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Weyl–Titchmarsh–Kodaira Theory for Dirac Operators with Strongly Singular Potentials

Verfasser

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"Mathematics knows no races or geographic boundaries;
for mathematics, the cultural world is one country."
David Hilbert, 1862–1943

ABSTRACT

The objective of the present work is to develop Weyl–Titchmarsh–Kodaira theory for one-dimensional Dirac operators with strongly singular potentials. In particular, we will show how to define a (singular) Weyl function in this case. Furthermore, we will establish an associated spectral transformation which maps our one-dimensional Dirac operator to a multiplication operator and we will show how the essential supports for the Lebesgue decomposition of the spectral measure can be obtained from the boundary behavior of the singular Weyl function. Moreover, we will derive an integral representation for the singular Weyl function and give a criterion when it is a generalized Nevanlinna function. If the endpoint a is limit circle, the singular Weyl function will turn out to be a Herglotz–Nevanlinna function. Finally, we will apply some of our results to a prototypical example of a Dirac operator with a strongly singular potential, namely the radial Dirac operator with a Coulomb potential which describes an electron in the electromagnetic field of a point nucleus.

ZUSAMMENFASSUNG

Das Ziel der vorliegenden Arbeit ist es, Weyl–Titchmarsh–Kodaira Theorie für eindimensionale Dirac Operatoren mit stark singulären Potentialen zu entwickeln. Insbesondere werden wir zeigen, wie man in diesem Fall eine (singuläre) Weyl Funktion definieren kann. Weiters werden wir eine zugehörige Spektraltransformation angeben, die unseren eindimensionalen Dirac Operator auf einen Multiplikationsoperator abbildet, und zeigen, wie man die wesentlichen Träger für die Lebesgue Zerlegung des Spektralmaßes aus dem Randverhalten der singulären Weyl Funktion erhalten kann. Darüberhinaus werden wir eine Integraldarstellung für die singuläre Weyl Funktion ableiten und ein Kriterium angeben, wann sie eine verallgemeinerte Nevanlinna Funktion ist. Liegt am Endpunkt a der Grenzkreisfall vor, so wird sich zeigen, dass die singuläre Weyl Funktion eine Herglotz–Nevanlinna Funktion ist. Schließlich werden wir einige unserer Resultate auf ein typisches Beispiel eines Dirac Operators mit einem stark singulären Potential anwenden, nämlich auf den radialen Dirac Operator mit Coulomb Potential, der ein Elektron im elektromagnetischen Feld eines punktförmigen Kerns beschreibt.

Contents

Chapter 0

Introduction

This thesis deals with the one-dimensional Dirac operator which provides a description of spin-1/2 particles (such as, e.g., electrons). It is consistent with the theory of quantum mechanics as well as with special relativity.

The differential expression for the one-dimensional Dirac operator is given by

$$\tau = \frac{1}{\mathrm{i}}\sigma_2 \frac{d}{dx} + \phi, \qquad x \in (a, b) \tag{1}$$

where ϕ represents a potential (cf. Definition 1.1). A self-adjoint operator H can be obtained from τ if one restricts its domain by imposing additional boundary conditions (if necessary, cf. Section 1.4).

The objective is to develop Weyl–Titchmarsh–Kodaira theory for the case of Dirac operators where both endpoints, a and b, are singular (cf. Definition 1.11). If at least one endpoint, say a, is regular, one can choose a boundary condition at this endpoint and introduce two solutions $c(z, x)$ and $s(z, x)$ of the Dirac differential equation $\tau u = zu$, $z \in \mathbb{C}$ which are entire with respect to z such that the solution $s(z, x)$ satisfies the boundary condition at the regular endpoint a and such that the Wronskian (cf. Definition 1.5) of these solutions satisfies $W(c(z), s(z)) = 1$.

If one has given such a system of solutions, one can define the so-called Weyl–Titchmarsh m-function $m(z)$ via the requirement that the solution $u_+(z, x)$ given by

$$u_+(z, x) = c(z, x) + m(z)s(z, x) \tag{2}$$

lies in the domain of H near b (cf. Section 1.5). The function $m(z)$ is a Herglotz–Nevanlinna function. A corresponding spectral measure $d\mu$ such that H is unitarily equivalent to multiplication by the identity function in $L^2(\mathbb{R}, d\mu)$ can be obtained from $m(z)$ by use of the Stieltjes inversion formula (cf. Theorem B.5).

If neither endpoint is regular, one can still consider some point $c \in (a, b)$ and obtain similar results, but then one has to deal with two by two Weyl matrices (cf. [We03]). This is unavoidable if the spectral multiplicity is two. The question is now if there are cases where a single function is sufficient and a singular Weyl function $M(z)$ can be introduced.

In order to define $M(z)$, we have to find an entire system of linearly independent solutions $\phi(z,x)$ and $\theta(z,x)$ of the Dirac equation $\tau u = zu$, $z \in \mathbb{C}$ such that $W(\theta(z), \phi(z)) = 1$. To make the connection with H, one solution, say $\phi(z,x)$, has to be chosen such that it lies in the domain of H near a. Similarly as above, once the system $\phi(z,x)$ and $\theta(z,x)$ is given, we can define $M(z)$ by requiring that

$$\psi(z,x) = \theta(z,x) + M(z)\phi(z,x) \tag{3}$$

lies in the domain of H near the endpoint b.

This is the starting point for the present work. It has been shown how to construct such a system of solutions if H is a one-dimensional Schrödinger operator (cf. [KST11]). The same construction works for Dirac operators as well after some small modifications. In particular, as in [KST11], the requirement that the spectrum of H restricted to some subinterval $(a,c) \subset (a,b)$ is purely discrete is necessary and sufficient for the existence of $\phi(z,x)$. We will construct the second solution $\theta(z,x)$ explicitly by use of the Mittag–Leffler theorem from complex analysis.

We will follow [KST11] and extend the main results to the case of one-dimensional Dirac operators. Sometimes, this turns out to be quite easy whereas sometimes, one needs more effort. We will reproduce the results of Section 2–4 and Appendix A, that is, in particular, we will establish a spectral transformation and investigate certain properties of $M(z)$. Furthermore, we will provide an example, the radial Dirac operator with a Coulomb potential, in order to illustrate some of our results. Below one can find a description of the content of each chapter.

Chapter 1 provides a short overview of one-dimensional Dirac operators. We will recall some basic definitions and see how to obtain a self-adjoint operator. Furthermore, we will have a look at the Weyl m-functions. The information provided in this chapter is essentially collected from [St10], [Te09], [Te98], [Tim95], [Th92] and [We03].

Chapter 2 is devoted to spectral theory for self-adjoint operators. The central object in this chapter is the spectral theorem. During considerations concerning the spectral theorem we will see that it is necessary to understand certain multiplication operators. Furthermore, we will have a look at the different spectral types. This chapter is a summary of [Te09, Chapter 3].

In **Chapter 3** we will construct a system of solutions of the Dirac equation such that one solution lies in the domain of H near the (in general singular) endpoint a and such that the Wronskian of the two solutions equals one. This will allow us to define a singular Weyl function. This chapter has to be compared with [KST11, Section 2].

In **Chapter 4** we will associate a measure with the singular Weyl function defined in Chapter 2 by making use of the Stieltjes inversion formula. We will establish a spectral transformation, that is, a unitary transformation which maps our one-dimensional Dirac operator to a multiplication operator. This will allow us to read off the different spectral types from the boundary behavior of the singular Weyl function as usual. In particular, we extend [KST11, Section 3] to the case of Dirac operators.

The aim of **Chapter 5** is to derive some properties of the singular Weyl function defined in Chapter 2. We will establish an integral representation, we will show that there is always a system of solutions such that the singular Weyl function is a Herglotz–Nevanlinna function and we will give a criterion when the singular Weyl function is a generalized Nevanlinna function with no nonreal poles and the only generalized pole of nonpositive type at infinity. In particular, the results included in this chapter have the same form as those from [KST11, Chapter 4].

In **Chapter 6** we will see how our considerations simplify in the special case where the endpoint a is limit circle and show that the singular Weyl function is a Herglotz–Nevanlinna function this case. This chapter is a generalization of [KST11, Appendix A].

In **Chapter 7** we consider the radial Dirac operator with a Coulomb potential which is an example of a Dirac operator with a strongly singular potential, that is, a potential with two singular endpoints. We will use this example to illustrate some of the results from the previous chapters. Our presentation in this chapter mainly follows [GTV07, Section 3].

The purpose of **Appendix A** is to recall some facts from Complex Analysis which are used throughout this theses. In particular, we give a proof of Weierstrass' product theorem and the theorem of Mittag-Leffler. The material included in this chapter is collected from [Mar85].

Appendix B provides some information about Herglotz–Nevanlinna and generalized Nevanlinna functions by compiling facts from [KST11], [Te09] and [Tim95].

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Last, but not least I wish to express my gratitude to my parents for supporting me in every way and to all my friends who have always been there when I needed them.

Chapter 1

A brief overview of Dirac operators

In this chapter we are going to recall some basic facts about Dirac operators. We will introduce the differential expression for the one-dimensional Dirac operator and give some information about the solutions of the underlying Dirac equation. We will discuss the behavior of these solutions at the boundary, shed some light at possible boundary conditions and we will see how to obtain a self-adjoint operator. Furthermore, we deal with the resolvent and the so-called Weyl m-functions. All material contained in this chapter is essentially collected from [St10], [Te09], [Te98], [Tim95], [Th92] and [We03]. Other good references are [LS91] and [We87].

1.1 The Dirac differential expression

In order to give a proper definition of the Dirac differential expression and to discuss its properties we need to introduce some notations and to recall some function spaces first.

(i) We write $(a, b) \subseteq \mathbb{R}$ for an arbitrary open interval with $-\infty \leq a < b \leq \infty$.

(ii) In $\mathbb{C}^2$ we will use the inner product

$$(u, v) = \langle u, v \rangle_{\mathbb{C}^2} = u_1^* v_1 + u_2^* v_2, \qquad u, v \in \mathbb{C}^2 \tag{1.1}$$

and the corresponding norm $\|u\|_{\mathbb{C}^2} = \sqrt{(u, u)}$.

