicitly denoted up to a phase factor. Let us also assume that $q(\cdot, t)$ is compactly supported for all (fixed) $t$, then we know by Theorem 4.1.2, with notation as in Theorem 4.2.7 that $f_n(x, t) = e^{-p_n x}$ for $x$ sufficiently large, i.e. outside the support of $q(\cdot, t)$. For such $x$ we have $B(t) = -4\frac{d^3}{dx^3}$ with the version as in Exercise 5.3.7, so that the phase factor has to be 1 and

$$\begin{aligned}
\frac{d}{dt}\psi_n(x, t) &= B(t)\psi_n(x, t) = -4\frac{d^3}{dx^3}N(t)e^{-p_n x} = 4p_n^3 N(t)e^{-p_n x}, \\
\frac{d}{dt}\psi_n(x, t) &= \frac{d}{dt}N_n(t)e^{-p_n x} = e^{-p_n x}\frac{dN_n}{dt}(t)
\end{aligned}$$

for sufficiently large $x$. So $\frac{dN_n}{dt}(t) = 4p_n^3 N(t)$, and $N_n(t) = \exp(4p_n^3 t)N_n(0)$ or $\rho_n(t) = \exp(8p_n^3 t)\rho_n(0)$. So this gives the time-development for the discrete part of the scattering data in terms of a simple linear first order differential equation.

For the time-dependency of the scattering and reflection coefficient we proceed in an analogous way. Take $\gamma \in \mathbb{R}$ and assume that $q(\cdot, t)$ satisfies the conditions of Theorem 4.2.7 for all $t$. Consider the solution $\psi_\gamma(x) = T(\gamma)\, f_\gamma^-(x) = f_{-\gamma}^+(x) + R(\gamma)\, f_\gamma^+(x)$ for the eigenvalue equation for Schrödinger solution at time zero for the eigenvalue $\gamma^2$, see Section 4.2. Then we know by Lax's Theorem 5.3.4 that $\Psi_\gamma(x, t) = V(t)\, \psi_\gamma(x)$ is a solution of the corresponding eigenvalue equation for the Schrödinger equation at time $t$. So we can write

$$\Psi_\gamma(x, t) = A(t)\, f_{-\gamma}^+(x, t) + E(t)\, f_\gamma^+(x, t) = C(t)\, f_{-\gamma}^-(x, t) + D(t)\, f_\gamma^-(x, t)$$

with $A(0) = 1$, $E(0) = R(\gamma)$, $C(0) = 0$, $D(0) = T(\gamma)$, where $f^{\pm}_{\pm\gamma}(x,t)$ denote the Jost solutions of the corresponding Schrödinger operator at time $t$. Moreover, assume that $q(\cdot,t)$ is compactly supported for all (fixed) $t$, so that $\Psi_\gamma(x,t) = A(t)\,e^{-i\gamma x} + E(t)\,e^{i\gamma x}$ for $x$ sufficiently large. Again for such $x$ we have $B(t) = -4\frac{d^3}{dx^3}$ and so

$$\begin{aligned}
\frac{d}{dt}\Psi_\gamma(x,t) &= B(t)\,\Psi_\gamma(x,t) = -4(-i\gamma)^3\,A(t)\,e^{-i\gamma x} - 4(i\gamma)^3\,E(t)\,e^{i\gamma x} \\
\frac{d}{dt}\Psi_\gamma(x,t) &= \frac{dA}{dt}(t)\,e^{-i\gamma x} + \frac{dE}{dt}(t)\,e^{i\gamma x}.
\end{aligned}$$

This gives $\frac{dA}{dt}(t) = -4i\gamma^3\,A(t)$, $A(0) = 1$ and $\frac{dE}{dt}(t) = 4i\gamma^3\,E(t)$, $E(0) = R(\gamma)$, hence $A(t) = \exp(-4i\gamma^3 t)$, $E(t) = \exp(4i\gamma^3 t)R(\gamma)$.

For $x$ sufficiently negative we find $\Psi_\gamma(x,t) = C(t)\,e^{i\gamma x} + D(t)\,e^{-i\gamma x}$, and

$$\begin{aligned}
\frac{d}{dt}\Psi_\gamma(x,t) &= B(t)\,\Psi_\gamma(x,t) = -4(i\gamma)^3\,C(t)\,e^{i\gamma x} - 4(-i\gamma)^3\,D(t)\,e^{-i\gamma x} \\
\frac{d}{dt}\Psi_\gamma(x,t) &= \frac{dC}{dt}(t)\,e^{i\gamma x} + \frac{dD}{dt}(t)\,e^{-i\gamma x}.
\end{aligned}$$

This gives $\frac{dC}{dt}(t) = 4i\gamma^3\,C(t)$, $C(0) = 0$ and $\frac{dD}{dt}(t) = -4i\gamma^3\,D(t)$, $D(0) = T(\gamma)$. Hence $C(t) = 0$, $D(t) = \exp(-4i\gamma^3 t)T(\gamma)$.

Combining this then gives

$$\Psi_\gamma(x,t) = e^{-4i\gamma^3 t}\,T(\gamma)\,f^-_\gamma(x,t) = e^{-4i\gamma^3 t}\,f^+_{-\gamma}(x,t) + e^{4i\gamma^3 t}\,R(\gamma)\,f^+_\gamma(x).$$

If we now denote the corresponding time-dependent Jost solutions, transmission and reflection coefficients by

$$\psi_\gamma(x,t) = T(\gamma,t)\,f^-_\gamma(x,t) = f^+_{-\gamma}(x,t) + R(\gamma,t)\,f^+_\gamma(x,t),$$

we obtain $e^{4i\gamma^3 t}\Psi_\gamma(x,t) = \psi_\gamma(x,t)$. This then immediately gives $T(\gamma,t) = T(\gamma)$, or the transmission coefficient is independent of time, and $R(\gamma,t) = e^{8i\gamma^3 t}\,R(\gamma)$.

**Theorem 5.4.2.** *Assume $q(x,t)$ is a solution to the KdV-equation* (5.1.1) *such that for each $t \geq 0$ the function $q(\cdot,t)$, $t \geq 0$, satisfies the conditions of Theorem 4.2.7 and such that $\frac{\partial^k q}{\partial x^k}(x,t)$ is bounded for $k \in \{0,1,2,3\}$ as $|x| \to \infty$ and $\lim_{|x|\to\infty} q(x,t) = \lim_{|x|\to\infty} q_x(x,t) = 0$. Then the scattering data of $L(t) = -\frac{d^2}{dx^2} + q(\cdot,t)$ satisfies*

$$T(\gamma,t) = T(\gamma), \qquad R(\gamma,t) = e^{8i\gamma^3 t}\,R(\gamma), \qquad p_n(t) = p_n(0), \qquad \rho_n(t) = \exp(8p_n^3 t)\rho_n(0).$$

Note that the theorem in particular shows that the poles of the transmission coefficient $T$, hence the eigenvalues of the Schrödinger operator, are time-independent.

In case $q(\cdot,t)$ is of compact support, then the above argumentation leads to the statements of Theorem 5.4.2. For the $N$-soliton solutions this is not the case, and we need Theorem 5.4.2 in the more general form. The idea of the proof is the same.

Note that Theorem 5.4.2 provides a solution scheme for the KdV-equation with initial condition (5.1.2) as long as the initial condition $q(\cdot,0)$ satisfies the conditions. Determine the scattering data at time $t$, and next use the Gelfand-Levitan-Marchenko integral equation as in Theorem 4.4.2 to determine $q(x,t)$.

## 5.5 Pure soliton solutions to the KdV-equation

We now look for specific solutions of the KdV-equation using Theorem 5.4.2. The pure $N$-soliton solution to the KdV-equation (5.1.1) is the solution that is determined using Theorem 5.4.2 starting with a reflectionfless potential and with $N$ discrete points in the spectrum at time $t = 0$. Note that by Theorem 5.4.2 the potential remains reflectionless in time, and the corresponding Schrödinger operator has $N$ discrete points in the spectrum in time. We only consider the cases $N = 1$ and $N = 2$.

We first consider the case $N = 1$ and $R(\gamma) = 0$ at time $t = 0$. By Proposition 4.5.1 the potential at time $t = 0$ equals $q(x, 0) = -2\cosh^{-2}(x + C)$, $C = \frac{1}{2}\ln 2$, see the derivation in the beginning of Section 4.5, but the constant $C$ can be scaled away. From Proposition 4.5.1 we see that $p = p_1 = 1$ and $\rho = \rho_1 = 1$ at time $t = 0$. Using Theorem 5.4.2 we find that at arbitrary time $t$ we have $p(t) = 1$ and $\rho(t) = e^{8t}$. So we can solve the potential $q(x, t)$ at time $t$ in the same way as in the beginning of Section 4.5, using $p = 1$, $\rho = e^{8t}$, or we can just use (4.5.1) with $\rho = e^{8t}$. This then gives $q(x, t) = -2\cosh^{-2}(x - 4t + C)$, which is precisely the solution for the KdV-equation given in Proposition 5.1.10 for $c = 4$, and we obtain the pure 1-soliton solution.

Next we consider the case $N = 2$, so that we require at time $t = 0$ the conditions $R(\gamma) = 0$, $p_1 = 1$, $p_2 = 2$, $\rho_1 = \frac{1}{2}$, $\rho_2 = 1$, $q(x, 0) = -6\cosh^{-2}(x)$, as follows from Proposition 4.5.1. Now the time evolution of the scattering data follows from Theorem 5.4.2, so that $R(\gamma, t) = 0$ for all $t$, $p_1(t) = p_1 = 1$, $p_2(t) = p_2 = 2$, $\rho_1(t) = \frac{1}{2}e^{8t}$, $\rho_2(t) = e^{64t}$. We then need to solve for the kernel $B(x, y; t)$ and the potential $q(x, t) = -\frac{d}{dx}B(x, 0)$ from the Gelfand-Levitan-Marchenko equation. For this we use Proposition 4.5.3 in the case $N = 2$. It follows that the determinant of the symmetric matrix $I + S(x, t)$, which is now time-dependent, is given by

$$\det(I + S(x, t)) = \frac{1}{6}e^{36t-3x}\Big(\cosh(3x - 36t + \ln(12)) + 3\cosh(x - 28t)\Big)$$

using the calculation given after Proposition 4.5.3 for the case $N = 2$. By replacing $x$ and $t$ by $x + a$, $t + b$ for suitable $a$ and $b$ we can reduce to the case that

$$\det(I + S(x, t)) = C\, e^{36t-3x}\big(\cosh(3x - 36t) + 3\cosh(x - 28t)\big)$$

for some constant $C$ independent of $x$ and $t$. Take the logarithm and deriving the resulting expression twice and multiplying by $-2$ to find the potential; $q(x, t) = 2\frac{(f'(x))^2 - f''(x)f(x)}{(f(x))^2}$, with $f(x) = \det(I + S(x, t))$. This shows that the potential $q(x, t)$ is indeed independent of $C$. Using a computer algebra system is handy, and in case one uses Maple, we find

$$q(x, t) = -12\,\frac{5\,\cosh(-x + 28\,t)\cosh(-3\,x + 36\,t) + 3 - 3\,\sinh(-x + 28\,t)\sinh(-3\,x + 36\,t)}{(3\,\cosh(-x + 28\,t) + \cosh(-3\,x + 36\,t))^2}.$$

Using the addition formula $\cosh(x \pm y) = \cosh(x)\cosh(y) \pm \sinh(x)\sinh(y)$ we obtain

$$q(x, t) = -12\frac{3 + 4\cosh(2x - 8t) + \cosh(4x - 64t)}{\big(3\cosh(x - 28t) + \cosh(3x - 36t)\big)^2}. \tag{5.5.1}$$

Note that indeed

$$q(x,0) = -12\frac{3+4\cosh(2x)+\cosh(4x)}{\big(3\cosh(x)+\cosh(3x)\big)^2} = \frac{-6}{\cosh^2(x)},$$

as can be done easily in e.g. Maple. Compare this with Proposition 4.5.3. The solution (5.5.1) is known as the pure 2-soliton solution.

So we have proved from Theorem 5.4.2 and the inverse scattering method described in Sections 4.4, 4.5 the following Proposition.

**Proposition 5.5.1.** *Equation* (5.5.1) *is a solution to the KdV-equation* (5.1.1) *with initial condition* $q(x,0) = \frac{-6}{\cosh^2(x)}$.

Having the solution (5.5.1) at hand, one can check by a direct computation, e.g. using a computer algebra system like Maple, that it solves the KdV-equation. However, it should be clear that such a solution cannot be guessed without prior knowledge.

In Figure 5.2 we have plotted the solution $q(x,t)$ for different times $t$. It seems that $q(\cdot,t)$ exists of two solitary waves for $t \gg 0$ and $t \ll 0$, and that the 'biggest' solitary wave travels faster than the 'smallest' solitary wave, and the 'biggest' solitary wave overtakes the 'smallest' at $t=0$. For $t \approx 0$ the waves interact, and then the shapes are not affected by this interaction when $t$ grows. This phenomenon is typical for soliton solutions.