(iii) Furthermore, we define the tensor product $u \otimes v \in \mathbb{C}^2$ of two vectors $u, v \in \mathbb{C}^2$ by

$$u \otimes v = \begin{pmatrix} u_1 v_1 & u_1 v_2 \\ u_2 v_1 & u_2 v_2 \end{pmatrix}. \tag{1.2}$$

(iv) By σ_1, σ_2 and σ_3 we denote the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.3}$$

(v) We write $L^1_{loc}((a,b),\mathbb{R})$ for the space of (equivalence classes of) locally integrable functions $f:(a,b)\to\mathbb{R}$, that is, the set of measurable functions $f:(a,b)\to\mathbb{R}$ which satisfy $\int_K |f(x)|dx<\infty$ for every compact set $K\subset(a,b)$.

(vi) By $AC_{loc}((a,b),\mathbb{C}^2)$ we denote the set of (equivalence classes of) functions $f:(a,b)\to\mathbb{C}^2$ which are locally absolutely continuous (i.e., both components f_j, $j=1,2$ are locally absolutely continuous). A function is absolutely continuous if and only if it can be written as the integral of some (locally) integrable function.

(vii) As Hilbert space we will use $L^2((a,b),\mathbb{C}^2)$, that is, the space (of equivalence classes) of square integrable functions $f:(a,b)\to\mathbb{C}^2$ (i.e., both components f_j, $j=1,2$ are square integrable), equipped with the inner product

$$\langle f,g\rangle_{L^2((a,b),\mathbb{C}^2)}=\int_a^b \left(f_1^*(x)g_1(x)+f_2^*(x)g_2(x)\right)dx,\qquad f,g\in L^2((a,b),\mathbb{C}^2)$$

and the corresponding norm $\|f\|_{L^2((a,b),\mathbb{C}^2)}=\sqrt{\langle f,f\rangle_{L^2((a,b),\mathbb{C}^2)}}$.

Now we are ready to introduce the differential expression for the one-dimensional Dirac operator.

Definition 1.1 (Dirac differential expression)**.** *A differential expression τ is called Dirac differential expression on (a,b) if it is of the form*

$$\tau=\frac{1}{\mathrm{i}}\sigma_2\frac{d}{dx}+\phi,\qquad x\in(a,b)\tag{1.4}$$

where $\phi\in\mathbb{R}^{2\times2}$ is a symmetric matrix.

The matrix ϕ represents a potential. It is given by

$$\phi(x)=\phi_{\mathrm{el}}(x)\mathbb{1}+\phi_{\mathrm{am}}(x)\sigma_1+(m+\phi_{\mathrm{sc}}(x))\sigma_3\tag{1.5}$$

and includes the mass m of the observed particle, the scalar potential ϕ_{sc}, the electrostatic magnetic moment ϕ_{el} and the anomalous magnetic moment ϕ_{am}. We require $m\in[0,\infty)$ and $\phi_{\mathrm{sc}},\phi_{\mathrm{el}},\phi_{\mathrm{am}}\in L^1_{loc}((a,b),\mathbb{R})$.

Explicitly, τ reads

$$\tau f=\begin{pmatrix}\phi_{11} & -\frac{d}{dx}+\phi_{12}\\ \frac{d}{dx}+\phi_{12} & \phi_{22}\end{pmatrix}\begin{pmatrix}f_1\\ f_2\end{pmatrix}=\begin{pmatrix}-f_2'+\phi_{12}f_2+\phi_{11}f_1\\ f_1'+\phi_{12}f_1+\phi_{22}f_2\end{pmatrix},\quad f\in AC_{loc}((a,b),\mathbb{C}^2)$$

where primes denote derivatives with respect to x and $\phi_{11}=\phi_{\mathrm{el}}+m+\phi_{\mathrm{sc}}$, $\phi_{12}=\phi_{21}=\phi_{\mathrm{am}}$, $\phi_{22}=\phi_{\mathrm{el}}-m-\phi_{\mathrm{sc}}$.

Remark 1.2. *The maximal domain of definition on which τ makes sense is given by*

$$\mathfrak{D}(\tau)=\{f\in L^2((a,b),\mathbb{C}^2)|f\in AC_{loc}((a,b),\mathbb{C}^2),\ \tau f\in L^2((a,b),\mathbb{C}^2)\}.\tag{1.6}$$

1.2 The Dirac differential equation

We are now interested in the solutions of the homogeneous Dirac equation

$$(\tau - z)u = 0, \qquad z \in \mathbb{C}. \tag{1.7}$$

Definition 1.3 (Solutions of the Dirac equation)**.** *We call a function $u : (a,b) \to \mathbb{C}^2$ a solution of (1.7) if $u \in AC_{loc}((a,b),\mathbb{C}^2)$ and $\tau u(z,x) = zu(z,x)$ is satisfied for almost every $x \in (a,b)$.*

The following theorem provides some information about the existence and uniqueness of solutions of the inhomogeneous Dirac equation.

Theorem 1.4 ([We03, Corollary 15.2])**.** *Suppose $g \in L^1_{loc}((a,b),\mathbb{C}^2)$. Then for all $z \in \mathbb{C}$, $x_0 \in (a,b)$ and $(y_1,y_2) \in \mathbb{C}^2$ the initial value problem*

$$(\tau - z)u = g, \qquad g(x_0) = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \tag{1.8}$$

is uniquely solvable. Furthermore, for all $x \in (a,b)$ the solution $u(z,x)$ is an entire function with respect to z.

The solutions of the homogeneous Dirac equation form a two-dimensional vector space.

Definition 1.5 (Wronski determinant)**.** *The Wronski determinant or Wronskian $W_x(u,v)$ of two functions $u, v \in \mathfrak{D}(\tau)$ is defined by*

$$W_x(u,v) = \det\begin{pmatrix} u_1(x) & v_1(x) \\ u_2(x) & v_2(x) \end{pmatrix} = \mathrm{i}\,(u(x)^*, \sigma_2 v(x)) = u_1(x)v_2(x) - u_2(x)v_1(x). \tag{1.9}$$

Furthermore, we define $W_a(u,v) = \lim_{x\to a} W_x(u,v)$ and $W_b(u,v) = \lim_{x\to b} W_x(u,v)$ whenever these limits exist.

Two solutions of (1.7) form a fundamental system of solutions of (1.7) if and only if their Wronskian does not vanish.

Lemma 1.6 (cf. [We03, p121])**.** *The Wronskian $W_x(u(z),v(z))$ of two solutions $u(z,x)$ and $v(z,x)$ of (1.7) is independent of x. In this case we write $W(u(z),v(z))$ instead of $W_x(u(z),v(z))$.*

Proof. The straightforward calculation

$$\begin{aligned} W_x(u(z),v(z))' &= (u_1(z,x)v_2(z,x) - u_2(z,x)v_1(z,x))' \\ &= \left(\frac{1}{\mathrm{i}}\sigma_2\frac{d}{dx}u(z,x)^*, v(z,x)\right) + \left(u(z,x)^*, \frac{1}{\mathrm{i}}\sigma_2\frac{d}{dx}v(z,x)\right) \\ &= ((z^*\mathbb{1} - \phi(x))u(z,x)^*, v(z,x)) + (u(z,x)^*, (z\mathbb{1} - \phi(x))v(z,x)) = 0 \end{aligned}$$

shows that the derivative of $W_x(u(z),v(z))$ with respect to x vanishes which clearly means that $W_x(u(z),v(z))$ is independent of x. □

Lemma 1.7 (cf. [We03, p122])**.** *Suppose $g \in L^1_{loc}((a,b),\mathbb{C}^2)$. Let $u_1(x)$ and $u_2(x)$ be a fundamental system of solutions of $(\tau - z_0)u = 0$ which satisfies $W(u_1,u_2) = 1$. Then all solutions of $(\tau - z)u = g$ are given by*

$$u(x) = \alpha u_1(x) + \beta u_2(x) + u_2(x)\int_c^x (u_1(y)^*, g(y))\, dy - u_1(x)\int_c^x (u_2(y)^*, g(y))\, dy \quad (1.10)$$

where $c \in (a,b)$ and $\alpha, \beta \in \mathbb{C}$ are constants.

Proof. This claim can be proved by using the method of variation of constants or simply by a straightforward calculation. □

Remark 1.8. *A fact which will turn out to be very useful later on is that the identity (the so-called Plücker identity)*

$$W_x(f_1,f_2)W_x(f_3,f_4) + W_x(f_1,f_3)W_x(f_4,f_2) + W_x(f_1,f_4)W_x(f_2,f_3) = 0 \quad (1.11)$$

holds for all $f_1, f_2, f_3, f_4 \in \mathfrak{D}(\tau)$.

1.3 Limit circle, limit point alternative

We will now shed some light at the possible behavior of the solutions of the homogeneous Dirac equation (1.7) at the endpoints a and b.

Definition 1.9 (Square integrable functions near an endpoint)**.** *Suppose $f : (a,b) \to \mathbb{C}^2$ is a measurable function.*

(i) The function f is said to be square integrable near a if there is some $c \in (a,b)$ such that $f|_{(a,c)} \in L^2((a,c),\mathbb{C}^2)$.

(ii) Analogously, f is said to be square integrable near b if there is some $c \in (a,b)$ such that $f|_{(c,b)} \in L^2((c,b),\mathbb{C}^2)$.

As we will always apply these definitions to solutions of (1.7), they hold either for all or for no $c \in (a,b)$.

Theorem 1.10 ([We03, Theorem 15.14])**.** *Suppose τ is a Dirac differential expression on (a,b). If every solution of of $(\tau - z_0)u = 0$ is square integrable near a (respectively b) for one $z_0 \in \mathbb{C}$, then every solution of $(\tau - z)u = 0$ is square integrable near a (respectively b) for all $z \in \mathbb{C}$.*

Proof. A proof is given in [We03] on page 55 for Sturm-Liouville expressions. The same proof holds for Dirac expressions if one modifies it like prescribed on page 128 in [We03]. □

Next, we distinguish between regular and singular endpoints. The title and the introduction of the present work may already disclose that we will be interested in potentials with two singular endpoints throughout the following chapters.

Definition 1.11 (Regular respectively singular endpoints). *Suppose τ is a Dirac differential expression on (a,b).*

(i) We call τ regular at a if $a > -\infty$ and if ϕ_{11}, ϕ_{12} and ϕ_{22} are integrable over $[a,c]$ for one/all $c \in (a,b)$. Analogously, we define being regular at b. τ is called regular if τ is regular at a and at b.

(ii) We call τ singular at a (respectively b) if it is not regular at a (respectively b), singular if it is not regular at a or b and strongly singular if it is not regular at a and b.

Concerning the behavior of solutions of (1.7) near the endpoints a respectively b we can distinguish between two cases as well.

Theorem 1.12 (Weyl alternative, [We03, Theorem 15.15]). *For every Dirac differential expression τ on (a,b) we have either*

(i) for all $z \in \mathbb{C}$ every solution of (1.7) is square integrable near a (respectively b), or

(ii) for all $z \in \mathbb{C}$ there exists at least one solution which is not square integrable near a (respectively b). In that case, for every $z \in \mathbb{C} \setminus \mathbb{R}$ there exists a up to a complex multiple uniquely determined solution of $\tau u = zu$ which is square integrable near a (respectively b).

Proof. A proof is given in [We03] on page 55 for the case that τ is a Sturm-Liouville expression. This proof also holds for the case that τ is a Dirac expression after the slight modification prescribed in [We03] on page 129. □

Definition 1.13 (Limit circle, limit point). *If (i) holds, we will say that τ is limit circle at a (respectively b). If (ii) holds, we call τ limit point at a (respectively b).*

The terms limit circle and limit point originate in the approach of Hermann Weyl. He considered the set of solutions of $\tau u = zu,\ z \in \mathbb{C} \setminus \mathbb{R}$ satisfying $W_x(u^*, u) = 0$. They lie on a circle which converges to a circle or a point as $x \to a$ or $x \to b$.

Theorem 1.14 ([Tim95, Theorem A.4]). *Let τ be a Dirac differential expression on (a,b).*

(i) If τ is regular at a (respectively b), then τ is limit circle at a (respectively b).

(ii) If $a = -\infty$ (respectively $b = \infty$), then τ is limit point at a (respectively b).

Proof. (i) At a regular endpoint, we are able to extend any solution of (1.7) continuously to this endpoint which means that it is therefore square integrable at this endpoint.
(ii) We show the second claim for the endpoint b. For the endpoint a the claim can be proved analogously. Let $b = \infty$. Suppose we had the limit circle case at b. Then there are two linearly independent solutions $u, v \in L^2((c,b), \mathbb{C}^2)$ of $\tau u = 0$. From the estimate

$$|W_x(u,v)| \leq |u_1(x)v_2(x)| + |u_2(x)v_1(x)| \leq |u_1(x)|^2 + |u_2(x)|^2 + |v_1(x)|^2 + |v_2(x)|^2$$

we obtain $W(u,v) \in L^1((c,b), \mathbb{R})$. On the other hand, as u and v satisfy $\tau u = 0$, one infers from the fact that the Wronskian of two solutions is independent of x that $W_x(u,v) \neq 0$ is constant which is a contradiction. □

1.4 Self-adjoint extensions

Our next goal is to obtain a self-adjoint operator associated with τ. Before we proceed, let us recall the definition of a self-adjoint operator.

Definition 1.15 (The adjoint, self-adjointness)**.** *Let $A : \mathfrak{D}(A) \to \mathfrak{H}$ be a linear operator whose domain $\mathfrak{D}(A)$ is dense in the (complex and separable) Hilbert space $\mathfrak{H}$.*

(i) The adjoint operator A^* of A is defined by

$$\mathfrak{D}(A^*) = \{\psi \in \mathfrak{H} | \exists \tilde{\psi} \in \mathfrak{H} : \langle \psi, A\varphi \rangle = \langle \tilde{\psi}, \varphi \rangle \ \forall \varphi \in \mathfrak{H}\}, \tag{1.12}$$

$$A^*\psi = \tilde{\psi}. \tag{1.13}$$

(ii) If we have $A^* = A$, that is, we have $\mathfrak{D}(A^*) = \mathfrak{D}(A)$ and $A\psi = A^*\psi$ for all $\psi \in \mathfrak{D}(A)$, we call A self-adjoint.

Note that any self-adjoint operator is necessarily symmetric which means that the identity $\langle \varphi, A\psi \rangle = \langle A\varphi, \psi \rangle$ holds for all $\varphi, \psi \in \mathfrak{D}(A)$. Using integration by parts yields the Lagrange identity

$$\int_a^b (g(t), (\tau f)(t))\, dt = W_a(g^*, f) - W_b(g^*, f) + \int_a^b ((\tau g)(t), f(t))\, dt \tag{1.14}$$

which shows that any operator associated with τ can only be symmetric if and only if $W_a(g^*, f) = W_b(g^*, f)$ is satisfied for all $g, f \in \mathfrak{D}(\tau)$.

If τ is limit point at both endpoints, a and b, then τ gives rise to a unique self-adjoint operator H when defined maximally (c.f. [LS91], [We87], [We03]). Therefore we do not need any further conditions in this case. If τ is limit circle at a, then let $v \in \mathfrak{D}(\tau)$ with $W_a(v^*, v) = 0$ such that $W_a(v, f) \neq 0$ for some $f \in \mathfrak{D}(\tau)$ and if τ is limit circle at b, then let $w \in \mathfrak{D}(\tau)$ with $W_b(w^*, w) = 0$ such that $W_b(w, f) \neq 0$ for some $f \in \mathfrak{D}(\tau)$. We fix the boundary conditions

$$BC_a(f) = W_a(v, f) \qquad \text{and} \qquad BC_b(f) = W_b(w, f) \tag{1.15}$$

at each endpoint where τ is limit circle. A self-adjoint operator H associated with τ is given by (cf. [St10], [Te98])

$$\begin{array}{rccl} H: & \mathfrak{D}(H) & \to & L^2((a,b), \mathbb{C}^2), \\ & f & \mapsto & \tau f \end{array} \tag{1.16}$$

where

$$\begin{aligned} \mathfrak{D}(H) = \{ f \in L^2((a,b), \mathbb{C}^2) | f \in AC_{loc}((a,b), \mathbb{C}^2), \tau f \in L^2((a,b), \mathbb{C}^2), \\ BC_a(f) = BC_b(f) = 0 \text{ if } \tau \text{ is limit circle at } a \text{ respectively } b\}. \end{aligned} \tag{1.17}$$

Definition 1.16 (Functions lying in the domain of H near an endpoint)**.** *We say that a function $f : (a,b) \to \mathbb{C}^2$ lies in the domain of H near a (respectively b) if f is square integrable near a (respectively b) and fulfills the boundary condition at a (respectively b).*

Next, we recall some definitions concerning the resolvent and the spectrum of an operator.

Definition 1.17 (Resolvents and spectra)**.** *Suppose again $A : \mathfrak{D}(A) \to \mathfrak{H}$ is a linear operator whose domain $\mathfrak{D}(A)$ is dense in the (complex and separable) Hilbert space $\mathfrak{H}$.*

(i) The resolvent set of A is defined by

$$\rho(A) = \{z \in \mathbb{C} | (A - z)^{-1} \in \mathfrak{L}(\mathfrak{H})\} \tag{1.18}$$

where $\mathfrak{L}(\mathfrak{H})$ is the set of all bounded linear operators from $\mathfrak{H}$ to itself. More precisely, $z \in \rho(A)$ if and only if $(A - z) : \mathfrak{D}(A) \to \mathfrak{H}$ is bijective and its inverse is bounded.

(ii) The map

$$\begin{array}{rlcl} R_A : & \rho(A) & \to & \mathfrak{L}(\mathfrak{H}) \\ & z & \mapsto & (A - z)^{-1} \end{array} \tag{1.19}$$

is called the resolvent of A.

(iii) The complement of the resolvent set of A is called the spectrum

$$\sigma(A) = \mathbb{C} \setminus \rho(A) \tag{1.20}$$

of A. The discrete spectrum $\sigma_d(A)$ is the set of all eigenvalues which are discrete points of the spectrum and whose corresponding eigenspaces are finite dimensional. The complement of the discrete spectrum is called the essential spectrum

$$\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A). \tag{1.21}$$

Remark 1.18. *The spectrum of any self-adjoint linear operator A satisfies $\sigma(A) \subseteq \mathbb{R}$.*

Making use of Theorem 1.12 we can already say something about the eigenvalues of the self-adjoint operator H given by (1.16) and (1.17).

Corollary 1.19 ([St10, Corollary 1.11])**.** *All eigenvalues of H are simple.*

Proof. If τ is limit point at a, then there is at most one (linearly independent) solution of (1.7) which is square integrable near a. If τ is limit circle at a, then the Wronskian of two solutions which satisfy the same boundary condition vanishes. Thus they are linearly dependent. The same arguments hold for b. □

Definition 1.20 (Weyl solutions)**.** *We define the Weyl solutions $u_\pm(z, x)$ by the following requirements (whenever such solutions exist):*

(i) $u_\pm(z, .) \in AC_{loc}((a, b), \mathbb{C}^2)$, $\tau u_\pm(z) = z u_\pm(z)$ and $u \not\equiv 0$.

(ii) $u_+(z, .)$ (respectively $u_-(z)$) is square integrable near b (respectively a) and satisfies the boundary condition of H at b (respectively a) if any (i.e., if τ is limit circle at b (respectively a)).

The resolvent $(H-z)^{-1}$ of the self-adjoint operator H given by (1.16) and (1.17) can be expressed in terms of the Weyl solutions $u_\pm(z,.)$ by

$$(H-z)^{-1}f(x) = \int_a^b G(z,x,y)f(y)dy, \qquad z \in \rho(H) \tag{1.22}$$

where

$$G(z,x,y) = \frac{u_\pm(z,x) \otimes u_\mp(z,y)}{W(u_+(z),u_-(z))}, \quad \pm(x-y) > 0 \tag{1.23}$$

denotes the Green function of H (cf. [Te98, Section 1]). Note that $W(u_+(z),u_-(z))$ can only vanish if $u_+(z,.)$ and $u_-(z,.)$ are linearly dependent. This can only be the case if $u_\pm(z,.)$ both exist and satisfy both boundary conditions which is equivalent to $z \in \sigma_d(H)$.