In order to see this from the explicit form (5.5.1) we introduce new variables $x_1 = x - 4p_1^2 t = x - 4t$ and $x_2 = x - 4p_2^2 t = x - 16t$, so Figure 5.2 suggest that the 'top' of the 'biggest' or 'fastest travelling' solitary wave occurs for $x_2 = 0$, and the top for the 'smallest' or 'slowest travelling' solitary wave occurs for $x_1 = 0$. So we see the 'biggest' solitary wave travel at four times the speed of the 'smallest' solitary wave.

We first consider the 'fastest travelling' solitary wave, so we rewrite

$$q_2(x_2,t) = q(x_2+16t,t) = -12\frac{3+4\cosh(2x_2+24t)+\cosh(4x_2)}{\big(3\cosh(x_2-12t)+\cosh(3x_2+12t)\big)^2},$$

so that for $t \to \infty$ we have

$$q_2(x_2,t) \sim -12\frac{2e^{2x_2+24t}}{\big(\frac{3}{2}e^{12t-x_2}+\frac{1}{2}e^{3x_2+12t}\big)^2} = \frac{-8}{\cosh^2(2x_2-\frac{1}{2}\ln(3))}$$

and for $t \to -\infty$ we have

$$q_2(x_2,t) \sim -12\frac{2e^{-2x_2-24t}}{\big(\frac{3}{2}e^{-12t+x_2}+\frac{1}{2}e^{-3x_2-12t}\big)^2} = \frac{-8}{\cosh^2(2x_2+\frac{1}{2}\ln(3))}.$$

From these asymptotic considerations, we see that the 'biggest' solitray wave undergoes a phase-shift, meaning that its top is shifted by $\ln(3)$ forward during the interaction with the 'smallest' solitary wave.

Similarly, we can study

$$q_1(x_1,t) = q(x_1+4t,t) = -12\frac{3+4\cosh(2x_1)+\cosh(4x_1-48t)}{\big(3\cosh(x_1-24t)+\cosh(3x_1-24t)\big)^2},$$

so that

$$q_1(x_1,t) \sim \begin{cases} -12\dfrac{\frac{1}{2}e^{48t-4x_1}}{(\frac{3}{2}e^{24t-x_1}+\frac{1}{2}e^{24t-3x_1})^2} = \dfrac{-2}{\cosh^2(x_1+\frac{1}{2}\ln(3))}, & t\to\infty, \\ -12\dfrac{\frac{1}{2}e^{-48t+4x_1}}{(\frac{3}{2}e^{-24t+x_1}+\frac{1}{2}e^{-24t+3x_1})^2} = \dfrac{-2}{\cosh^2(x_1-\frac{1}{2}\ln(3))}, & t\to-\infty. \end{cases}$$

So the ‘smallest’ wave undergoes the same phase-shift, but in the opposite direction.

So we can conclude that

$$q(x,t) \sim \frac{-2}{\cosh^2(x-4t\pm\frac{1}{2}\ln(3))} + \frac{-8}{\cosh^2(x-16t\mp\frac{1}{2}\ln(3))}, \qquad t\to\pm\infty.$$

This also suggests that one can build new solutions out of known solutions, even though the Korteweg-de Vries equation (5.1.1) is non-linear. This is indeed the case, we refer to [2], [6] for more information.

**Remark 5.5.2.** It is more generally true that a solution which exhibits a solitary wave in its solution for $t \gg 0$, then the speed of this solitary wave equals $-4\lambda$ for some $\lambda < 0$ in the discrete spectrum of the corresponding Schrödinger operator.

**Remark 5.5.3.** It is clear that for $N \geq 3$ the calculations become more and more cumbersome. There is a more unified treatment of soliton solutions possible, using the so-called $\tau$-functions. For an introduction of these aspects of the KdV-equation in relation also to vertex algebras one can consult [8].

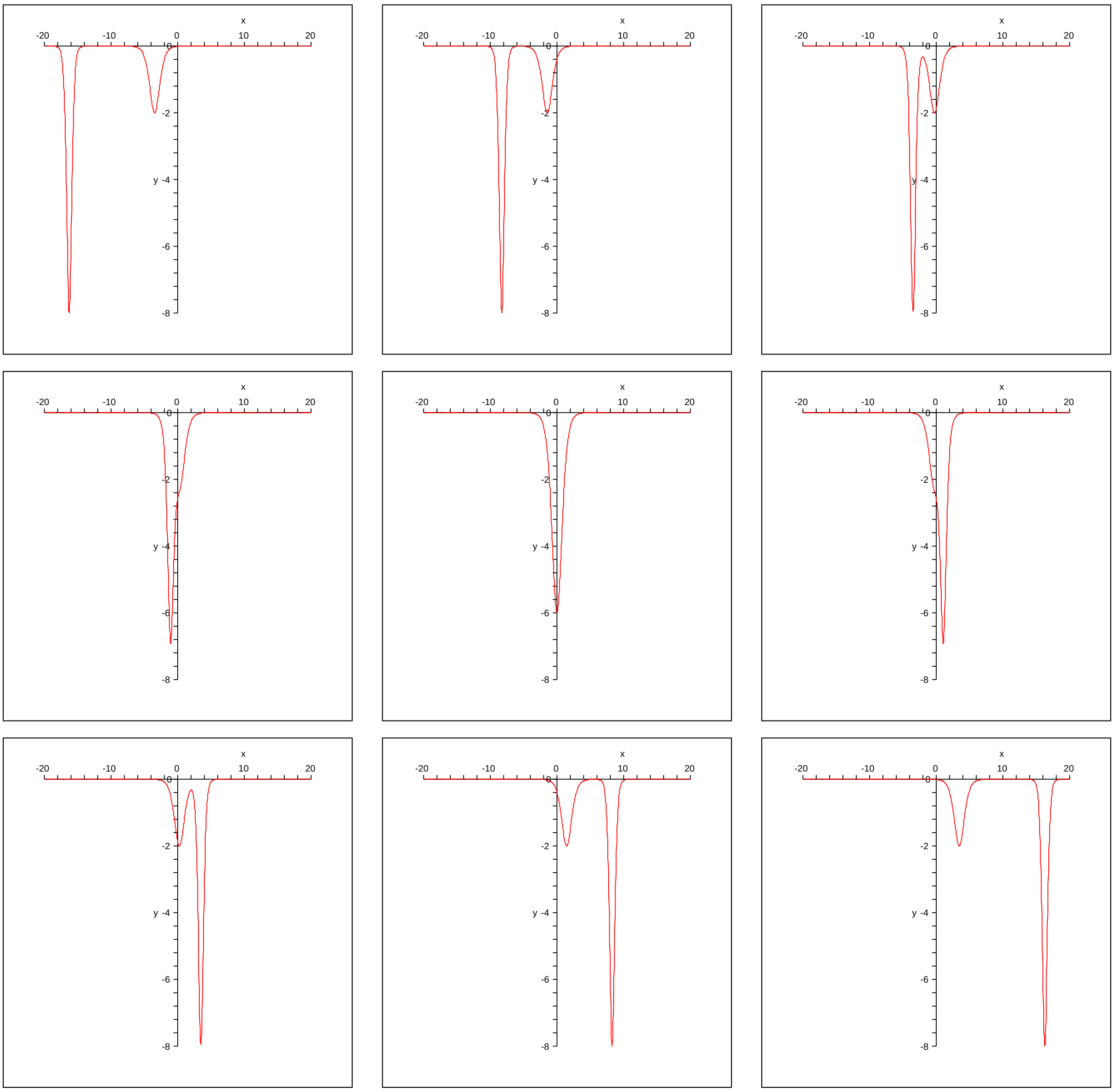


Figure 5.2: $N = 2$-soliton solution for $t = -1$, $t = -0.5$, $t = -0.2$ (first row), $t = -0.05$, $t = 0$, $t = 0.05$ (second row) and $t = 0.2$, $t = 0.5$, $t = 1$ (third row).

# Chapter 6

# Preliminaries and results from functional analysis

In this Chapter we recall several notions from functional analysis in order to fix notations and to recall standard results. Most of the unproved results can be found in Lax [7], Werner [11] or in course notes for a course in Functional Analysis. Some of the statements are equipped with a proof, notably in Section 6.5 for the description of the spectrum and the essential spectrum.

## 6.1 Hilbert spaces

A Banach[1] space $\mathcal{X}$ is a vector space (over $\mathbb{C}$) equipped with a norm, i.e. a mapping $\|\cdot\|\colon \mathcal{X} \to \mathbb{R}$ such that

- $\|\alpha x\| = |\alpha|\,\|x\|$, $\forall\, \alpha \in \mathbb{C}$, $\forall x \in \mathcal{X}$,
- $\|x + y\| \leq \|x\| + \|y\|$, $\forall\, x, y \in \mathcal{X}$, (triangle inequality)
- $\|x\| = 0 \iff x = 0$,

such that $\mathcal{X}$ is complete with respect to the metric topology induced by $d(x, y) = \|x - y\|$. Completeness means that any Cauchy[2] sequence, i.e. a sequence $\{x_n\}_{n=1}^{\infty}$ in $\mathcal{X}$ such that $\forall \varepsilon > 0\ \exists N \in \mathbb{N}\ \forall n, m \geq N\ \|x_n - x_m\| < \varepsilon$, converges in $\mathcal{X}$ to some element $x \in \mathcal{X}$, i.e. $\forall \varepsilon > 0$ $\exists N \in \mathbb{N}\ \forall n \geq N\ \|x_n - x\| < \varepsilon$. If $x_n \to x$ in $\mathcal{X}$, then $\|x_n\| \to \|x\|$ by the reversed triangle inequality $|\|x\| - \|y\|| \leq \|x - y\|$.

An inner product on a vector space $\mathcal{H}$ is a mapping $\langle \cdot, \cdot \rangle\colon \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ such that

- $\langle \alpha x + \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle$ $\forall \alpha, \beta \in \mathbb{C}$, $\forall x, y, z \in \mathcal{H}$,
- $\langle x, y \rangle = \overline{\langle y, x \rangle}$, $\forall x, y \in \mathcal{H}$,

[1] Stefan Banach (30 March 1892 — 31 August 1945), Polish mathematician, who is one of the founding fathers of functional analysis.

[2] Augustin Louis Cauchy (21 August 1789 — 23 May 1857), French mathematician.

- $\langle x, x\rangle \geq 0\ \forall x \in \mathcal{H}$ and $\langle x, x\rangle = 0 \iff x = 0$.

It can be shown that $\|x\| = \sqrt{\langle x, x\rangle}$ induces a norm on $\mathcal{H}$, and we call $\mathcal{H}$ a Hilbert[3] space if it is complete. The standard inequality is the Cauchy-Schwarz[4] inequality;

$$|\langle x, y\rangle| \leq \|x\|\,\|y\|. \tag{6.1.1}$$

A linear map $\phi\colon \mathcal{H} \to \mathbb{C}$ on a Hilbert space $\mathcal{H}$, also known as a functional, is continuous if and only if $|\phi(x)| \leq C\|x\|$ for some constant $C$. Note that (6.1.1) implies that $x \mapsto \langle x, y\rangle$ is continuous. The Riesz[5] representation theorem states that any continuous functional $\phi\colon \mathcal{H} \to \mathbb{C}$ is of this form, i.e. $\exists y \in \mathcal{H}$ such that $\phi(x) = \langle x, y\rangle$. A sequence $\{x_n\}_{n=1}^\infty$ in $\mathcal{H}$ is weakly convergent to $x \in \mathcal{H}$ if $\lim_{n\to\infty}\langle x_n, y\rangle = \langle x, y\rangle$, $\forall y \in \mathcal{H}$. By the Cauchy-Schwarz inequality (6.1.1) we see that convergence in $\mathcal{H}$, i.e. with respect to the norm, implies weak convergence. The converse is not true in general. In general, a bounded sequence in a Hilbert space does not need have a convergent subsequence (e.g. take any orthonormal sequence $\{x_n\}_{n=1}^\infty$ in an infinite dimensional Hilbert space, since then $\|x_n\| = 1$ and $\|x_n - x_m\| = \sqrt{2}$, $n \neq m$, by the Pythagorean[6] theorem), but it has a weakly convergent subsequence (e.g. in the example $x_n \to 0$ weakly). This is known as weak compactness. This is actually weak sequentially compact, but the Eberlein-Smulian theorem states that a weakly closed, bounded set $A$ in a Banach space $\mathcal{X}$ is weakly compact if and only if any sequence in $A$ has a convergent subsequence.