1.5 The Weyl m-functions

We choose an arbitrary, but fixed point $x \in (a,b)$ and call it the base point. We write $H_{x,-}$ and $H_{x,+}$ for self-adjoint operators associated with τ which are obtained by restricting H to (a,x) and (x,b), respectively. Furthermore, we impose the additional boundary condition $f_1(x) = 0$. Let $G_{x,\pm}(z,.,.)$ denote the resolvent kernel of $H_{x,\pm}$. We set $G(z,x,x) = \lim_{\varepsilon\to 0}(G(z,x+\varepsilon,x) + G(z,x-\varepsilon,x))/2$.

Definition 1.21 (Weyl m-functions)**.** *We define the Weyl m-functions $m_{x,\pm}(z)$ (with respect to the base point x) by*

$$G_{x,\pm}(z,x,x) = \begin{pmatrix} 0 & \pm\frac{1}{2} \\ \pm\frac{1}{2} & m_{x,\pm}(z) \end{pmatrix}. \tag{1.24}$$

The Weyl m-functions are Herglotz–Nevanlinna functions. We will now show that the Weyl solutions $u_\pm(z,x)$ exist if we are away from the essential spectrum.

Lemma 1.22 (cf. [Te98, Lemma 1.1])**.** *The solutions $u_\pm(z,x)$ exist for $z \in \mathbb{C}\setminus\sigma_{ess}(H_{x_0,\pm})$. and can be assumed to be real analytic with respect to $z \in \mathbb{C}\setminus\sigma_{ess}(H_{x_0,\pm})$.*

Proof. If $U(z,x,x_0)$, $z \in \mathbb{C}$ is a fundamental matrix solution for (1.7) (i.e., $U(z,x_0,x_0) = \mathbb{1}$, $x_0 \in (a,b)$) and $m_{x_0,\pm}(z)$ are the Weyl m-functions with respect to the base point x_0, we can choose

$$u_\pm(z,x) = U(z,x,x_0)\begin{pmatrix} 1 \\ m_{x_0,\pm}(z) \end{pmatrix}.$$

By removing the corresponding poles of $m_{x_0,\pm}(z)$ we can include any number of isolated eigenvalues in the domain of holomorphy of $u_\pm(z,x)$. This is possible as Weierstrass' theorem (Theorem A.13) does not only hold in the whole complex plane, but also in arbitrary domains $G \subseteq \mathbb{C}$. □

Remark 1.23. *The Weyl solutions $u_\pm(z,x)$ do not only exist for $z \in \mathbb{C}\setminus\sigma_{ess}(H_{x_0,\pm})$, but also if $z \in \sigma_{ess}(H)$ is an eigenvalue.*

From now on we fix $c \in (a, b)$ as our base point. Restricting H to (a, c) and (c, b) yields the operators $H_{(a,c)}$ and $H_{(c,b)}$, respectively. As a fundamental system for (1.7) we choose the functions

$$c(z, x) = \begin{pmatrix} c_1(z, x) \\ c_2(z, x) \end{pmatrix} \quad \text{and} \quad s(z, x) = \begin{pmatrix} s_1(z, x) \\ s_2(z, x) \end{pmatrix} \tag{1.25}$$

which are assumed to be solutions corresponding to the initial conditions

$$c_1(z, c) = 1, \; c_2(z, c) = 0 \quad \text{and} \quad s_1(z, c) = 0, s_2(z, c) = 1. \tag{1.26}$$

Our fundamental matrix solution $U(z, x, x_0)$ from the proof of Lemma 1.22 is then of the form

$$U(z, x, c) = \begin{pmatrix} c_1(z, x) & s_1(z, x) \\ c_1(z, x) & s_2(z, x) \end{pmatrix}, \qquad U(z, c, c) = \mathbb{1}, \tag{1.27}$$

and thus we can define the Weyl solutions

$$u_-(z, x) = \begin{pmatrix} u_{-1}(z, x) \\ u_{-2}(z, x) \end{pmatrix} \quad \text{and} \quad u_+(z, x) = \begin{pmatrix} u_{+1}(z, x) \\ u_{+2}(z, x) \end{pmatrix} \tag{1.28}$$

as usual by

$$\begin{aligned} u_-(z, x) &= c(z, x) - m_-(z)s(z, x), \qquad & z \in \mathbb{C} \setminus \sigma(H_{(a,c)}), \\ u_+(z, x) &= c(z, x) + m_+(z)s(z, x), \qquad & z \in \mathbb{C} \setminus \sigma(H_{(c,b)}). \end{aligned} \tag{1.29}$$

Here, $m_\pm(z)$ are the Weyl m-functions corresponding to the base point c and associated with the operators $H_{(a,c)}$ and $H_{(c,b)}$, respectively. The different sign in front of $m_-(z)$ is introduced such that $m_-(z)$ is a Herglotz–Nevanlinna function as well.

Chapter 2

Spectral theory for self-adjoint operators

The purpose of this chapter is to give an overview of spectral theory for self-adjoint operators. In the first section we are going to deal with the spectral theorem for self-adjoint operators which is in some sense an analogue to the diagonalization of a symmetric matrix. During the considerations towards the spectral theorem we will see that, in order to understand self-adjoint operators, we need to shed some light on certain multiplication operators. Finally, in the last section, we will generalize some results which hold for these multiplication operators to arbitrary self-adjoint operators.

The presentation in this chapter strictly follows [Te09, Chapter 3]. There, more details on this topic and the proofs of the results mentioned in the following sections can be found. In order to refresh the necessary background concerning measure theory, the reader is recommended to have a look at [Te09, Appendix A].

2.1 The spectral theorem

We begin with establishing integration with respect to projection-valued measures and observe that we can assign a self-adjoint operator with every projection-valued measure. We will see that, in further consequence, the converse is also true, that is, we can assign a projection-valued measure P_A, the so-called spectral projection, to any self-adjoint operator A. This fundamental result is known as the spectral theorem for self-adjoint operators as the spectral projection P_A contains all the information about the spectrum of A.

Let $\mathfrak{H}$ be a (complex and separable) Hilbert space which is equipped with the inner product $\langle .,. \rangle$ and the norm $\|.\|$. Furthermore, we denote the Borel sigma algebra of $\mathbb{R}$ by $\mathfrak{B}$.

Definition 2.1 (Projection-valued measures). *A projection-valued measure P is a map*

$$P : \mathfrak{B} \to \mathfrak{L}(\mathfrak{H}), \qquad \Omega \mapsto P(\Omega) \tag{2.1}$$

from the Borel sets to the set of orthogonal projections P, that is, P satisfies $P(\Omega)^* = P(\Omega)$ and $P(\Omega)^2 = P(\Omega)$, such that the following two conditions hold:

(i) $P(\mathbb{R}) = \mathbb{1}$.

(ii) *If* $\Omega = \bigcup_{n=1}^{\infty} \Omega_n$ *with* $\Omega_n \cap \Omega_m = \emptyset$ *for* $n \neq m$*, then* $\sum_{n=1}^{\infty} P(\Omega_n)\psi = P(\Omega)\psi$ *for every* $\psi \in \mathfrak{H}$ *(strong* σ*-additivity).*

Remark 2.2. *Suppose* $\Omega, \Omega_1, \Omega_2 \in \mathfrak{B}$*. For any projection-valued measure* P *the following identities hold:*

(i) $P(\emptyset) = 0$, $P(\mathbb{R} \setminus \Omega) = \mathbb{1} - P(\Omega)$.

(ii) $P(\Omega_1 \cup \Omega_2) + P(\Omega_1 \cap \Omega_2) = P(\Omega_1) + P(\Omega_2)$.

(iii) $P(\Omega_1)P(\Omega_2) = P(\Omega_1 \cap \Omega_2)$.

Futhermore, a projection-valued measure is monotone, that is, $\Omega_1 \subseteq \Omega_2$ *implies* $P(\Omega_1) \leq P(\Omega_2)$ *in the sense that* $\langle \psi, P(\Omega_1)\psi \rangle \leq \langle \psi, P(\Omega_2)\psi \rangle$ *for two Borel sets* Ω_1 *and* Ω_2*.*

With every projection-valued measure we can associate a resolution of the identity

$$P(\lambda) = P((-\infty, \lambda]). \tag{2.2}$$

Recall that a sequence A_n of linear operators which is defined on a dense domain $\mathfrak{D}(A_n) \subset \mathfrak{H}$ is said to converge strongly to a linear operator A (defined on $\mathfrak{D}(A) \subseteq \mathfrak{D}(A_n)$) and write $\text{s-lim}_{n\to\infty} A_n = A$ if we have $A_n\psi \to A\psi$ for every $\psi \in \mathfrak{D}(A) \subseteq \mathfrak{D}(A_n)$.

Remark 2.3. $P(\lambda)$ *has the following properties:*

(i) $P(\lambda)$ *is an orthogonal projection,*

(ii) $P(\lambda_1) \leq P(\lambda_2)$ *for* $\lambda_1 \leq \lambda_2$,

(iii) $\text{s-lim}_{\lambda_n \downarrow \lambda} P(\lambda_n) = P(\lambda)$,

(iv) $\text{s-lim}_{\lambda\to-\infty} P(\lambda) = 0$ *and* $\text{s-lim}_{\lambda\to+\infty} P(\lambda) = \mathbb{1}$.

Choosing $\psi \in \mathfrak{H}$ yields a Borel measure $\mu_\psi(\Omega) = \langle \psi, P(\Omega)\psi \rangle = \|P(\Omega)\|^2$ with $\mu_\psi(\mathbb{R}) = \|\psi\|^2 < \infty$. The distribution function corresponding to μ_ψ is given by $\mu_\psi(\lambda) = \langle \psi, P(\lambda)\psi \rangle$. For every distribution function there is a uniquely determined Borel measure (cf. [Te09, Theorem A.2]) and therefore, for every resolution of the identity there exists a unique projection-valued measure. By invoking the polarization identity, we obtain the complex Borel measures

$$\mu_{\varphi,\psi}(\Omega) = \langle \varphi, P(\Omega)\psi \rangle = \frac{1}{4}(\mu_{\varphi+\psi}(\Omega) - \mu_{\varphi-\psi}(\Omega) + \mathrm{i}\mu_{\varphi-\mathrm{i}\psi}(\Omega) - \mathrm{i}\mu_{\varphi+\mathrm{i}\psi}(\Omega)). \tag{2.3}$$

By the inequality of Cauchy-Schwarz we get $|\mu_{\varphi,\psi}(\Omega)| \leq \|\varphi\|\|\psi\| < \infty$. The next step is to establish integration with respect to our projection-valued measure. First, we define integration with respect to the projection-valued measure P for any simple function $f = \sum_{j=1}^{n} \alpha_j \chi_{\Omega_j}$ (where $\Omega_j = f^{-1}(\alpha_j)$) by setting

$$P(f) \equiv \int_{\mathbb{R}} f(\lambda) dP(\lambda) = \sum_{j=1}^{n} \alpha_j P(\Omega_j). \tag{2.4}$$

In particular, we have $P(\chi_\Omega) = P(\Omega)$. Then, by $\langle\varphi, P(f)\psi\rangle = \sum_{j=1}^\infty \alpha_j \mu_{\varphi,\psi}(\Omega_j)$ we infer

$$\langle\varphi, P(f)\psi\rangle = \int_{\mathbb{R}} f(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{2.5}$$

Invoking the linearity of the integral, we see that the operator P is a linear map from the set of simple functions to the set of bounded linear operators on $\mathfrak{H}$. Moreover, $\|P(f)\psi\|^2 = \sum_{j=1}^\infty |\alpha_j|^2 d\mu_\psi(\Omega_j)$ (where $\Omega_i \cap \Omega_j = \emptyset$ for $i \neq j$) shows

$$\|P(f)\psi\|^2 = \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi(\lambda). \tag{2.6}$$

We equip the set of simple functions with the sup norm $\|.\|_\infty$ and get $\|P(f)\psi\| \leq \|f\|_\infty \|\psi\|$ which allows us to conclude $\|P\| = 1$. The set of simple functions is a dense subset of the Banach space of bounded Borel functions $B(\mathbb{R})$ and therefore it exists a unique extension of P to a bounded linear operator $P : B(\mathbb{R}) \to \mathfrak{L}(\mathfrak{H})$ (with $\|P\| = 1$) from the bounded Borel functions on $\mathbb{R}$ (equipped with $\|.\|_\infty$) to the set $\mathfrak{L}(\mathfrak{H})$ of bounded linear operators on $\mathfrak{H}$. In particular, (2.5) and (2.6) remain true. Thus we have established integration with respect to our projection-valued measure for bounded Borel functions.

We want now to define integration for unbounded Borel functions as well. As we expect the resulting operator to be unbounded, we cannot define it on the entire Hilbert space $\mathfrak{H}$ which means that we need to find suitable (dense) domain. Inspired by (2.6), we set

$$\mathfrak{D}_f = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} |f(\lambda)|^2 d\mu_\psi(\lambda) < \infty\}. \tag{2.7}$$

Note that $\mathfrak{D}_f$ forms a linear subspace of $\mathfrak{H}$ since $\mu_{\alpha\psi}(\Omega) = |\alpha|^2 \mu_\psi(\Omega)$ and since $\mu_{\varphi+\psi}(\Omega) = \|P(\Omega)(\varphi + \psi)\|^2 \leq 2(\|P(\Omega)\varphi\| + \|P(\Omega)\psi\|^2) = 2(\mu_\varphi(\Omega) + \mu_\psi(\Omega))$.

We define the sequence of bounded Borel functions

$$f_n = \chi_{\Omega_n} f, \qquad \Omega_n = \{\lambda | \, |f(\lambda)| \leq n\} \tag{2.8}$$

which is a Cauchy sequence converging to f in the sense of $L^2(\mathbb{R}, d\mu_\psi)$ for every $\psi \in \mathfrak{D}_f$. From (2.6) we conclude that the vectors $\psi_n = P(f_n)\psi$ form a Cauchy sequence in $\mathfrak{H}$ (cf. [Te09, p91]). Thus the limit of the sequence (2.8) exists and we are allowed to set

$$P(f)\psi = \lim_{n\to\infty} P(f_n)\psi, \qquad \psi \in \mathfrak{D}_f. \tag{2.9}$$

By construction, $P(f)$ is a linear operator which satisfies (2.6). Note that (2.5) remains true at least for $\varphi = \psi$ as $f \in L^1(\mathbb{R}, d\mu_\psi)$ where μ_ψ is finite. Furthermore, $\mathfrak{D}_f$ is dense (cf. [Te09, p91]).

Definition 2.4 (Normal operators)**.** *Suppose A is an unbounded operator and denote by A^* the adjoint of A. We call A normal if $\mathfrak{D}(A) = \mathfrak{D}(A^*)$ and $\|A\psi\| = \|A^*\psi\|$.*

Theorem 2.5 ([Te09, Theorem 3.2]). *For any Borel function f, the operator*

$$P(f) \equiv \int_{\mathbb{R}} f(\lambda) dP(\lambda), \qquad \mathfrak{D}(P(f)) = \mathfrak{D}_f \tag{2.10}$$

is normal and satisfies $P(f)^* = P(f^*)$.

These considerations seem to indicate some kind of correspondence between the operators $P(f)$ in $\mathfrak{H}$ and f in $L^2(\mathbb{R}, d\mu_\psi)$.

Definition 2.6 (Unitary operators, unitary equivalence). *Suppose $\tilde{\mathfrak{H}}$ is another (separable and complex) Hilbert space equipped with the norm $\|.\|_{\tilde{\mathfrak{H}}}$.*

(i) An operator $U : \mathfrak{H} \to \tilde{\mathfrak{H}}$ is called unitary if it is a bijection which preserves norms, that is, $\|U\psi\|_{\tilde{\mathfrak{H}}} = \|\psi\|$ (hence U also preserves scalar products).

(ii) Two operators $A : \mathfrak{H} \to \mathfrak{H}$ and $\tilde{A} : \tilde{\mathfrak{H}} \to \tilde{\mathfrak{H}}$ are called unitarily equivalent if $UA = \tilde{A}\,U$ and $U\mathfrak{D}(A) = \mathfrak{D}(\tilde{A})$.

Note that A is self-adjoint if and only if $\tilde{A}$ is and $\sigma(A) = \sigma(\tilde{A})$ holds. Now, we return to our original problem. Consider the subspace

$$\mathfrak{H}_\psi = \{P(g)\psi | g \in L^2(\mathbb{R}, d\mu_\psi)\} \subseteq \mathfrak{H}. \tag{2.11}$$

This subspace is closed as $L^2(\mathbb{R}, d\mu_\psi)$ is and as $\psi_n = P(g_n)\psi$ is convergent in $\mathfrak{H}$ if and only if the sequence g_n is convergent in $L^2(\mathbb{R}, d\mu_\psi)$.

Lemma 2.7 ([Te09, Lemma 3.3]). *The subspace $\mathfrak{H}_\psi$ reduces $P(f)$, that is, $P_\psi P(f) \subseteq P(f)P_\psi$. Here P_ψ is the projection onto $\mathfrak{H}_\psi$.*

In particular, we can decompose $P(f) = P(f)\big|_{\mathfrak{H}_\psi} \oplus P(f)\big|_{\mathfrak{H}_\psi^\perp}$. Note that we have

$$P_\psi \mathfrak{D}_f = \mathfrak{D}_f \cap \mathfrak{H}_\psi = \{P(g)\psi | g, fg \in L^2(\mathbb{R}, d\mu_\psi)\} \tag{2.12}$$

and $P(f)P(g)\psi = P(fg)\psi \in \mathfrak{H}_\psi$ in this case. By (2.6), the relation

$$U_\psi(P(f)\psi) = f \tag{2.13}$$

defines a unique unitary operator $U_\psi : \mathfrak{H} \to L^2(\mathbb{R}, d\mu_\psi)$ such that the identity

$$U_\psi P(f)\big|_{\mathfrak{H}_\psi} = fU_\psi \tag{2.14}$$

holds. Here f is identified with its corresponding multiplication operator. If f is unbounded, we have $U_\psi(\mathfrak{D}_f \cap \mathfrak{H}_\psi) = \mathfrak{D}_f = \{g \in L^2(\mathbb{R}, d\mu_\psi) | fg \in L^2(\mathbb{R}, d\mu_\psi)\}$ (as $\varphi = P(f)\psi$ implies $d\mu_\varphi = |f|^2 d\mu_\psi$) and therefore, the above equation still holds.

Definition 2.8 (Cyclic vector). *A vector $\psi \in \mathfrak{H}$ is called cyclic if we have $\mathfrak{H}_\psi = \mathfrak{H}$.*

If $\psi \in \mathfrak{H}$ is cyclic, our picture is complete. If this is not the case, we need to extend our approach.

Definition 2.9 (Spectral vector, spectral basis). *We will call a set $\{\psi_j\}_{j\in J}$ ($\psi_j \in \mathfrak{H}$, J some index set) a set of spectral vectors if $\|\psi_j\| = 1$ and $\mathfrak{H}_{\psi_i} \perp \mathfrak{H}_{\psi_j}$ for all $i \neq j$. A set of spectral vectors is called a spectral basis if $\bigoplus_j \mathfrak{H}_{\psi_j} = \mathfrak{H}$.*

The following Lemma gives a positive answer to the question whether such a spectral basis always exists.

Lemma 2.10 ([Te09, Lemma 3.4]). *For every projection-valued measure P there is an (at most countable) spectral basis $\{\psi_n\}$ such that*

$$\mathfrak{H} = \bigoplus_n \mathfrak{H}_{\psi_n}, \tag{2.15}$$

and a corresponding unitary operator

$$U = \bigoplus_n U_{\psi_n} : \ \mathfrak{H} \to \bigoplus_n L^2(\mathbb{R}, d\mu_{\psi_n}) \tag{2.16}$$

such that we have for any Borel function f

$$UP(f) = fU, \qquad U\mathfrak{D}_f = \mathfrak{D}(f). \tag{2.17}$$

The cardinality of a spectral basis is not well-defined.