**Exercise 6.1.1.** In this exercise we sketch a proof of the weak sequentially compactness of a bounded set in a Hilbert space $\mathcal{H}$. Let $\{x_n\}_{n=1}^\infty$ be a bounded sequence, say $\|x_n\| \leq 1$. We have to show that there exists a subsequence $\{x_{n_k}\}_{k=1}^\infty$ and a $x \in \mathcal{H}$ such that $\lim_{k\to\infty}\langle x_{n_k}, y\rangle = \langle x, y\rangle$ for all $y \in \mathcal{H}$.

- Fix $m$, and use $|\langle x_n, x_m\rangle| \leq 1$ to find a subsequence $\{x_{n_i}\}_{i=1}^\infty$ such that $\langle x_{n_i}, x_m\rangle$ converges as $i \to \infty$.
- Find a subsequence, say $\{y_n\}_{n=1}^\infty$ such that $\langle y_n, x_m\rangle$ converges for all $m$ as $n \to \infty$. Conclude that $\langle y_n, u\rangle$ converges for all $u$ in the linear span $\mathcal{U}$ of the elements $x_n$, $n \in \mathbb{N}$.
- Show that $\langle y_n, u\rangle$ converges for all $u$ in the closure $\overline{\mathcal{U}}$ of the linear span $\mathcal{U}$
- By writing an arbitrary $w \in \mathcal{H}$ as $w = u + z$, $u \in \overline{\mathcal{U}}$, $z \in \mathcal{U}^\perp$, show that $\langle y_n, w\rangle$ converges for all $w \in \mathcal{H}$ as $n \to \infty$.
- Define $\phi\colon \mathcal{H} \to \mathbb{C}$ as $\phi(w) = \lim_{n\to\infty}\langle y_n, w\rangle$. Show that $\phi$ is a continuous linear functional.

[3]David Hilbert (23 January 1862 —14 February 1943), German mathematician. Hilbert is well-known for his list of problems presented at the ICM 1900, some still unsolved.

[4]Hermann Amandus Schwarz (25 January 1843 — 30 November 1921), German mathematician.

[5]Frigyes Riesz (22 January 1880 — 28 February 1956), Hungarian mathematician, who made many contributions to functional analysis.

[6]Pythagoras of Samos (approximately 569 BC – 475 BC), Greek philosopher.

- Use the Riesz representation theorem to find $x \in \mathcal{H}$ such that the subsequence $\{y_n\}_{n=1}^{\infty}$ converges weakly to $x$.

**Example 6.1.2.** Using the Lebesgue[7] integral, we put for $1 \le p < \infty$

$$L^p(\mathbb{R}) = \{f \colon \mathbb{R} \to \mathbb{C} \text{ measurable } \mid \int_{\mathbb{R}} |f(x)|^p \, dx < \infty\}.$$

This is a Banach space with respect to the norm $\|f\|_p = \left(\int_{\mathbb{R}} |f(x)|^p \, dx\right)^{1/p}$. The case $p = \infty$ is $L^\infty(\mathbb{R}) = \{f \colon \mathbb{R} \to \mathbb{C} \text{ measurable } \mid \operatorname{ess\,sup}_{x\in\mathbb{R}} |f(x)| < \infty\}$, which is a Banach space for the norm $\|f\|_\infty = \operatorname{ess\,sup}_{x\in\mathbb{R}} |f(x)|$. Here we follow the standard convention of identifying two functions that are equal almost everywhere.

The case $p = 2$ gives a Hilbert space $L^2(\mathbb{R})$ with inner product given by

$$\langle f, g\rangle = \int_{\mathbb{R}} f(x)\, \overline{g(x)} \, dx$$

Since we work mainly with the Hilbert space $L^2(\mathbb{R})$, we put $\|f\| = \|f\|_2$. In this case the Cauchy-Schwarz inequality states

$$\left|\int_{\mathbb{R}} f(x)\overline{g(x)} \, dx\right| \le \left(\int_{\mathbb{R}} |f(x)|^2 \, dx\right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} |g(x)|^2 \, dx\right)^{\frac{1}{2}},$$

which is also known as Hölder's inequality. The converse Hölder's inequality states for measurable function $f$ such that

$$\sup\left|\int_{\mathbb{R}} f(x)\overline{g(x)} \, dx\right| = C < \infty,$$

where the supremum is taken over all functions $g$ such that $\|g\| \le 1$ and $\int_{\mathbb{R}} f(x)\overline{g(x)} dx$ exists, we have $f \in L^2(\mathbb{R})$ and $\|f\| = C$.

We recall some basic facts from Lebesgue's integration theory. We also recall that for a convergent sequence $\{f_n\}_{n=1}^{\infty}$ to $f$ in $L^p(\mathbb{R})$, $1 \le p \le \infty$ there exists a convergent subsequence $\{f_{n_k}\}_{k=1}^{\infty}$ that converges pointwise almost everywhere to $f$.

**Theorem 6.1.3** (Lebesgue's Dominated Convergence Theorem)**.** *If $\{f\}_{n=1}^{\infty}$ is a sequence of measurable functions on $\mathbb{R}$, such that $f_n \to f$ pointwise almost everywhere on a measurable set $E \subset \mathbb{R}$. If there exists a function $g$ integrable on $E$ such that $|f_n| \le g$ almost everywhere on $E$, then*

$$\lim_{n\to\infty} \int_E f_n(x) \, dx = \int_E f(x) \, dx.$$

[7]Henri Lon Lebesgue (28 June 1875 — 26 July 1941), French mathematician, and inventor of modern integration theory.

The Dominated Convergence Theorem 6.1.3 is needed to show that the $L^p(\mathbb{R})$ spaces are complete. Another useful result is the following.

**Theorem 6.1.4** (Lebesgue's Differentiation Theorem). *For $f \in L^1(\mathbb{R})$ its indefinite integral $\int_{-\infty}^x f(y)\,dy$ is differentiable with derivative $f(x)$ almost everywhere.*

A Banach space is separable if there exists a denumerable dense set. The examples $L^p(\mathbb{R})$, $1 \leq p < \infty$, are separable, but $L^\infty(\mathbb{R})$ is not separable. In these lecture notes the Hilbert spaces are assumed to be separable.

Another example of a Banach space is $C(\mathbb{R})$, the space of continuous functions $f\colon \mathbb{R} \to \mathbb{C}$ with respect to the supremum norm, $\|f\|_\infty = \sup_{x\in\mathbb{R}} |f(x)|$. The Arzelà-Ascoli[8] theorem states that $M \subset C(\mathbb{R})$ with the properties (i) $M$ bounded, (ii) $M$ closed, (iii) $M$ is uniformly continuous (i.e. $\forall \varepsilon > 0\ \exists \delta > 0\ \forall f \in M$: $|x-y| < \delta \Rightarrow |f(x) - f(y)| < \varepsilon$), then $M$ is compact in $C(\mathbb{R})$.

## 6.2 Operators

An operator is a linear map $T$ from its domain $D(T)$, a linear subspace of a Banach space $\mathcal{X}$, to a Banach space $\mathcal{Y}$, denoted by $T\colon \mathcal{X} \supset D(T) \to \mathcal{Y}$ or by $T\colon D(T) \to \mathcal{Y}$ or by $(T, D(T))$ if $\mathcal{X}$ and $\mathcal{Y}$ are clear from the context, or simply by $T$. We say that $(T, D(T))$ is an extension of $(S, D(S))$, in notation $S \subset T$, if $D(S) \subset D(T)$ and $Sx = Tx$ for all $x \in D(S)$. Two operators $S$ and $T$ are equal if $S \subset T$ and $T \subset S$, so that in particular the domains have to be equal. By $\mathrm{Ker}(T)$ we denote the kernel of $T$, $\mathrm{Ker}(T) = \{x \in D(T) \mid Tx = 0\}$, and by $\mathrm{Ran}(T)$ we denote its range, $\mathrm{Ran}(T) = \{y \in \mathcal{Y} \mid \exists x \in D(T) \text{ such that } Tx = y\}$. The graph norm on $D(T)$ is given by $\|x\|_T = \|x\| + \|Tx\|$.

The operator $(T, D(T))$ is densely defined if the closure of its domain is the whole Banach space, $\overline{D(T)} = \mathcal{X}$. We define the sum of two operators $S$ and $T$ by $(S+T)x = Sx + Tx$ for $x \in D(T+S) = D(T) \cap D(S)$, and the composition is defined as $(ST)x = S(Tx)$ with domain $D(ST) = \{x \in D(T) \mid Tx \in D(S)\}$. Note that it might happen that the domains of the sum or composition are trivial, even if $S$ and $T$ are densely defined.

A linear operator $T\colon \mathcal{X} \to \mathcal{Y}$ is continuous if and only if $T$ is bounded, i.e. there exists a constant $C$ such that $\|Tx\| \leq C\|x\|$ for all $x \in \mathcal{X}$. The operator norm is defined by

$$\|T\| = \sup_{x\in\mathcal{X}} \frac{\|Tx\|}{\|x\|}$$

and the space $B(\mathcal{X}, \mathcal{Y}) = \{T\colon \mathcal{X} \to \mathcal{Y} \mid T \text{ bounded}\}$ is a Banach space with respect to the operator norm $\|T\|$. If $(T, D(T))$ is densely defined and $\exists C$ such that $\|Tx\| \leq C\|x\|$ $\forall x \in D(T)$, then $T$ can be extended uniquely to a bounded operator $T\colon \mathcal{X} \to \mathcal{Y}$ with $\|T\| \leq C$. We put $B(\mathcal{X}) = B(\mathcal{X}, \mathcal{X})$. For an operator $T \in B(\mathcal{X})$ with operator norm $\|T\| < 1$, we check that $\sum_{n=0}^\infty T^n$ converges with respect to the operator norm and this gives an inverse to $1 - T$,

[8]Cesare Arzelà (6 March 1847 — 15 March 1912), Italian mathematician. Ascoli Italian mathematician.

where $1 \in B(\mathcal{X})$ is the identity operator $x \mapsto x$. For Hilbert spaces we use apart from the operator norm on $B(\mathcal{H})$ also the strong operator topology, in which $T_n \to$T if $T_n x \to Tx$ for all $x \in \mathcal{H}$, and the weak operator topology, in which $T_n \to T$ if $\langle T_n x, y\rangle \to \langle Tx, y\rangle$ for all $x, y \in \mathcal{H}$. Note that convergence in operator norm implies convergence in strong operator topology, which in turn implies convergence in weak operator topology.

For $T \in B(\mathcal{H})$, $\mathcal{H}$ Hilbert space, the adjoint operator $T^* \in B(\mathcal{H})$ is defined by $\langle Tx, y\rangle = \langle x, T^* y\rangle$ for all $x, y \in \mathcal{H}$. We call $T \in B(\mathcal{H})$ a self-adjoint (bounded) operator if $T^* = T$. If a self-adjoint operator $T$ satisfies $\langle Tx, x\rangle \geq 0$ for all $x \in \mathcal{H}$, then $T$ is a positive operator, $T \geq 0$. $T \in B(\mathcal{H})$ a unitary operator if $T^*T = 1 = TT^*$. An isometry is an operator $T \in B(\mathcal{H})$, which preserves norms; $\|Tx\| = \|x\|$ for all $x \in \mathcal{H}$. A surjective isometry is unitary. An orthogonal projection is a self-adjoint operator $P \in B(\mathcal{H})$ such that $P^2 = P$, so that $P$ projects onto $\mathrm{Ran}(P)$, a closed subspace of $\mathcal{H}$, or $P|_{\mathrm{Ran}(P)}$ is the identity and $\mathrm{Ker}(P) = \mathrm{Ran}(P)^\perp$, the orthogonal complement. In particular $P$ is a positive operator. A partial isometry $U \in B(\mathcal{H})$ is an element such that $UU^*$ and $U^*U$ are orthogonal projections. The range of the projection $U^*U$ is the inital subspace, say $D$, and the range of the projection $UU^*$ is the final subspace, say $R$, and we can consider $U$ as a unitary map from $D$ to $R$.

An operator $T\colon \mathcal{H} \supset D(T) \to \mathcal{H}$ is symmetric if $\langle Tx, y\rangle = \langle x, Ty\rangle$ for all $x, y \in D(T)$. For a densely defined operator $(T, D(T))$ we define

$$D(T^*) = \{x \in \mathcal{H} \mid y \mapsto \langle Ty, x\rangle \text{ is continuous on } D(T)\}.$$

Since $D(T)$ is dense in $\mathcal{H}$ it follows that $y \mapsto \langle Ty, x\rangle$ extends to a continuous functional on $\mathcal{H}$, which, by the Riesz representation theorem, is equal to $y \mapsto \langle Ty, x\rangle = \langle y, z\rangle$ for some $z \in \mathcal{H}$. Then we define $T^*x = z$. An operator $(T, D(T))$ is self-adjoint if $(T, D(T))$ equals $(T^*, D(T^*))$. So in particular, a self-adjoint operator is densely defined. A self-adjoint operator $(T, D(T))$ is positive if $\langle Tx, x\rangle \geq 0$ for all $x \in D(T)$. Note that a densely defined symmetric operator satisfies $T \subset T^*$, and that a self-adjoint operator is symmetric, but not conversely. For a self-adjoint operator $(T, D(T))$ we have $\langle Tx, x\rangle \in \mathbb{R}$ for all $x \in D(T)$. Note that the definition of self-adjointness coincides with the definition of self-adjointness in case the operator $T$ is bounded, since then $D(T) = \mathcal{H} = D(T^*)$.