Definition 2.11 (Spectral multiplicity, simple spectrum). *The minimal cardinality of a spectral basis is called the spectral multiplicity of P. If the spectral multiplicity is one, the spectrum is called simple.*

The above considerations show that we can assign a self-adjoint operator

$$A = \int_{\mathbb{R}} \lambda dP(\lambda) \tag{2.18}$$

to every projection-valued measure P. Our next aim is to show that we can invert this map. We consider the resolvent

$$R_A(z) = \int_{\mathbb{R}} (\lambda - z)^{-1} dP(\lambda) \tag{2.19}$$

whose quadratic form is given by

$$F_\psi(z) = \langle \psi, R_A(z)\psi \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_\psi(\lambda). \tag{2.20}$$

This expression is exactly the Borel transform of the measure μ_ψ (cf. Definition B.1). Furthermore, in Appendix B.1 is shown that $F_\psi(z)$ is an analytic map from the upper half plane to itself and thus a Herglotz–Nevanlinna function. The measure μ_ψ can be reconstructed from $F_\psi(z)$ by the Stieltjes inversion formula (cf. Theorem B.5)

$$\mu_\psi(\lambda) = \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{\pi} \int_{-\infty}^{\lambda+\delta} \mathrm{Im}(F_\psi(t + \mathrm{i}\varepsilon)) dt. \tag{2.21}$$

Conversely, if $F_\psi(z)$ is a Herglotz–Nevanlinna function which fulfills the growth estimate $|F_\psi(z)| \leq \frac{M}{\mathrm{Im}(z)}$, it is the Borel transform of a unique measure μ_ψ (which is given by the Stieltjes inversion formula) satisfying $\mu_\psi(\mathbb{R}) \leq M$ (cf. Theorem B.4).

Suppose now A is some given self-adjoint operator. We consider the expectation of the resolvent of A,

$$F_\psi(z) = \langle \psi, R_A(z)\psi \rangle. \tag{2.22}$$

This function is holomorphic for $z \in \rho(A)$ and satisfies

$$F_\psi(z^*) = F_\psi(z)^* \quad \text{and} \quad |F_\psi(z)| \leq \frac{\|\psi\|^2}{\mathrm{Im}(z)}. \tag{2.23}$$

Moreover, $F_\psi(z)$ is a Herglotz–Nevanlinna function. Thus, by the above remarks, we can associate a measure $\mu_\psi(\lambda)$ with $F_\psi(z)$ which is given by the Stieltjes inversion formula.

Definition 2.12 (Spectral measure)**.** *The measure $\mu_\psi(\lambda)$ is called the spectral measure corresponding to $\psi \in \mathfrak{H}$.*

More generally, by polarization, we get a corresponding complex measure $\mu_{\varphi,\psi}$ for each $\varphi, \psi \in \mathfrak{H}$ such that

$$\langle \varphi, R_A(z)\psi \rangle = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu_{\varphi,\psi}(\lambda). \tag{2.24}$$

The measure $\mu_{\varphi,\psi}$ is conjugate linear in φ and linear in ψ. We define a family of operators via the sesquilinear forms

$$s_\Omega(\varphi, \psi) = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{2.25}$$

The associated quadratic form is nonnegative. Indeed, we have $q_\Omega(\psi) = s_\Omega(\psi, \psi) = \mu_\psi(\Omega) \geq 0$ for every $\psi \in \mathfrak{H}$. The inequality of Cauchy-Schwarz for sesquilinear forms then implies

$$|s_\Omega(\varphi,\psi)| \leq q_\Omega(\varphi)^{1/2} q_\Omega(\psi)^{1/2} = \mu_\varphi(\Omega)^{1/2}\mu_\psi(\Omega)^{1/2} \leq \mu_\varphi(\mathbb{R})^{1/2}\mu_\psi(\mathbb{R})^{1/2} \leq \|\varphi\|\|\psi\|.$$

Recall that, for every bounded sesquilinear form s, there is a unique bounded operator A such that $s(\varphi, \psi) = \langle A\varphi, \psi \rangle$ is satisfied (cf. [Te09, Corollary 1.9]). Hence there exists a family of nonnegative ($0 \leq \langle \psi, P_A(\Omega)\psi) \rangle \leq 1$) and self-adjoint operators $P_A(\Omega)$ which satisfy

$$\langle \varphi, P_A(\Omega)\psi \rangle = \int_{\mathbb{R}} \chi_\Omega(\lambda) d\mu_{\varphi,\psi}(\lambda). \tag{2.26}$$

The family of operators $P_A(\Omega)$ forms a projection-valued measure (cf. [Te09, Lemma 3.6]).

Theorem 2.13 (Spectral theorem, [Te09, Theorem 3.7])**.** *To every self-adjoint operator A there corresponds a unique projection-valued measure P_A such that*

$$A = \int_{\mathbb{R}} \lambda dP_A(\lambda). \tag{2.27}$$

The quadratic form of A is given by

$$q_A(\psi) = \int_{\mathbb{R}} \lambda d\mu_\psi(\lambda) \tag{2.28}$$

and can be defined for every ψ in the form domain

$$\mathfrak{Q}(A) = \mathfrak{D}(|A|^{1/2}) = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} |\lambda| d\mu_\psi(\lambda) < \infty\}. \tag{2.29}$$

This extends our previous definition to nonnegative operators. Note that $\mathfrak{Q}(A)$ is larger than $\mathfrak{D}(A) = \{\psi \in \mathfrak{H} | \int_{\mathbb{R}} \lambda^2 d\mu_\psi(\lambda) < \infty\}$. If the operators A and $\tilde{A}$ are unitarily equivalent, then we have $UR_A(z) = R_{\tilde{A}}(z)U$ and thus $d\mu_\psi = d\tilde{\mu}_{U\psi}$.

The spectrum of A can be characterized in terms of the associated projectors.

Theorem 2.14 ([Te09, Theorem 3.8])**.** *The spectrum of A is given by*

$$\sigma(A) = \{\lambda \in \mathbb{R} | P_A((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \textit{ for all } \varepsilon > 0\}. \tag{2.30}$$

In particular, $P_A((\lambda_1, \lambda_2)) = 0$ if and only if $(\lambda_1, \lambda_2) \subseteq \rho(A)$.

Corollary 2.15 ([Te09, Corollary 3.9])**.** *We have*

$$P_A(\sigma(A)) = \mathbb{1} \qquad \textit{and} \qquad P_A(\mathbb{R} \cap \rho(A)) = 0. \tag{2.31}$$

By the simple observation

$$P_A(f) = P_A(\sigma(A))P_A(f) = P_A(\chi_{\sigma(A)} f) \tag{2.32}$$

we see that $P_A(f)$ is not affected by the values of f on $\mathbb{R} \setminus \sigma(A)$. From now on we will write $f(A)$ instead of $P_A(f)$.

2.2 Multiplication operators

We have seen that, in order to understand self-adjoint operators, we need to understand multiplication operators on $L^2(\mathbb{R}, d\mu)$ where $d\mu$ is a finite Borel measure.

Definition 2.16 (Spectrum of a measure)**.** *We define the set of all growth points $\sigma(\mu)$ by*

$$\sigma(\mu) = \{\lambda \in \mathbb{R} | \mu((\lambda - \varepsilon, \lambda + \varepsilon)) > 0 \textit{ for all } \varepsilon > 0\} \tag{2.33}$$

and call it the spectrum of μ.

Note that the spectrum $\sigma = \sigma(\mu)$ supports μ, that is, $\mu(\mathbb{R} \setminus \sigma) = 0$. As we have already noticed, the Borel transform of μ,

$$F(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda), \tag{2.34}$$

plays an important role in our considerations. The Borel transform of a finite Borel measure is a Herglotz–Nevanlinna function which is holomorphic in $\mathbb{C} \setminus \sigma(\mu)$ and satisfies $F(z^*) = F(z)^*$ (cf. Theorem B.3). Furthermore, note that F cannot be holomorphically extended to a larger domain. Indeed, if F is holomorphic in a neighborhood of some $\lambda \in \mathbb{R}$, then we have $\operatorname{Im}(F(\lambda)) = 0$ (as $F(\lambda) = F(\lambda^*)$) and from the Stieltjes inversion formula (Theorem B.5) we get $\lambda \in \mathbb{R} \setminus \sigma(\mu)$.

Associated with the measure μ is the operator

$$Af(\lambda) = \lambda f(\lambda), \qquad \mathfrak{D}(A) = \{f \in L^2(\mathbb{R}, d\mu) | \lambda f(\lambda) \in L^2(\mathbb{R}, d\mu)\}. \tag{2.35}$$

By Theorem 2.14 the spectrum of A coincides with the spectrum of μ, that is,

$$\sigma(A) = \sigma(\mu). \tag{2.36}$$

What can we say about the function $f(A)$ (which is precisely the multiplication operator by f) of A? We just consider the case where f is real-valued and introduce the measure

$$(f_\star \mu)(\Omega) = \mu(f^{-1}(\Omega)). \tag{2.37}$$

Then we have

$$\int_{\mathbb{R}} g(\lambda) d(f_\star \mu)(\lambda) = \int_{\mathbb{R}} g(f(\lambda)) d\mu(\lambda). \tag{2.38}$$

It is sufficient to check this identity for simple functions g which follows from $\chi_\Omega \circ f = \chi_{f^{-1}(\Omega)}$. In particular, we have

$$P_{f(A)}(\Omega) = \chi_{f^{-1}(\Omega)}. \tag{2.39}$$

We have that $f(A)$ is unitarily equivalent to multiplication by λ in $L^2(\mathbb{R}, d(f_\star \mu))$ via the map

$$L^2(\mathbb{R}, d(f_\star \mu)) \to L^2(\mathbb{R}, d\mu), \qquad g \mapsto g \circ f \tag{2.40}$$

if $L^2(\mathbb{R}, d\mu)$ is its range (cf. [Te09, Lemma 3.11]).

Lemma 2.17 ([Te09, Lemma 3.12])**.** *Let f be real-valued. The spectrum of $f(A)$ is given by*

$$\sigma(f(A)) = \sigma(f_\star \mu). \tag{2.41}$$

In particular,

$$\sigma(f(A)) \subseteq \overline{f(\sigma(A))} \tag{2.42}$$

where equality holds if f is continuous and the closure can be dropped if, in addition, $\sigma(A)$ is bounded.