We now switch back to operators from a Banach space $\mathcal{X}$ to a Banach space $\mathcal{Y}$. An operator $K$ is compact if the closure of the image of the unit ball $\{x \in \mathcal{X} \mid \|x\| \leq 1\}$ is compact in $\mathcal{Y}$, and we denote the compact operators by $K(\mathcal{X}, \mathcal{Y})$. It follows that $K(\mathcal{X}, \mathcal{Y}) \subset B(\mathcal{X}, \mathcal{Y})$, i.e. each compact operator is bounded. Compactness can be restated as follows: for each bounded sequence $\{x_n\}_{n=1}^\infty$ in $\mathcal{X}$, the sequence $\{Kx_n\}_{n=1}^\infty$ has a convergent subsequence. Any operator with finite dimensional range is compact, we denote these operators by $F(\mathcal{X}, \mathcal{Y})$. A typical example is the rank one operator $x \mapsto \langle x, y\rangle\, z$ for fixed $y, z \in \mathcal{H}$, For a Hilbert space $\mathcal{H}$ we have that $K(\mathcal{H}) = K(\mathcal{H}, \mathcal{H})$ is the operator norm closure of $F(\mathcal{H}) = F(\mathcal{H}, \mathcal{H})$, and $K(\mathcal{H})$ is a closed two-sided ideal in $B(\mathcal{H})$, i.e. $K \in K(\mathcal{H})$ and $S \in B(\mathcal{H})$ implies $SK, KS \in K(\mathcal{H})$.

An operator $T\colon \mathcal{X} \supset D(T) \to \mathcal{Y}$ is closed if for a sequence $\{x_n\}_{n=1}^\infty$ in $D(T)$ with the properties that $x_n \to x$ in $\mathcal{X}$ and $Tx_n \to y$ in $\mathcal{Y}$ we may conclude that $x \in D(T)$ and $Tx = y$. This is equivalent to the assumption that the graph of $T$, i.e. $G(T) = \{(x, Tx) \mid x \in D(T)\}$ is closed in $\mathcal{X} \times \mathcal{Y}$. An operator $(T, D(T))$ is closable if there exists a closed operator $(S, D(S))$

such that $S$ extends $T$, $T \subset S$. The smallest (with respect to extensions) closed operator of a closable operator is its closure, denoted $(\bar{T}, D(\bar{T}))$. For closed operator $(T, D(T))$ its domain is complete with respect to the graph norm $\|\cdot\|_T$.

**Theorem 6.2.1** (Closed Graph Theorem)**.** *A closed operator $(T, D(T))$ with $D(T) = \mathcal{X}$ is bounded, $T \in B(\mathcal{X})$.*

A closed operator $(T, D(T))$ from one Hilbert space $\mathcal{H}_1$ to another Hilbert space $\mathcal{H}_2$ has a polar decomposition, i.e. $T = U|T|$, where $D(|T|) = D(T)$ and $(|T|, D(|T|))$ is self-adjoint operator on $\mathcal{H}_1$ and $U\colon \mathcal{H}_1 \to \mathcal{H}_2$ is a partial isometry with initial space $(\operatorname{Ker} T)^\perp$ and final space $\overline{\operatorname{Ran} T}$. The condition $\operatorname{Ker} T = \operatorname{Ker}|T|$ determine $U$ and $|T|$ uniquely.

For an operator on a Hilbert space $\mathcal{H}$ we have that $(T, D(T))$ is closable if and only its adjoint $(T^*, D(T^*))$ is densely defined and then its closure is $(T^{**}, D(T^{**}))$. In particular, any densely defined symmetric operator is closable, its closure being $T^{**}$. In particular, if $(T, D(T))$ is self-adjoint, then it is a closed operator. For a closed, densely defined operator $(T, D(T))$ on a Hilbert space $\mathcal{H}$, the linear space $D(T)$ is a Hilbert space with respect to $\langle x, y\rangle_T = \langle x, y\rangle + \langle Tx, Ty\rangle$. The corresponding norm is the graph norm.

The following lemma gives necessary and sufficient conditions for a densely defined, closed, symmetric operator $(T, D(T))$ to be a self-adjoint operator on the Hilbert space $\mathcal{H}$.

**Lemma 6.2.2.** *Let $(T, D(T))$ be densely defined, symmetric operator, then the following are equivalent.*

1. *Its closure $(\bar{T}, D(\bar{T}))$ is a self-adjoint operator,*
2. $\operatorname{Ker}(T^* + i) = \{0\} = \operatorname{Ker}(T^* - i)$,
3. $\overline{\operatorname{Ran}(T + i)} = \mathcal{H} = \overline{\operatorname{Ran}(T - i)}$,
4. $\operatorname{Ker}(T^* - z) = \{0\}$ *for all* $z \in \mathbb{C}\backslash\mathbb{R}$,
5. $\overline{\operatorname{Ran}(T - z)} = \mathcal{H}$ *for all* $z \in \mathbb{C}\backslash\mathbb{R}$.

*In case $(T, D(T))$ is closed, the spaces* $\operatorname{Ran}(T \pm i)$, $\operatorname{Ran}(T - z)$ *are closed.*

In fact for a closed, densely defined, symmetric operator $T$ the dimension of $\operatorname{Ker}(T^* - z)$ and $\operatorname{Ran}(T - z)$ is constant in the upper half plane $\Im z > 0$ and in the lower half plane $\Im z < 0$.

A densely defined, symmetric operator $(T, D(T))$ whose closure is self-adjoint, is known as an essentially self-adjoint operator.

*Sketch of proof.* We prove Lemma 6.2.2 in case $T$ is closed and for the equivalence of the first three assumptions. Note that $5 \Rightarrow 3$ and $4 \Rightarrow 2$.

First, for $y \in \operatorname{Ran}(T + z)^\perp$ we have $\langle Tx, y\rangle + z\langle x, y\rangle = \langle (T + z)x, y\rangle = 0$ for all $x \in D(T)$, so that in particular by definition $y \in D(T^*)$ and $\langle (T^* + \bar{z})y, x\rangle = 0$ for all $x \in D(T)$. Since $D(T)$ is dense, it follows that $(T^* + \bar{z})y = 0$ or $y \in \operatorname{Ker}(T^* + \bar{z})$. The reverse conclusion can be obtained by reversing the argument. This shows that $2 \Leftrightarrow 3$, and also $4 \Leftrightarrow 5$.

Note that $\langle Tx, x\rangle \in \mathbb{R}$, $x \in D(T)$, for $T$ symmetric, so that

$$\|(T+i)x\|^2 = \langle (T+i)x, (T+i)x\rangle = \|Tx\|^2 + \|x\|^2 + 2\Re\langle Tx, ix\rangle = \|Tx\|^2 + \|x\|^2 \geq \|x\|^2.$$

In particular, $(T+i)x = 0$ implies $x = 0$, or $\mathrm{Ker}(T+i) = \{0\}$. Similarly, $\mathrm{Ker}(T-i) = \{0\}$, so $1 \Rightarrow 2$. Another consequence of this inequality is that $(T+i)^{-1}\colon \mathrm{Ran}(T+i) \to D(T)$ exists and $\|(T+i)^{-1}\| \leq 1$. Let $\{y_n\}_{n=1}^\infty$ be a Cauchy sequence in $\mathrm{Ran}(T+i)$, put $y_n = (T+i)x_n$ and let $y_n \to y$ in $\mathcal{H}$. Then $\{x_n\}_{n=1}^\infty$ is a Cauchy sequence in $\mathcal{H}$, with limit, say, $x$. Then $Tx_n = y_n - ix_n \to y - ix$. Since $T$ is closed, it follows that $y \in D(T)$ and $Tx = y - ix$ or $(T+i)x = y \in \mathrm{Ran}(T+i)$. Similarly one establishes the closedness of the other ranges.

To prove $3 \Rightarrow 1$ it suffices to check that $D(T^*) \subset D(T)$, since we already have $T \subset T^*$, since $T$ is a densely defined symmetric operator. So take $y \in D(T^*)$ arbitrary, and consider $(T^* - i)y = (T-i)x$ for some $x \in D(T)$, since $\mathrm{Ran}(T-i) = \mathcal{H}$ by the previous paragraph. Since $T \subset T^*$, it follows that $(T^*-i)y = (T^*-i)x$ or $y - x \in \mathrm{Ker}(T^*-i) = \mathrm{Ran}(T+i)^\perp = \{0\}$, by the already established equivalence $2 \Leftrightarrow 3$. Hence $y = x \in D(T)$. $\square$

**Exercise 6.2.3.** Consider the operator $T = i\frac{d}{dx}$.

- Take $\mathcal{H} = L^2(\mathbb{R})$ and $D(T) = C_c^1(\mathbb{R})$, the space of continuously differentiable functions with compact support. You may assume that $C_c^1(\mathbb{R})$ is dense in $L^2(\mathbb{R})$. Show that $(T, D(T))$ is essentially self-adjoint.
  - Show that $(T, D(T))$ is symmetric.
  - Fix $z \in \mathbb{C}\backslash\mathbb{R}$ arbitrary. Show that $\int_\mathbb{R} e^{izx} f(x)\, dx = 0$ for $f \in \mathrm{Ran}(T-z)$ by solving $iu' - zu = f$.
  - Conversely, if $f$ is a continuous function with compact support and $\int_\mathbb{R} e^{izx} f(x)\, dx = 0$, then $f \in \mathrm{Ran}(T-z)$. (Hint: consider $u(x) = -i\int_{-\infty}^x e^{iz(y-x)} f(y)\, dy$.)
  - Show that the space consisting of continuous functions $f$ with compact support with $\int_\mathbb{R} e^{izx} f(x)\, dx = 0$ is dense in $L^2(\mathbb{R})$, and conclude, using Lemma 6.2.2, that $(T, D(T))$ is essentially self-adjoint.

- Take $\mathcal{H} = L^2([0,\infty])$, and $D(T) = C_c^1(0,\infty)$, the space of continuously differentiable functions with compact support in $(0,\infty)$. You may assume that $C_c^1(0,\infty)$ is dense in $L^2([0,\infty])$. Show that $T$ is not essentially self-adjoint.
  - Show that $(T, D(T))$ is symmetric.
  - Show that $\int_\mathbb{R} e^{izx} f(x)\, dx = 0$ for $f \in \mathrm{Ran}(T-z)$ by solving $iu' - zu = f$.
  - Show that for $\Im z > 0$, $\mathrm{Ran}(T-z)$ is not dense in $\mathcal{H}$.
  - Conclude that $(T, D(T))$ is not essentially self-adjoint

  In this case one can show that there doesn't exist a self-adjoint $(S, D(S))$ such that $T \subset S$, or $T$ has no self-adjoint extensions.

There is an abundance of positive self-adjoint operators, where $(T, D(T))$ is a positive operator if $\langle Tx, x\rangle \geq 0$ for all $x \in D(T)$.

**Lemma 6.2.4.** *Let $(T, D(T))$ be a closed, densely defined operator on $\mathcal{H}$. Then $T^*T$ with its domain $D(T^*T) = \{x \in D(T) \mid Tx \in D(T^*)\}$ is a densely defined self-adjoint operator on $\mathcal{H}$. Moreover, this operator is positive and its spectrum $\sigma(T^*T) \subset [0, \infty)$.*

See Section 6.4 for the definition of the spectrum. We only apply Lemma 6.2.4 in case $T$ is a self-adjoint operator, and in this case Lemma 6.2.4 follows from the Spectral Theorem 6.4.1.

## 6.3 Fourier transform and Sobolev spaces

For an integrable function $f \in L^1(\mathbb{R})$ we define its Fourier[9] transform as

$$\mathcal{F}f(\lambda) = \hat{f}(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x)\, e^{-i\lambda x}\, dx. \tag{6.3.1}$$

If $f', f \in L^1(\mathbb{R})$ we have, by integration by parts, $\mathcal{F}(f')(\lambda) = i\lambda(\mathcal{F}f)(\lambda)$, so the Fourier transform intertwines differentiation and multiplication. The Riemann[10]-Lebesgue lemma states that $\mathcal{F}\colon L^1(\mathbb{R}) \to C_0(\mathbb{R})$, where $C_0(\mathbb{R})$ is the space of continuous functions on $\mathbb{R}$ that vanish at infinity. For $f \in L^1(\mathbb{R})$ such that $\mathcal{F}f \in L^1(\mathbb{R})$ we have the Fourier inversion formula $f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} (\mathcal{F}f)(\lambda)\, e^{i\lambda x}\, d\lambda$. We put

$$\mathcal{F}^{-1} f(\lambda) = \check{f}(\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x)\, e^{i\lambda x}\, dx.$$

For $f \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$ one can show that $\int_{-n}^{n} f(x) e^{\pm i\lambda x}\, dx$ converges in $L^2(\mathbb{R})$-norm as $n \to \infty$. This defines $\mathcal{F}, \mathcal{F}^{-1}\colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$, and then Parseval's[11] identity holds;

$$\langle f, g\rangle = \langle \mathcal{F}f, \mathcal{F}g\rangle. \tag{6.3.2}$$

In particular, $\mathcal{F}\colon L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is unitary, $\|\mathcal{F}f\| = \|f\|$, which is Plancherel's[12] identity.

Using the Fourier transform we define the Sobolev[13] space

$$W^m(\mathbb{R}) = \{f \in L^2(\mathbb{R}) \mid \lambda \mapsto (i\lambda)^p (\mathcal{F}f)(\lambda) \in L^2(\mathbb{R}),\ \forall p \in \{0, 1, 2, \cdots, m\}\} \tag{6.3.3}$$

[9] Jean Baptiste Joseph Fourier (21 March 1768 — 16 May 1830), French mathematician, who invented Fourier series, and used it to solve the heat equation.

[10] Georg Friedrich Bernhard Riemann (17 September 1826 — 20 July 1866), German mathematician, who made important contributions to many different areas of mathematics, and posed the Riemann hypothesis, one of the most famous open problems.

[11] Marc-Antoine Parseval des Chênes (27 April 1755 — 16 August 1836), French mathematician.

[12] Michel Plancherel (16 January 1885 — 4 March 1967), Swiss mathematician.

[13] Sergei Lvovich Sobolev (6 October 1908 — 3 January 1989), Russian mathematician.

The Sobolev space is a Hilbert space for the inner product

$$\langle f, g \rangle_{W^m(\mathbb{R})} = \sum_{p=0}^{m} \langle (i\lambda)^p (\mathcal{F}f), (i\lambda)^p (\mathcal{F}g) \rangle_{L^2(\mathbb{R})}.$$

We can also define the Sobolev space using weak derivatives . We say that $f \in L^2(\mathbb{R})$ has a weak derivative of order $p \in \mathbb{N}$ in case $C_c^\infty(\mathbb{R}) \ni \phi \mapsto (-1)^p \langle f, \frac{d^p\phi}{dx^p} \rangle$ is continuous (as a functional on the Hilbert space $L^2(\mathbb{R})$). Here $C_c^\infty(\mathbb{R})$ is the space of infinitely many times differentiable functions having compact support. This space is dense in $L^p(\mathbb{R})$, $1 \leq p < \infty$. By the Riesz representation theorem there exists $g \in L^2(\mathbb{R})$ such that $\langle g, \phi \rangle = (-1)^p \langle f, \frac{d^p\phi}{dx^p} \rangle$, and we define the $p$-th weak derivative of $f$ as $D^p f = g$. Then one can show that

$$\begin{aligned} W^m(\mathbb{R}) &= \{ f \in L^2(\mathbb{R}) \mid D^p f \in L^2(\mathbb{R}) \text{ exists}, \forall p \in \{0, 1, 2, \cdots, m\} \}, \\ \langle f, g \rangle_{W^m(\mathbb{R})} &= \sum_{p=0}^{m} \langle D^p f, D^p g \rangle_{L^2(\mathbb{R})} \end{aligned}$$

By abuse of notation we put $f' = Df$, $f'' = D^2 f$, etc. for weak derivatives.

Note that $C_c^\infty(\mathbb{R}) \subset W^m(\mathbb{R})$, and since $C_c^\infty(\mathbb{R})$ is dense in $L^2(\mathbb{R})$, it follows that the Sobolev spaces $W^m(\mathbb{R})$ are dense in $L^2(\mathbb{R})$.

**Lemma 6.3.1** (Sobolev imbedding)**.** *For $m, k \in \mathbb{N}$ such that $m > k + \frac{1}{2}$ we have $W^m(\mathbb{R}) \subset C^k(\mathbb{R})$, with $C^k(\mathbb{R})$ the space of $k$-times continuous differentiable functions on $\mathbb{R}$.*

Note that this means, that $f \in W^m(\mathbb{R})$ can be identified with a function in $C^k$ after changing it on a set of measure zero. In fact this inclusion is even continuous, and a proof for the case $m = 2$, $k = 1$ is given in the proof of Theorem 2.3.4.

We also require a classical theorem of Paley and Wiener concerning the Fourier transform. A function analytic in the open complex upper half plane is an element of the Hardy[14] class $H_2^+$ if

$$C = \sup_{y>0} \int_{\mathbb{R}} |f(x + iy)|^2 \, dx < \infty.$$

Then $\sqrt{C}$ is the corresponding $H_2^+$-norm of $f$.

**Theorem 6.3.2** (Paley[15]-Wiener[16])**.** *$f \in H_2^+$ if and only if $f$ is the inverse Fourier transform of $F \in L^2(\mathbb{R})$ with $\operatorname{supp}(F) \subset [0, \infty)$,*

$$f(z) = \frac{1}{\sqrt{2\pi}} \int_0^\infty F(\lambda) e^{iz\lambda} \, d\lambda, \quad z \in \mathbb{C}, \, \Im z > 0.$$

[14] Godfrey Harold Hardy (7 February 1877 – 1 December 1947), English mathematician, also famous for his quote "There is no permanent place in the world for ugly mathematics.".

[15] Raymond Edward Alan Christopher Paley (7 January 1907 — 7 April 1933), English mathematician, killed by an avalanche while skiing during his visit to Wiener.

[16] Norbert Wiener (26 November 1894 — 18 March 1964), American mathematician, who made numerous contributions to different areas in mathematics.

*Moreover, the following Plancherel formula holds;*

$$\int_0^\infty |F(\lambda)|^2 \, d\lambda = \sup_{y>0} \int_{\mathbb{R}} |f(x+iy)|^2 \, dx,$$

*i.e. the $L^2$-norm of $F$ is the $H_2^+$-norm of $f$, and $\lim_{b\downarrow 0} f(\cdot + ib) = \mathcal{F}^{-1}F$ in $L^2(\mathbb{R})$.*

*Proof.* First, if $f$ is the inverse Fourier transform of $F$ supported on $[0,\infty)$, then $f$ is an analytic function in the open upper half plane since, writing $z = a+ib$,

$$f(z) = f(a+ib) = \frac{1}{\sqrt{2\pi}} \int_0^\infty F(\lambda) e^{-b\lambda} e^{ia\lambda} \, d\lambda$$

and this integral converges absolutely in the open upper half plane. Then $\int_C f(z)\, dz = 0$ for any closed curve in the open upper half plane by interchanging integrations and $e^{i\lambda z}$ being analytic. So $f$ is analytic by Morera's theorem. By the Plancherel identity we have

$$\sup_{b>0} \|a \mapsto f(a+ib)\| = \sup_{b>0} \|\lambda \mapsto e^{-b\lambda} F(\lambda)\| = \|F\|,$$

and

$$\|f(\cdot + ib) - \mathcal{F}^{-1}F\|^2 = \|\mathcal{F}^{-1}\Big(\lambda \mapsto (1-e^{-b\lambda})F(\lambda)\Big)\|^2 = \int_0^\infty (1-e^{-b\lambda})^2 \, |F(\lambda)|^2 \, d\lambda \to 0,$$

as $b \downarrow 0$ by the Dominated Convergence Theorem 6.1.3.

To finish the proof, we have to show that any element $f$ in the Hardy class $H_2^+$ can be written in this way. Define $f_b(x) = f(x+ib)$, i.e. the function restricted to the line $\Im z = b$. Then $f_b \in L^2(\mathbb{R})$, and $\|f_b\| \leq C$ independent of $b$. Consider

$$e^{b\lambda}\mathcal{F}(f_b)(\lambda) = \frac{e^{b\lambda}}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\lambda x} f_b(x)\, dx = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-i\lambda(x+ib)} f_b(x)\, dx = \frac{1}{\sqrt{2\pi}} \int_{\Im z = b} e^{-i\lambda z} f(z)\, dz$$

We claim that this expression is independent of $b > 0$ as functions in $L^2(\mathbb{R})$. Assuming this claim is true, we define $F(\lambda) = e^{b\lambda}\mathcal{F}(f_b)(\lambda)$, then

$$\int_{\mathbb{R}} e^{-2b\lambda} |F(\lambda)|^2 \, d\lambda = \|e^{-b\lambda}F\|^2 = \|\mathcal{F}f_b\|^2 = \|f_b\|^2 \leq C^2$$

independent of $b$. From this we can observe the following; (i) $F(\lambda) = 0$ for $\lambda < 0$ (almost everywhere) by considering $b \to \infty$, (ii) $F \in L^2(\mathbb{R})$ by taking the limit $b \downarrow 0$, and (iii), as identity in $L^2(\mathbb{R})$,

$$\begin{aligned} f(z) &= f(a+ib) = f_b(a) = \mathcal{F}^{-1}\Big(\mathcal{F}f_b\Big)(a) = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\lambda a} (\mathcal{F}f_b)(\lambda)\, d\lambda \\ &= \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\lambda a} e^{-b\lambda} F(\lambda)\, d\lambda = \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{i\lambda z} F(\lambda)\, d\lambda. \end{aligned}$$

The proof of the claim is as follows. Let $\mathcal{C}_\alpha$, $\alpha > 0$, be the rectangle with vertices at $\pm\alpha + i$ and $\pm\alpha + ib$, then $\int_{\mathcal{C}_\alpha} e^{-i\lambda z} f(z)\, dz = 0$ by analyticity of the integrand in the open upper half plane. Put $I(\alpha) = \int_{\alpha+i}^{\alpha+ib} e^{-i\lambda z} f(z)\, dz$ in case $b > 1$ (the other case is similar). Then

$$|I(\alpha)|^2 = |i \int_1^b e^{-i\lambda(\alpha+it)} f(\alpha+it)\, dt|^2 \leq \int_1^b |f(\alpha+it)|^2\, dt \int_1^b e^{2t\lambda}\, dt,$$

where the first integral is independent of $\lambda$. Since $f \in H_2^+$ it follows

$$\int_{\mathbb{R}} \big( \int_1^b |f(\alpha+it)|^2\, dt \big)\, d\alpha = \int_1^b \int_{\mathbb{R}} |f(\alpha+it)|^2\, d\alpha\, dt \leq C^2\, |b-1|,$$

with $C$ the Hardy space norm of $f$. Or $\alpha \mapsto G(\alpha) = \int_1^b |f(\alpha+it)|^2\, dt$ is in $L^1(\mathbb{R})$, there exist sequence $\beta_n \to \infty$ and $\gamma_n \to -\infty$ such that $G(\beta_n) \to 0$ and $G(\gamma_n) \to 0$, and hence $I(\beta_n) \to 0$ and $I(\gamma_n) \to 0$. Note that these sequences are independent of $\lambda$ by the estimate above. We now define

$$g_n(b,\lambda) = \frac{1}{\sqrt{2\pi}} \int_{\gamma_n}^{\beta_n} f(x+ib)\; e^{-i\lambda x}\, dx,$$

so that

$$\lim_{n\to\infty} e^{\lambda b} g_n(b,\lambda) - e^{\lambda} g_n(1,\lambda) = 0.$$

By the Plancherel theorem we have $\lim_{n\to\infty} \|\mathcal{F}(f_b) - g_n(b,\cdot)\| = 0$, so that we can find a subsequence of $\{g_n(b,\cdot)\}_{n=1}^\infty$ that converges pointwise to $\mathcal{F}(f_b)$ almost everywhere, and by restricting the previous limit to this subsequence we see that $e^{b\lambda}\mathcal{F}(f_b)(\lambda)$ is independent of $b$ as claimed. $\square$

In the last part of the proof we have used the fact that if $\{f_n\}$ is a Cauchy sequence in $L^2(\mathbb{R})$ converging to $f \in L^2(\mathbb{R})$, then there exists a subsequence $\{f_{n_k}\}$ such that $f_{n_k} \to f$, $k \to \infty$, pointwise almost everywhere.

## 6.4 Spectral theorem

We consider densely defined operators $(T, D(T))$ on a Hilbert space $\mathcal{H}$. Then $z \in \mathbb{C}$ is in the resolvent set if $T - z$ is invertible in $B(\mathcal{H})$, i.e. there exists a bounded linear operator $R(z;T)$ such that $R(z;T)\colon \mathcal{H} \to D(T) \subset \mathcal{H}$ such that $R(z;T)(T-z) \subset (T-z)R(z;T) = 1$. Note that this implies $T - z$ to be a bijection $D(T) \to \mathcal{H}$. The resolvent set is denoted by $\rho(T)$, and its complement $\sigma(T)$ is its spectrum. The spectrum is always closed in $\mathbb{C}$. If for $\lambda \in \mathbb{C}$ there exists an element $x \in D(T) \subset \mathcal{H}$ such that $Tx = \lambda x$, then we say that $\lambda \in \sigma_p(T)$, point spectrum, and $\sigma_p(T) \subset \sigma(T)$. Then $x$ is an eigenvector for the eigenvalue $\lambda \in \sigma_p(T)$.