Definition 2.18 (Absolutely continuous, mutually absolutely continuous and singular measures)**.** *Suppose μ_1 and μ_2 are two Borel measures.*

(i) We call μ_1 absolutely continuous with respect to μ_2 (in symbols $\mu_1 \ll \mu_2$) if $\mu_2(A) = 0$ implies $\mu_1(A) = 0$ for every Borel set A.

(ii) The measures μ_1 *and* μ_2 *are called mutually absolutely continuous if* $\mu_1 \ll \mu_2$ *and* $\mu_2 \ll \mu_1$.

(iii) Moreover, μ_1 *and* μ_2 *are called mutually singular if they are supported on disjoint sets.*

One can now read off the unitary equivalence of two operators with simple spectrum from the corresponding measures.

Lemma 2.19 ([Te09, Lemma 3.13])**.** *Let* A_1 *and* A_2 *be self-adjoint operators with simple spectrum and corresponding spectral measures* μ_1 *and* μ_2 *of cyclic vectors. Then,* A_1 *and* A_2 *are unitarily equivalent if and only if* μ_1 *and* μ_2 *are mutually absolutely continuous.*

Next we recall that one can decompose μ with respect to the Lebesgue measure (cf. [Te09, Theorem A.29]),

$$d\mu = d\mu_{ac} + d\mu_s. \tag{2.43}$$

Here μ_{ac} is absolutely continuous with respect to the Lebesgue measure (i.e., we have $\mu_{ac}(B) = 0$ for all B with Lebesgue measure zero) and μ_s is singular with respect to the Lebesgue measure (i.e., μ_s is supported, $\mu_s(\mathbb{R} \setminus B) = 0$, on a set B with Lebesgue measure zero). One can decompose the singular part μ_s into two further parts, a (singularly) continuous and a pure point part,

$$d\mu_s = d\mu_{sc} + d\mu_{pp} \tag{2.44}$$

where μ_{sc} is continuous on $\mathbb{R}$ and μ_{pp} is a step function. The measures $d\mu_{ac}$, $d\mu_{sc}$ and $d\mu_{pp}$ are mutually singular. Hence their supports Σ_{ac}, Σ_{sc} and Σ_{pp} are mutually singular. These sets are not unique. They are chosen such that Σ_{pp} is the set of all jumps of $\mu(\lambda)$ and such that Σ_{sc} is a set of Lebesgue measure zero.

To the sets Σ_{ac}, Σ_{sc} and Σ_{pp} correspond projectors $P^{ac} = \chi_{\Sigma_{ac}(A)}$, $P^{sc} = \chi_{\Sigma_{sc}(A)}$ and $P^{pp} = \chi_{\Sigma_{pp}(A)}$ satisfying $P^{ac} + P^{sc} + P^{pp} = \mathbb{1}$. Therefore we can decompose both, our Hilbert space

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sc}) \oplus L^2(\mathbb{R}, d\mu_{pp}) \tag{2.45}$$

and our operator

$$A = (AP^{ac}) \oplus (AP^{sc}) \oplus (AP^{pp}). \tag{2.46}$$

We call the corresponding spectra

$$\sigma_{ac}(A) = \sigma(\mu_{ac}), \qquad \sigma_{sc}(A) = \sigma(\mu_{sc}) \qquad \text{and} \qquad \sigma_{pp}(A) = \sigma(\mu_{pp}) \tag{2.47}$$

the absolutely continuous, singularly continuous, and pure point spectrum of A, respectively. Note that, in general, $\sigma_{pp}(A)$ is not equal to the set of eigenvalues

$$\sigma_p(A) = \{\lambda \in \mathbb{R} | \lambda \text{ is an eigenvalue of } A\} \tag{2.48}$$

since we only have $\sigma_{pp}(A) = \overline{\sigma_p(A)}$.

Finally, the spectrum can be read off from the boundary values of $\mathrm{Im}(F)$ towards the real line. We define the sets

$$\Sigma_{ac} = \{\lambda | 0 < \limsup_{\varepsilon \downarrow 0} \mathrm{Im}(F(\lambda + \mathrm{i}\varepsilon)) < \infty\}, \tag{2.49}$$

$$\Sigma_{s} = \{\lambda | \limsup_{\varepsilon \downarrow 0} \mathrm{Im}(F(\lambda + \mathrm{i}\varepsilon)) = \infty\}, \tag{2.50}$$

$$\Sigma = \Sigma_{ac} \cup \Sigma_s = \{\lambda | 0 < \limsup_{\varepsilon \downarrow 0} \mathrm{Im}(F(\lambda + \mathrm{i}\varepsilon))\} \tag{2.51}$$

which are minimal supports for μ_{ac}, μ_s and μ, respectively (cf. [Te09, Theorem 3.23]). We could even restrict ourselves to values of λ where the lim sup is a lim (finite or infinite).

Lemma 2.20 ([Te09, Lemma 3.14]). *The spectrum of μ is given by*

$$\sigma(\mu) = \overline{\Sigma}. \tag{2.52}$$

Recall that the essential closure of a Borel set $\Omega \subseteq \mathbb{R}$ is defined by

$$\overline{\Omega}^{ess} = \{\lambda \in \mathbb{R} || (\lambda - \varepsilon, \lambda + \varepsilon)| > 0 \text{ for all } \varepsilon > 0\}. \tag{2.53}$$

Lemma 2.21 ([Te09, Lemma 3.15]). *The absolutely continuous spectrum of μ is given by*

$$\sigma(\mu_{ac}) = \overline{\Sigma}_{ac}^{ess}. \tag{2.54}$$

2.3 Spectral types

The aim of this section is to transfer the above results to arbitrary self-adjoint operators.

We will make use of Lemma 2.10. Therefore we need a spectral measure containing the information from all measures in a spectral basis.

Definition 2.22 (Maximal spectral vector). *A vector $\psi \in \mathfrak{H}$ is called maximal spectral vector of A and μ_ψ if for every $\varphi \in \mathfrak{H}$ the spectral measure μ_φ is absolutely continuous with respect to μ_ψ*

If a maximal spectral vector exists, there is a spectral measure which contains the information from all measures in a spectral basis. Luckily, for every self-adjoint operator A there is a maximal spectral vector (cf. [Te09, Lemma 3.16]).

Definition 2.23 (Set of ordered spectral vectors). *A set $\{\psi_j\}$ of spectral vectors is called ordered if ψ_k is a maximal spectral vector for A restricted to $(\bigoplus_{j=1}^{k-1} \mathfrak{H}_{\psi_j})^\perp$.*

We can even deduce that, for every self-adjoint operator, there is an ordered spectral basis (cf. [Te09, Theorem 3.17]). Next, we define the spaces

$$\mathfrak{H}_{ac} = \{\psi \in \mathfrak{H} | \mu_\psi \text{ is absolutely continous}\}, \tag{2.55}$$

$$\mathfrak{H}_{sc} = \{\psi \in \mathfrak{H} | \mu_\psi \text{ is singularly continous}\}, \tag{2.56}$$

$$\mathfrak{H}_{pp} = \{\psi \in \mathfrak{H} | \mu_\psi \text{ is pure point}\}. \tag{2.57}$$

Lemma 2.24 ([Te09, Lemma 3.19]). *We have*

$$\mathfrak{H} = \mathfrak{H}_{ac} \oplus \mathfrak{H}_{sc} \oplus \mathfrak{H}_{pp}. \tag{2.58}$$

There are Borel sets Σ_{xx} such that the projector onto $\mathfrak{H}_{xx}$ is given by $P^{xx} = \chi_{\Sigma_{xx}}(A)$, $xx \in \{ac,\ sc,\ pp\}$. In particular, the subspaces $\mathfrak{H}_{xx}$ reduce A. For the sets Σ_{xx} one can choose the corresponding supports of some maximal spectral measure μ.

We define the absolutely continuous, singularly continuous and pure point spectrum of A as

$$\sigma_{ac} = \sigma(A|_{\mathfrak{H}_{ac}}), \qquad \sigma_{sc} = \sigma(A|_{\mathfrak{H}_{sc}}) \qquad \text{and} \qquad \sigma_{pp} = \sigma(A|_{\mathfrak{H}_{pp}}), \tag{2.59}$$

respectively. Suppose μ is a maximal spectral measure. Then we have

$$\sigma_{ac}(A) = \sigma(\mu_{ac}), \qquad \sigma_{sc}(A) = \sigma(\mu_{sc}) \qquad \text{and} \qquad \sigma_{pp}(A) = \sigma(\mu_{pp}). \tag{2.60}$$

If A and $\tilde{A}$ are unitarily equivalent via a map U, then so are $A|_{\mathfrak{H}_{xx}}$ and $A|_{\tilde{\mathfrak{H}}_{xx}}$. In particular, we have $\sigma_{xx}(A) = \sigma_{xx}(\tilde{A})$.

Chapter 3

The singular Weyl function

The aim of this chapter is to define a Weyl function at the (in general singular) endpoint a. To this end, we have to find an analogous system of solutions to the Weyl solutions introduced in Section 1.5. We are going to construct such a system of entire solutions $\theta(z,x)$ and $\phi(z,x)$ for (1.7) such that $\phi(z,x)$ lies in the domain of H near a and such that the Wronskian of $\theta(z,x)$ and $\phi(z,x)$ satisfies $W(\theta(z),\phi(z)) = 1$. This will, in further consequence, enable us to define a singular Weyl function at the endpoint a. In particular, we extend [KST11, Section 2] to the case of one-dimensional Dirac operators. Some background concerning Complex Analysis which is helpful to understand this chapter can be found in Appendix A.

We will use the same notations as in Section 1.5, that is, we choose a base point $c \in (a,b)$ and consider the operators $H_{(a,c)}$ and $H_{(c,b)}$ which are obtained by restricting H to (a,c) and (c,b), respectively. We recall the solutions $c(z,x)$ and $s(z,x)$ corresponding to the initial conditions (1.26) and define the Weyl solutions $u_-(z,x)$ and $u_+(z,x)$ as in (1.29).