For $(T, D(T))$ a self-adjoint operator we have $\sigma(T) \subset \mathbb{R}$, and for a positive self-adjoint operator we have $\sigma(T) \subset [0,\infty)$.

Recall that a $\sigma$-algebra on a space $X$ is a collection $\mathcal{M}$ of subsets of $X$, such that (i) $X \in \mathcal{M}$, (ii) for $A \in \mathcal{M}$ its complement $A^c = X \backslash A \in \mathcal{M}$ (iii) if $A_i \in \mathcal{M}$ then $\cup_{n=1}^\infty A_i \in \mathcal{M}$.

The Borel[17] sets on $\mathbb{R}$ are the smallest $\sigma$-algebra that contain all open intervals. A (positive) measure is a map $\mu\colon \mathcal{M} \to [0,\infty]$ such that $\mu$ is countably additive, i.e. for all sets $A_i \in \mathcal{M}$ with $A_i \cap A_j = \emptyset$ for $i \neq j$ we have $\mu(\cup_{i=1}^\infty A_i) = \sum_{i=1}^\infty \mu(A_i)$. A complex measure is a countably additive map $\mu\colon \mathcal{M} \to \mathbb{C}$.

For the Spectral Theorem 6.4.1 we need the notion of spectral measure, which is a orthogonal projection valued measure on the Borel sets of $\mathbb{R}$. So, denoting the spectral measure by $E$, this means that for any Borel set $A \subset \mathbb{R}$, $E(A) \in B(\mathcal{H})$ is an orthogonal projection such that $E(\emptyset) = 0$, $E(\mathbb{R}) = 1$ (the identity element of $B(\mathcal{H})$) and for pairwise disjoint Borel sets $A_1, A_2, \cdots$ we have

$$\sum_{i=1}^\infty E(A_i)\, x = E(\cup_{i=1}^\infty A_i)\, x, \qquad \forall\, x \in \mathcal{H}.$$

This can be restated as that the series $\sum_{i=1}^\infty E(A_i)$ converges in the strong operator topology of $B(\mathcal{H})$ to $E(\cup_{i=1}^\infty A_i)$. One can show that e.g. $E(A \cap B) = E(A)E(B)$, so that spectral projections commute.

In particular, for $E$ a spectral measure and $x, y \in \mathcal{H}$ we can define a complex-valued Borel measure $E_{x,y}$ on $\mathbb{R}$ by $E_{x,y}(A) = \langle E(A)x, y\rangle$ for $A \subset \mathbb{R}$ a Borel set. Note that $E_{x,x}(A)$ is a positive Borel measure, since $E(A) = E(A)^2 = E(A)^*$;

$$E_{x,x}(A) = \langle E(A)x, x\rangle = \langle E(A)^2 x, x\rangle = \langle E(A)x, E(A)x\rangle = \|E(A)x\|^2 \geq 0.$$

**Theorem 6.4.1** (Spectral Theorem)**.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there exists a uniquely determined spectral measure $E$ such that*

$$\langle Tx, y\rangle = \int_{\mathbb{R}} \lambda\, dE_{x,y}(\lambda), \qquad \forall x \in D(T),\ \forall y \in \mathcal{H},$$

*and the support of the complex measure $E_{x,y}$ is contained in the spectrum $\sigma(T)$. For any bounded measurable function $f$ there is a uniquely defined operator $f(T)$ defined by*

$$\langle f(T)x, y\rangle = \int_{\mathbb{R}} f(\lambda)\, dE_{x,y}(\lambda),$$

*such that the map $\mathcal{B}(\mathbb{R}) \ni f \mapsto f(T) \in B(\mathcal{H})$ is a $*$-algebra homomorphism from the space $\mathcal{B}(\mathbb{R})$ of bounded measurable functions to the space of bounded linear operators, i.e. $(fg)(T) = f(T)g(T)$, $(af+bg)(T) = af(T) + bg(T)$, $\bar{f}(T) = f(T)^*$, for all $f, g \in \mathcal{B}(\mathbb{R})$, $a, b \in \mathbb{C}$, and where $\bar{f}(x) = \overline{f(x)}$. Moreover, for a measurable real-valued function $f\colon \mathbb{R} \to \mathbb{R}$ define*

$$D = \{x \in \mathcal{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2\, dE_{x,x}(\lambda) < \infty\},$$
$$\langle f(T)x, y\rangle = \int_{\mathbb{R}} f(\lambda)\, dE_{x,y}(\lambda),$$

*then $(f(T), D)$ is a self-adjoint operator. Moreover, $S \in B(\mathcal{H})$ commutes with $T$, $ST \subset TS$, if and only if $S$ commutes with all spectral projections $E(A)$, $A$ Borel set of $\mathbb{R}$.*

[17] Félix Edouard Justin Émile Borel (7 January 1871 — 3 February 1956), French mathematician.

The map $f \mapsto f(T)$ is known as the functional calculus for bounded measurable functions. This can be extended to unbounded measurable functions. All integrals can be restricted to the spectrum $\sigma(T)$, i.e. the spectral measure is supported on the spectrum.

The Spectral Theorem 6.4.1 in particular characterises the domain in terms of the spectral measure, since

$$D(T) = \{x \in \mathcal{H} \mid \int_{\mathbb{R}} \lambda^2 \, dE_{x,x}(\lambda) < \infty\}.$$

Note also that $\|f(T)x\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 \, dE_{x,x}(\lambda) \geq 0$ since $E_{x,x}$ is a positive measure.

In particular, it follows from the Spectral Theorem 6.4.1, that for a self-adjoint $(T, D(T))$ on the Hilbert space $\mathcal{H}$ and the function $\exp(-itx)$, $t \in \mathbb{R}$, we get a bounded operator $U(t) = \exp(-itT)$. From the functional calculus it follows immediately that $U(t+s) = U(t)U(s)$, $U(0) = 1$, $U(t)^* = U(-t)$, so that $t \mapsto U(t)$ is a 1-parameter group of unitary operators in $B(\mathcal{H})$. Stone's[18] Theorem 6.4.2 states that the converse is also valid.

**Theorem 6.4.2** (Stone)**.** *Assume $\mathbb{R} \ni t \mapsto U(t)$ is a 1-parameter group of unitary operators, i.e. $U(s)U(t) = U(s+t)$ for all $s, t \in \mathbb{R}$, and $U(t)$ is a unitary operator in $B(\mathcal{H})$ for each $t \in \mathbb{R}$. Assume moreover that $\mathbb{R} \ni t \mapsto U(t)x \in \mathcal{H}$ is continuous for all $x \in \mathcal{H}$. Then there exists a unique self-adjoint operator $(T, D(T))$ such that $U(t) = \exp(-itT)$, and the operator $T$ is defined by*

$$D(T) = \{x \in \mathcal{H} \mid \lim_{t \to 0} \frac{U(t)x - x}{t} \text{ converges}\} \qquad Tx = i \lim_{t \to 0} \frac{U(t)x - x}{t}, \qquad x \in D(T).$$

$U(t)$ as in Stone's Theorem 6.4.2 is called a strongly continuous 1-parameter group of unitary operators.

## 6.5 Spectrum and essential spectrum for self-adjoint operators

In this subsection we recall some facts that are usually not parts of a standard course in functional analysis. So we provide some of the statements of proofs.

We start with characterising the spectrum of a self-adjoint operator. Theorem 6.5.1 can be extended to normal operators, i.e. $T^*T = TT^*$ (also for unbounded operators $T$).

**Theorem 6.5.1.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and $\lambda \in \mathbb{R}$. Then $\lambda \in \sigma(T)$ if and only if the following condition holds: there exists a sequence $\{x_n\}_{n=1}^{\infty}$ in $D(T)$ such that*

1. *$\|x_n\| = 1$,*

2. *$\lim_{n \to \infty} (T - \lambda)x_n = 0$.*

[18] Marshall Harvey Stone (8 April 1903 — 9 January 1989), American mathematician.

In particular, for $\lambda \in \sigma_p(T)$ we can take the sequence constant $x_n = x$ with $x$ an eigenvector of norm one for the eigenvalue $\lambda$. In general, for a closed operator $(T, D(T))$ we say that $\lambda$ is in the approximate point spectrum if there exists a sequence $\{x_n\}_{n=1}^\infty$ in $D(T)$ such that $\|x_n\| = 1$ and $\lim_{n\to\infty}(T-\lambda)x_n = 0$. Theorem 6.5.1 states that for a self-adjoint operator the approximate point spectrum is its spectrum.

*Proof.* Let us first assume that such a sequence exists. We have to prove that $\lambda \in \sigma(T)$. Suppose not, then $\lambda$ is element of the resolvent, and so there exists $R(\lambda; T) \in B(\mathcal{H})$ such that $R(\lambda; T)(T-\lambda) \subset 1$. So

$$1 = \|x_n\| = \|R(\lambda; T)(T-\lambda)x_n\| \leq \|R(\lambda; T)\| \, \|(T-\lambda)x_n\|$$

and since $\|R(\lambda; T)\|$ is independent of $n$, the right hand side can be made arbitrarily small since $(T-\lambda)x_n \to 0$. This is a contradiction, so that $\lambda \notin \rho(T)$, or $\lambda \in \sigma(T)$. Note that this implication is independent of $(T, D(T))$ being self-adjoint, so we have proved that in general the approximate point spectrum is part of the spectrum.

We prove the converse statement by negating it. So we assume such a sequence does not exist, and we have to show that $\lambda \in \rho(T)$. First we claim that there exists a $C > 0$ such that

$$\|x\| \leq C \, \|(T-\lambda)x\| \quad \forall x \in D(T). \tag{6.5.1}$$

To see why (6.5.1) is true, we assume that there exists a sequence $\{y_n\}_{n=1}^\infty$ in $D(T)$ such that

$$\frac{\|y_n\|}{\|(T-\lambda)y_n\|} \to \infty, \qquad n \to \infty.$$

Putting $x_n = y_n/\|y_n\|$, noting that $y_n \neq 0$, this gives $\|x_n\| = 1$ and $\frac{\|x_n\|}{\|(T-\lambda)x_n\|} \to \infty$, so $\|(T-\lambda)x_n\| \to 0$, which is precisely the statement whose negation we assume to be true.

As an immediate corollary to (6.5.1) we see that $T - \lambda$ is injective. Indeed, assume $(T-\lambda)x_1 = y = (T-\lambda)x_2$, then $0 = \|y - y\| = C\|(T-\lambda)(x_1 - x_2)\| \geq \|x_1 - x_2\| \geq 0$ and $\|x_1 - x_2\| = 0$ or $x_1 = x_2$.

Another consequence of (6.5.1) is $\mathrm{Ran}(T-\lambda)$ is closed. Indeed, take any sequence $\{y_n\}_{n=1}^\infty$ in $\mathrm{Ran}(T-\lambda)$, and assume $y_n \to y$ in $\mathcal{H}$. We need to show that $y \in \mathrm{Ran}(T-\lambda)$. By the previous observation we can pick unique $x_n \in D(T)$ with $(T-\lambda)x_n = y_n$. Then (6.5.1) and $y_n \to y$ imply that $\{x_n\}_{n=1}^\infty$ is a Cauchy sequence, hence convergent to, say, $x \in \mathcal{H}$. For any $z \in D(T)$ we have

$$\langle (T-\lambda)z, x\rangle = \lim_{n\to\infty} \langle (T-\lambda)z, x_n\rangle = \lim_{n\to\infty} \langle z, (T-\lambda)x_n\rangle = \lim_{n\to\infty} \langle z, y_n\rangle = \langle z, y\rangle$$

since $x_n \in D(T^*) = D(T)$ and $\lambda \in \mathbb{R}$. This implies by definition that $x \in D((T-\lambda)^*) = D(T^*) = D(T)$ and that $(T-\lambda)^* x = y$, or $(T-\lambda)x = y$, or $y \in \mathrm{Ran}(T-\lambda)$.

Summarising, $T-\lambda$ is an injective map onto the closed subspace $\mathrm{Ran}(T-\lambda)$. We now show that $\mathrm{Ran}(T-\lambda)$ is the whole Hilbert space $\mathcal{H}$. Fix an element $z \in \mathcal{H}$. We define a functional

$\phi\colon \mathrm{Ran}(T-\lambda) \to \mathbb{C}$ by $\phi(y) = \langle x, z\rangle$ with $x \in D(T)$ uniquely defined by $(T-\lambda)x = y$. Then $\phi$ is indeed linear. Using (6.5.1) and the Cauchy-Schwarz inequality (6.1.1) we see

$$|\phi(y)| \, = \, |\langle x, z\rangle| \, \le \, \|x\| \, \|z\| \, \le \, C \, \|(T-\lambda)x\| \, \|z\| = C \, \|y\| \, \|z\|$$

or $\phi$ is a continuous linear functional on $\mathrm{Ran}(T-\lambda)$ as a closed subspace of $\mathcal{H}$, so that the Riesz representation theorem gives $\phi(y) = \langle y, w\rangle$ for some $w \in \mathcal{H}$. This is $\langle (T-\lambda)x, w\rangle = \langle x, z\rangle$ and since this is true for all $x \in D(T)$ we see that $w \in D((T-\lambda)^*) = D(T^*) = D(T)$ and $z = (T-\lambda)^* w = (T-\lambda)w$ since $T$ is self-adjoint and $\lambda \in \mathbb{R}$. This shows that $z \in \mathrm{Ran}(T-\lambda)$, and since $z \in \mathcal{H}$ is arbitrary, it follows that $\mathrm{Ran}(T-\lambda) = \mathcal{H}$ as claimed.

So now we have $T-\lambda$ as an injective map from $D(T)$ to $\mathcal{H} = \mathrm{Ran}(T-\lambda)$, and we can define its inverse $(T-\lambda)^{-1}$ as a map from $\mathcal{H}$ to $D(T)$. Now (6.5.1) implies that $(T-\lambda)^{-1}$ is bounded, hence $(T-\lambda)^{-1} \in B(\mathcal{H})$ and so $\lambda \in \rho(T)$. □

The Spectral Theorem 6.4.1 for the case of a compact operator is well-known, and we recall it.

**Theorem 6.5.2** (Spectral theorem for compact operators)**.** *Let $K \in K(\mathcal{H})$ be self-adjoint. Then its spectrum is a denumerable set in $\mathbb{R}$ with $0$ as the only possible point of accumulation. Each non-zero point in the spectrum is an eigenvalue of $K$, and the corresponding eigenspace is finite dimensional. Denoting the spectrum by $|\lambda_1| \ge |\lambda_2| \ge |\lambda_3| \cdots$ (each $\lambda \in \sigma(K)$ occurring as many times as $\dim(\mathrm{Ker}(K-\lambda))$) and $\{e_i\}_{i\ge1}$, $\|e_i\| = 1$, the corresponding eigenvectors, then*

$$\mathcal{H} = \mathrm{Ker}(K) \oplus \bigoplus_{i\ge1} \mathbb{C}\, e_i, \qquad Kx = \sum_{i\ge1} \lambda_i \, \langle x, e_i\rangle \, e_i.$$

The essential spectrum of a self-adjoint operator is the part of the spectrum that is not influenced by compact perturbations. Suppose e.g. that $\lambda \in \sigma_p(T)$ with corresponding eigenvector $e$ such that the self-adjoint operator $x \mapsto Tx - \lambda\langle x, e\rangle e$ has $\lambda$ in its resolvent, then we see that this part of the spectrum is influenced by a compact (in this case even rank-one) perturbation. The definition of the essential spectrum is as follows. The essential spectrum is also known as the Weyl spectrum.

**Definition 6.5.3.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$, then the essential spectrum is*

$$\sigma_{ess}(T) = \bigcap_{K\in K(\mathcal{H}),\ K^*=K} \sigma(T+K).$$

Obviously, $\sigma_{ess}(T) \subset \sigma(T)$ by taking $K$ equal to the zero operator. Also note that the essential spectrum only makes sense for infinite dimensional Hilbert spaces. For $\mathcal{H}$ finite dimensional the essential spectrum of any self-adjoint operator is empty.

**Theorem 6.5.4.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and take $\lambda \in \mathbb{R}$. Then the following statements are equivalent:*

1. $\lambda \in \sigma_{ess}(T)$;

2. *there exists a sequence* $\{x_n\}_{n=1}^\infty$ *in the domain* $D(T)$ *such that*
   - $\|x_n\| = 1$,
   - $\{x_n\}_{n=1}^\infty$ *has no convergent subsequence,*
   - $(T-\lambda)x_n \to 0$;
3. *there exists a sequence* $\{x_n\}_{n=1}^\infty$ *in the domain* $D(T)$ *such that*
   - $\|x_n\| = 1$,
   - $x_n \to 0$ *weakly,*
   - $(T-\lambda)x_n \to 0$.

*Proof.* (3) $\Rightarrow$ (2): Assume that $\{x_n\}_{n=1}^\infty$ has a convergent subsequence, we relabel and we can assume that the sequence converges to $x$. Since $\|x_n\| = 1$, we have $\|x\| = 1$. Since $x_n \to x$ we also have $x_n \to x$ weakly, and since also $x_n \to 0$ weakly we must have $x = 0$ contradicting $\|x\| = 1$.

(2) $\Rightarrow$ (3): Since $\|x_n\| = 1$ is a bounded sequence, it has a weakly convergent subsequence, which, by relabeling, may be assumed to be the original sequence, see Exercise 6.1.1. Denote its weak limit by $x$. Since by assumption there is no convergent subsequence, there exists $\delta > 0$ so that $\|x_n - x\| \geq \delta$ for all $n \in \mathbb{N}$ (by switching to a subsequence if necessary). Since the sequence is from $D(T)$, the self-adjointness implies

$$\langle (T-\lambda)y, x_n\rangle = \langle y, (T-\lambda)x_n\rangle$$

for all $y \in D(T)$. Since $(T-\lambda)x_n \to 0$ and $x_n \to x$ weakly we find by taking $n \to \infty$ that $\langle (T-\lambda)y, x\rangle = 0$ for all $y \in D(T)$. Since this is obviously continuous as a functional in $y$, we see that $x \in D((T-\lambda)^*) = D(T)$, since $T$ is self-adjoint, and that $(T-\lambda)^*x = (T-\lambda)x = 0$.

We now define $z_n = (x_n - x)/\|x_n - x\|$, which can be done since $\|x_n - x\| \geq \delta > 0$. Then by construction $\|z_n\| = 1$ and $z_n \to 0$ weakly. Moreover, since $x \in \mathrm{Ker}(T-\lambda)$,

$$\|(T-\lambda)z_n\| = \frac{1}{\|x_n - x\|}\|(T-\lambda)x_n\| \leq \frac{1}{\delta}\|(T-\lambda)x_n\| \to 0.$$

So the sequence $\{z_n\}_{n=1}^\infty$ satisfies the conditions of (3).

(2) $\Rightarrow$ (1): We prove the negation of this statement. Assume $\lambda \notin \sigma_{ess}(T)$, and let $K$ be a self-adjoint compact operator such that $\lambda \in \rho(T+K)$. So in particular $R(\lambda; T+K)\colon \mathcal{H} \to D(T+K) = D(T)$ is bounded, or

$$\begin{aligned} &\|R(\lambda; T+K)x\| \leq \|R(\lambda; T+K)\|\,\|x\| \\ \Longrightarrow &\|y\| \leq \|R(\lambda; T+K)\|\,\|(T+K-\lambda)y\| \end{aligned}$$

by switching $x$ to $(T+K-\lambda)y$, $y \in D(T)$ arbitrary. Now take any sequence $\{x_n\}_{n=1}^\infty$ satisfying the first and last condition of (2). Then by the above observation, with $C = \|R(\lambda; T+K)\|$,

$$\begin{aligned} \|x_n - x_m\| &\leq C\,\|(T+K-\lambda)(x_n - x_m)\| \\ &\leq C\,\|(T-\lambda)x_n\| + C\,\|(T-\lambda)x_m\| + C\,\|K(x_n - x_m)\| \end{aligned}$$

and the first two terms on the right hand side tend to zero by assumption. Since $K$ is compact, and the sequence $\{x\}_{n=1}^{\infty}$ is bounded by 1 there is a convergent subsequence of $\{Kx_n\}_{n=1}^{\infty}$. By relabeling we may assume that the sequence $\{Kx_n\}_{n=1}^{\infty}$ is convergent, and then the final term on the right hand side tends to zero. This means that $\{x_n\}_{n=1}^{\infty}$ is a Cauchy sequence, hence convergent. So the three conditions in (2) cannot hold.

(1) $\Rightarrow$ (2) We consider two possibilities; $\dim \mathrm{Ker}(T-\lambda) < \infty$ or $\dim \mathrm{Ker}(T-\lambda) = \infty$. In the last case we pick an orthonormal sequence $\{x_n\}_{n=1}^{\infty}$ in $\mathrm{Ker}(T-\lambda) \subset D(T)$. Then obviously, $\|x_n\| = 1$ and $(T-\lambda)x_n = 0$ for all $n$, and this sequence cannot have a convergent subsequence, since $\|x_n - x_m\| = \sqrt{2}$ by the Pythagorean theorem, cf. Section 6.1.

In case $\mathrm{Ker}(T-\lambda)$ is finite-dimensional, we claim that there exists a sequence $\{x_n\}_{n=1}^{\infty}$ in $D(T)$ such that $x_n \perp \mathrm{Ker}(T-\lambda)$, $\|x_n\| = 1$ and $(T-\lambda)x_n \to 0$. In order to prove the claim we first observe that $D(T) \cap \mathrm{Ker}(T-\lambda)^{\perp}$ is dense in $\mathrm{Ker}(T-\lambda)^{\perp}$. Indeed, let $P$ denote the orthogonal projection on $\mathrm{Ker}(T-\lambda)$ and take arbitrary $x \in \mathrm{Ker}(T-\lambda)^{\perp}$, $\varepsilon > 0$, so that $\exists y \in D(T)$ such that $\|x - y\| < \varepsilon$. Write $y = Py + (1-P)y$, then $Py \in \mathrm{Ker}(T-\lambda) \subset D(T)$ so that with $y \in D(T)$ and $D(T)$ being a linear space, also $(1-P)y \in D(T)$. Now $\|x - (1-P)y\| = \|(1-P)(x-y)\| \leq \|x-y\| < \varepsilon$, so the density follows.

In order to see why the claim in the previous paragraph is true, note that $P$ is self-adjoint and, since this is a finite rank operator, $P$ is compact. Note that $T+P$ is a self-adjoint operator. If such a sequence would not exist, then we can conclude, by restricting to $\mathrm{Ker}(T-\lambda)^{\perp}$, as in the proof of Theorem 6.5.1, cf. (6.5.1), that there exists a $C$ such that for all $x \perp \mathrm{Ker}(T-\lambda)$, $x \in D(T)$ we have $\|x\| \leq C\|(T-\lambda)x\|$. For $x \in D(T) \cap \mathrm{Ker}(T-\lambda)^{\perp}$ we have

$$\langle (T-\lambda)x, Px\rangle = \langle x, (T-\lambda)Px\rangle = 0,$$

so that, using this orthogonality in the last equality,

$$\begin{aligned} \|x\|^2 &= \|(1-P)x\|^2 + \|Px\|^2 \leq C^2\|(T-\lambda)x\|^2 + \|Px\|^2 \\ &\leq \max(C^2,1)\big(\|(T-\lambda)x\|^2 + \|Px\|^2\big) = \max(C^2,1)\, \|(T+P-\lambda)x\|^2. \end{aligned}$$

This implies that $T+P-\lambda$ has a bounded inverse, so that $\lambda \in \rho(T+P)$ or $\lambda \notin \sigma_{ess}(T)$.

Now the claim can be used to finish the proof as follows. We have to show that $\{x_n\}_{n=1}^{\infty}$ does not have a convergent subsequence. Suppose, that it does have a convergent subsequence, which we denote by $\{x_n\}_{n=1}^{\infty}$ as well, and say that $x_n \to x$. Then $\|x\| = 1$, and $x \in \mathrm{Ker}(T-\lambda)^{\perp}$. On the other hand, $(T-\lambda)x_n \to 0$, and since $T$ is self-adjoint, hence closed, we see that $T-\lambda$ is closed. This means that $x \in D(T)$ and $x \in \mathrm{Ker}(T-\lambda)$. So $x \in \mathrm{Ker}(T-\lambda)\cap\mathrm{Ker}(T-\lambda)^{\perp} = \{0\}$, which contradicts $\|x\| = 1$. $\square$

The essential spectrum can be obtained from the spectrum by "throwing out the point spectrum". Below we mean by an isolated point $\lambda$ of a subset $\sigma$ of $\mathbb{R}$ that there does not exists a sequence $\{\lambda_n\}_{n=1}^{\infty}$ of points in $\sigma$ such that $\lambda_n \to \lambda$ in $\mathbb{R}$.

**Theorem 6.5.5.** *Let $(T, D(T))$ be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then we have*

1. *If $\lambda \in \sigma(T)\backslash\sigma_{ess}(T)$, then $\lambda$ is an isolated point in $\sigma(T)$.*

*2. If $\lambda \in \sigma(T)\backslash\sigma_{ess}(T)$, then $\lambda \in \sigma_p(T)$.*

*Proof.* To prove the first statement assume that $\lambda$ is not isolated in $\sigma(T)$, so there exists a sequence $\{\lambda_n\}_{n=1}^\infty$, $\lambda_n \neq \lambda$, $\lambda_n \in \sigma(T)$ and $\lambda_n \to \lambda$. By invoking Theorem 6.5.1 we can find for each $n \in \mathbb{N}$ an element $x_n \in \mathcal{H}$ such that $\|x_n\| = 1$ and $\|(T-\lambda_n)x_n\| < \frac{1}{n}|\lambda-\lambda_n|$ for $n \in \mathbb{N}$. Then

$$\|(T-\lambda)x_n\| \leq \|(T-\lambda_n)x_n\| + |\lambda-\lambda_n|\,\|x\| < (1+\frac{1}{n})\,|\lambda-\lambda_n| \to 0, \qquad n \to \infty,$$

In order to show that $\lambda \in \sigma_{ess}(T)$, we can use Theorem 6.5.4. It suffices to show that the constructed sequence $\{x_n\}_{n=1}^\infty$ has no convergent subsequence. So suppose it does have a convergent subsequence, again denoted by $\{x_n\}_{n=1}^\infty$, say $x_n \to x$. Then $\|x\| = 1$, and by closedness of $T-\lambda$, $x \in D(T)$ and $x \in \mathrm{Ker}(T-\lambda)$. On the other hand,

$$\begin{aligned} &|(\lambda-\lambda_n)|\,|\langle x_n, x\rangle| = |\langle x_n, \lambda x\rangle - \lambda_n \langle x_n, x\rangle| = |\langle x_n, Tx\rangle - \lambda_n \langle x_n, x\rangle| \\ =\,&|\langle (T-\lambda_n)x_n, x\rangle| \leq \frac{1}{n}|\lambda-\lambda_n| \end{aligned}$$

and since $\lambda \neq \lambda_n$ we see that $\langle x_n, x\rangle \to 0$. But by assumption $\langle x_n, x\rangle \to \|x\|^2 = 1$, so this give the required contradiction.

For the second statement we use Theorem 6.5.1 to get a sequence $\{x_n\}_{n=1}^\infty$ such that $\|x_n\| = 1$ and $(T-\lambda)x_n \to 0$. Since $\lambda \notin \sigma_{ess}(T)$, Theorem 6.5.4 implies that this sequence must have a convergent subsequence, again denoted $\{x_n\}_{n=1}^\infty$ with $x_n \to x$. Since $T$ is self-adjoint, $T-\lambda$ is closed and hence $x \in D(T)$ and $(T-\lambda)x = 0$. Now $\|x\| = 1$ shows that $\mathrm{Ker}(T-\lambda)$ is non-trivial, and hence $\lambda \in \sigma_p(T)$. □

## 6.6 Absolutely continuous and singular spectrum

Let $\lambda$ denote Lebesgue measure restricted to the $\sigma$-algebra of the Borel sets on $\mathbb{R}$. An arbitrary measure in this Section is a finite complex measure. Recall that a measure $\mu$ is absolutely continuous (with respect to Lebesgue measure $\lambda$) if for all Borel sets $B$ with $\lambda(B) = 0$ we have $\mu(B) = 0$, and the measure $\mu$ is singular (with respect to Lebesgue measure $\lambda$) if there exists a Borel set $Z$ such that $\lambda(Z) = 0$ and $\mu(Z^c) = 0$, where $Z^c = \mathbb{R}\backslash Z$ is its complement in $\mathbb{R}$. So the singular measure is supported on $Z$. The Lebesgue Decomposition Theorem states that any measure $\mu$ can be uniquely decomposed as $\mu = \mu_{ac} + \mu_s$ with $\mu_{ac}$ absolutely continuous and $\mu_s$ singular. Knowing the support $Z$ of the singular measure, the Lebesgue decomposition is given by $\mu_s(B) = \mu(B \cap Z)$, $\mu_{ac}(B) = \mu(B \cap Z^c)$ for any Borel set $B$. Also, the sum of two absolutely continuous, respectively singular, measures is again absolutely continuous, respectively singular.

Recall that for a self-adjoint operator $(T, D(T))$ the Spectral Theorem 6.4.1 gives a finite complex measure $E_{x,y}$ for any pair $x, y \in \mathcal{H}$ by $E_{x,y}(B) = \langle E(B)x, y\rangle$, where $E$ is the spectral measure, and in case $x = y$ we have that $E_{x,x}$ is a positive measure.

**Definition 6.6.1.** *Given a self-adjoint operator $(T, D(T))$ we define*

$$\begin{aligned}\mathcal{H}_{ac} &= \mathcal{H}_{ac}(T) = \{x \in \mathcal{H} \mid E_{x,x} \text{ is absolutely continuous}\},\\ \mathcal{H}_{s} &= \mathcal{H}_{s}(T) = \{x \in \mathcal{H} \mid E_{x,x} \text{ is singular}\}.\end{aligned}$$

*$\mathcal{H}_{ac}$ is the absolutely continuous subspace and $\mathcal{H}_s$ is the singular subspace.*

We call $x \in \mathcal{H}_{ac}$ an absolutely continuous element, and $x \in \mathcal{H}_s$ a singular element of $\mathcal{H}$.

**Theorem 6.6.2.** *Consider a self-adjoint operator $(T, D(T))$ on $\mathcal{H}$, then*

1. *$\mathcal{H} = \mathcal{H}_{ac} \oplus \mathcal{H}_s$, so in particular $\mathcal{H}_{ac}$ and $\mathcal{H}_s$ are closed subspaces,*
2. *$\mathcal{H}_{ac}$ and $\mathcal{H}_s$ reduce $T$.*

Recall the definition of reducing spaces as in Definition 3.2.10 for the second statement. Using Theorem 6.6.2(2) we can define the absolutely continuous spectrum of a self-adjoint operator $(T, D(T))$ as $\sigma_{ac}(T) = \sigma(T\big|_{\mathcal{H}_{ac}})$ and the singular spectrum $\sigma_s(T) = \sigma(T\big|_{\mathcal{H}_s})$. Using Theorem 6.6.2 it follows that $\sigma(T) = \sigma_{ac}(T) \cup \sigma_s(T)$.

*Proof.* First observe that, using $\langle E(B)x, y\rangle = \langle E(B)x, E(B)y\rangle$ since $E(B)$ is self-adjoint projection, we have

$$|\langle E(B)x, y\rangle|^2 \leq \langle E(B)x, x\rangle \langle E(B)y, y\rangle \tag{6.6.1}$$

by the Cauchy-Schwarz inequality (6.1.1). Now (6.6.1) shows that for $x \in \mathcal{H}_{ac}$ and any Borel set $B$ with $\lambda(B) = 0$ we also have $\langle E(B)x, y\rangle = 0$, or $E_{x,y}$ is absolutely continuous. If $x \in \mathcal{H}_s$ we have a Borel set $B$ such that $\lambda(B) = 0$ and $E_{x,x}(B^c) = 0$, and (6.6.1) implies that $E_{x,y}(B^c) = 0$ as well, so $E_{x,y}$ is singular as well.

Observe that $E_{cx,cx} = |c|^2 E_{x,x}$ for any $c \in \mathbb{C}$, so that with $x$ also $cx$ are in $\mathcal{H}_{ac}$, respectively $\mathcal{H}_c$. Next let $x, y \in \mathcal{H}_{ac}$, then for any Borel set $B$

$$E_{x+y,x+y}(B) = \langle E(B)(x+y), x+y\rangle = \langle E(B)x, x\rangle + \langle E(B)y, y\rangle + \langle E(B)x, y\rangle + \langle E(B)y, x\rangle$$

and the first two measures are absolutely continuous by assumption, and the last two are absolutely continuous by the reasoning in the previous paragraph. So $x + y \in \mathcal{H}_{ac}$. Similarly, $\mathcal{H}_s$ is a linear space.

To see that $\mathcal{H}_{ac} \perp \mathcal{H}_s$ take $x \in \mathcal{H}_{ac}$, $y \in \mathcal{H}_s$ and consider the measure $E_{x,y}$. This measure is absolutely continuous, since $x \in \mathcal{H}_{ac}$, and singular, since $y \in \mathcal{H}_s$, so it has to be the measure identically equal to zero. So $\langle E(B)x, y\rangle = 0$ for all Borel sets $B$, and taking $B = \mathbb{R}$ and recalling $E(\mathbb{R}) = 1$ in $B(\mathcal{H})$, we see that $\langle x, y\rangle = 0$.

To finish the proof of the first statement we show that any element, say $z \in \mathcal{H}$, can be written as $z = x + y$ with $x \in \mathcal{H}_{ac}$ and $y \in \mathcal{H}_s$. Use the Lebesgue decomposition theorem to write $E_{z,z} = \mu_{ac} + \mu_s$, and let $Z$ be the Borel set such that $\lambda(Z) = 0$ and $\mu_s(Z^c) = 0$. Put $x = E(Z^c)z$, $y = E(Z)z$, and it remains to show that these elements are the required ones.

First, $x + y = E(Z)z + E(Z^c)z = E(\mathbb{R})z = z$ by additivity of the spectral measure. Next for an arbitrary Borel set $B$

$$\begin{aligned} E_{x,x}(B) &= \langle E(B)x, x\rangle = \langle E(B)E(Z^c)z, E(Z^c)z\rangle \\ &= \langle E(Z^c)E(B)E(Z^c)z, z\rangle = \langle E(B \cap Z^c)z, z\rangle = E_{z,z}(B \cap Z^c), \end{aligned}$$

so that $E_{x,x} = \mu_{ac}$ and hence $x \in \mathcal{H}_{ac}$. Similarly, $y \in \mathcal{H}_s$.

To prove the second statement, we take $z \in D(T) \subset \mathcal{H}$ and write $z = x + y$, $x \in \mathcal{H}_{ac}$, $y \in \mathcal{H}_s$. We claim that $x, y \in D(T)$. To see this, recall that $E_{x,x}$, $E_{y,y}$ and $E_{z,z}$ are positive measures satisfying $E_{z,z} = E_{x,x} + E_{y,y}$, so that

$$\int_{\mathbb{R}} \lambda^2 \, dE_{x,x}(\lambda) \leq \int_{\mathbb{R}} \lambda^2 \, dE_{z,z} < \infty,$$

implying that $x \in D(T)$ using the Spectral Theorem 6.4.1. Similarly, $y \in D(T)$. For $x \in D(T) \cap \mathcal{H}_{ac}$, $y \in \mathcal{H}$, we have, again by the Spectral Theorem 6.4.1,

$$E_{Tx,y}(B) = \int_B \lambda \, dE_{x,y}, \tag{6.6.2}$$

so that $E_{Tx,y}$ is absolutely continuous with respect to $E_{x,y}$, in fact its Radon-Nikodym derivative is $\lambda$. Since $E_{x,y}$ is absolutely continuous, it follows that $E_{Tx,Tx}$ –take $y = Tx$– is absolutely continuous, hence $Tx \in \mathcal{H}_{ac}$. We can reason in a similar way for the singular subspace $H_s$, or we can use the first statement and $T$ being self-adjoint to see that $T\colon D(T) \cap \mathcal{H}_s \to \mathcal{H}_s$. □

In case $T$ has an eigenvector $x$ for the eigenvalue $\lambda$, then $E_{x,x}$ is a measure with $E_{x,x}(\{\lambda\}) > 0$ and $E_{x,x}(\mathbb{R}\backslash\{\lambda\}) = 0$. So in particular, all eigenspaces are contained in $\mathcal{H}_s$. Define $\mathcal{H}_{pp} = \mathcal{H}_{pp}(T)$ as the closed linear span of all eigenvectors of $T$, so that $\mathcal{H}_{pp} \subset \mathcal{H}_s$. Again, $\mathcal{H}_{pp}$ reduces $T$. We denote by $\mathcal{H}_{cs} = \mathcal{H}_{cs}(T)$ the orthocomplement of $\mathcal{H}_{pp}$ in $\mathcal{H}_s$, then $\mathcal{H}_{cs}$ also reduces $T$. So we get the decomposition

$$\mathcal{H} = \mathcal{H}_{pp} \oplus \mathcal{H}_{cs} \oplus \mathcal{H}_{ac}.$$

Here 'pp' stands for 'pure point' and 'cs' for 'continuous singular'. Since these spaces reduce $T$, we have corresponding spectra, $\sigma_{pp}(T) = \sigma(T\big|_{\mathcal{H}_{pp}})$ and $\sigma_{sc}(T) = \sigma(T\big|_{\mathcal{H}_{sc}})$. In general, $\sigma_{pp}(T)$ is not equal to $\sigma_p(T)$, but $\sigma_{pp}(T) = \overline{\sigma_p(T)}$.

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