We start with a Hypothesis which will turn out to be equivalent to the existence of the announced system of solutions $\theta(z,x)$ and $\phi(z,x)$ such that $\phi(z,x)$ lies in the domain of H near a and such that the Wronskian satisfies $W(\theta(z),\phi(z)) = 1$.

Hypothesis 3.1. *Suppose that the spectrum of $H_{(a,c)}$ is purely discrete for one (and hence for all) $c \in (a,b)$.*

Lemma 3.2. *There exists a (nontrivial) solution*

$$\phi(z,x) = \begin{pmatrix} \phi_1(z,x) \\ \phi_2(z,x) \end{pmatrix}$$

of $\tau u = zu$ which is in the domain of H near a and which is entire with respect to z if and only if Hypothesis 3.1 is satisfied. Furthermore, $\phi(z,x)$ can be chosen such that we have

$$\phi(z,x) = \alpha(z)c(z,x) + \beta(z)s(z,x) \tag{3.1}$$

where $\alpha(z)$ and $\beta(z)$ are real entire functions with no common zeros.

Proof. Suppose Hypothesis 3.1 is satisfied. Then $m_-(z)$ is meromorphic with poles at the points in $\sigma(H_{(a,c)})$. As these poles are simple, one can construct a (real) entire function $\alpha(z)$ with simple zeros (and no other zeros) at the poles of $m_-(z)$ by Weierstrass' theorem (Theorem A.13). By setting $\phi(z,x) = \alpha(z)u_-(z,x)$ we are done.
Conversely, let $\phi(z,x) = \alpha(z)c(z,x) + \beta(z)s(z,x)$ be entire. Then $\alpha(z) = \phi_1(z,c)$ is entire. Consider

$$\beta(z) = \frac{\phi_1(z,x) - \alpha(z)c_1(z,x)}{s_1(z,x)} = \frac{\phi_2(z,x) - \alpha(z)c_2(z,x)}{s_2(z,x)}.$$

All possible poles of $\beta(z)$ on the real line are removable because the left-hand side of this formula is independent of x and the possible poles on the right-hand side vary as x varies. Thus $\beta(z)$ is also entire. Note that we have

$$\alpha(z) = \phi_1(z,c) \quad \text{and} \quad \beta(z) = \phi_2(z,c). \tag{3.2}$$

Due to Theorem 1.12, $\phi(z,x)$ and $u_-(z,x)$ are both square integrable near a and satisfy the boundary condition at a if H is limit circle at a. If H is limit point at a, the square integrable solution is uniquely determined up to a multiple. Therefore we can set $\phi(z,x) = c(z)u_-(z,x)$ for any real entire function $c(z)$ which implies that $\phi_2(z,c) = c(z)$ must hold as well. Finally, using (1.29), obtain that

$$m_-(z) = -u_{-2}(z,c) = \frac{\phi_2(z,c)}{c(z)} = -\frac{\phi_2(z,c)}{\phi_1(z,c)} = -\frac{\beta(z)}{\alpha(z)} \tag{3.3}$$

is meromorphic which means that Hypothesis 3.1 holds. □

Corollary 3.3. *The function $\phi(z,x)$ constructed in Lemma 3.2 is uniquely determined up to a real entire function without zeros, that is, if $\tilde{\phi}(z,x)$ is another real entire solution which is nontrivial for all $z \in \mathbb{C}$ and in the domain of H near a, we have*

$$\tilde{\alpha}(z) = \mathrm{e}^{g(z)}\alpha(z) \qquad \text{and} \qquad \tilde{\beta}(z) = \mathrm{e}^{g(z)}\beta(z) \tag{3.4}$$

where $g(z)$ is some real entire function.

It remains to find the second solution $\theta(z,x)$ such that the Wronskian of $\theta(z,x)$ and $\phi(z,x)$ satisfies $W(\theta(z),\phi(z)) = 1$.

Lemma 3.4. *Suppose Hypothesis 3.1 holds. Then there is a second solution*

$$\theta(z,x) = \begin{pmatrix} \theta_1(z,x) \\ \theta_2(z,x) \end{pmatrix}$$

which satisfies

$$\theta(z,x) = \gamma(z)c(z,x) + \delta(z)s(z,x) \tag{3.5}$$

where $\gamma(z)$ and $\delta(z)$ are real entire functions with no common zeros. Furthermore, the Wronskian of $\theta(z,x)$ and $\phi(z,x)$ satisfies

$$W(\theta(z),\phi(z)) = \gamma(z)\beta(z) - \alpha(z)\delta(z) = 1. \tag{3.6}$$

Proof. The ansatz

$$\gamma(z) = \frac{\beta(z)}{\alpha(z)^2 + \beta(z)^2} - \eta(z)\alpha(z) \qquad \text{and} \qquad \delta(z) = \frac{-\alpha(z)}{\alpha(z)^2 + \beta(z)^2} - \eta(z)\beta(z) \tag{3.7}$$

will turn out to work. Here, $\eta(z)$ should be a meromorphic function which has poles at the the zeros of $\alpha(z)^2 + \beta(z)^2$. Our first goal is to determine $\eta(z)$.
By $\{z_j\}$ we denote the zeros of the entire function $\alpha(z)^2 + \beta(z)^2$. Suppose z_j is a zero of order $n_j \in \mathbb{N}$. Then, at each z_j,

$$\beta^{(k)}(z_j) = \sigma_j \mathrm{i} \alpha^{(k)}(z_j), \qquad 0 \leqslant k < n_j \tag{3.8}$$

holds for some $\sigma_j \in \{\pm 1\}$. In order to obtain entire functions, we choose $\eta(z)$ such that the principal part of $\eta(z)$ near z_j matches the one from $\sigma_j \mathrm{i}(\alpha(z)^2 + \beta(z)^2)^{-1}$, that is, we have

$$\frac{\sigma_j \mathrm{i}}{\alpha(z)^2 + \beta(z)^2} = \eta(z) + O(z - z_j)^0.$$

Such a function can be constructed due to Mittag-Leffler's theorem (Theorem A.15). Then we compute

$$\begin{aligned} \gamma(z) &= \frac{\beta(z)}{\alpha(z)^2 + \beta(z)^2} - \eta(z)\alpha(z) \\ &= \frac{\sigma_j \mathrm{i}\alpha(z) + O(z - z_j)^{n_j}}{\alpha(z)^2 + \beta(z)^2} - \frac{\sigma_j \mathrm{i}\alpha(z)}{\alpha(z)^2 + \beta(z)^2} + O(z - z_j)^0 = O(z - z_j)^0 \end{aligned}$$

which shows that all poles of $\gamma(z)$ are removable. By a similar computation

$$\begin{aligned} \delta(z) &= \frac{-\alpha(z)}{\alpha(z)^2 + \beta(z)^2} - \eta(z)\beta(z) \\ &= \frac{-\alpha(z)}{\alpha(z)^2 + \beta(z)^2} - \frac{(\sigma_j i)^2\alpha(z) + O(z - z_j)^{n_j}}{\alpha(z)^2 + \beta(z)^2} + O(z - z_j)^0 = O(z - z_j)^0 \end{aligned}$$

we see that all poles of $\delta(z)$ are removable. Finally, by use of (1.26) and (3.7) we have

$$\begin{aligned} W(\theta(z), \phi(z)) &= \theta_1(z,c)\phi_2(z,c) - \theta_2(z,c)\phi_1(z,c) \\ &= (\gamma(z)c_1(z,c) + \delta(z)s_1(z,c))(\alpha(z)c_2(z,c) + \beta(z)s_2(z,c)) \\ &\quad - (\gamma(z)c_2(z,c) + \delta(z)s_2(z,c))(\alpha(z)c_1(z,c) + \beta(z)s_1(z,c) \\ &= \gamma(z)\beta(z) - \delta(z)\alpha(z) \\ &= 1 \end{aligned}$$

as stated. If $\gamma(z)$ or $\delta(z)$ are not real, they have to be replaced by $\frac{1}{2}(\gamma(z) + \gamma(z^*)^*)$ and $\frac{1}{2}(\delta(z) + \delta(z^*)^*)$, respectively. □

Note that similarly to (3.2) we have

$$\gamma(z) = \theta_1(z,c) \qquad \text{and} \qquad \delta(z) = \theta_2(z,c). \tag{3.9}$$

Corollary 3.5. *Given a system of solutions $\phi(z,x)$ and $\theta(z,x)$ as above, any other real entire solution $\tilde{\theta}(z,x)$ for which $W(\tilde{\theta}(z),\phi(z)) = 1$ holds as well can be written as*

$$\tilde{\theta}(z,x) = \theta(z,x) - f(z)\phi(z,x) \tag{3.10}$$

where $f(z)$ is some real entire function.

Definition 3.6 (Singular Weyl function)**.** *Suppose we have given a system of real entire solutions $\phi(z,x)$ and $\theta(z,x)$ as in Lemma 3.4. We define the singular Weyl function*

$$M(z) = -\frac{W(\theta(z),u_+(z))}{W(\phi(z),u_+(z))} = -\frac{\gamma(z)m_+(z)-\delta(z)}{\alpha(z)m_+(z)-\beta(z)} \tag{3.11}$$

such that the solution which is in the domain of H near b (cf. (1.29)*) is given by*

$$u_+(z,x) = a(z)\big(\theta(z,x) + M(z)\phi(z,x)\big) \tag{3.12}$$

where $a(z) = -W(\phi(z),u_+(z)) = \beta(z) - m_+(z)\alpha(z)$.

This definition immediately enables us to prove two properties of $M(z)$.

Lemma 3.7. *The singular Weyl function $M(z)$ is analytic in $\mathbb{C}\backslash\mathbb{R}$. Moreover, the identity $M(z) = M(z^*)^*$ holds.*

Proof. Note that $m_+(z)$ is analytic in $\mathbb{C}\backslash\mathbb{R}$. All the other functions are entire by construction. Thus it follows from (3.11) that $M(z)$ is meromorphic in $\mathbb{C}\backslash\mathbb{R}$. Moreover, every zero of the Wronskian $W(\phi(z),u_+(z))$ corresponds to a complex eigenvalue of H. As H is self-adjoint, there are only real eigenvalues and we have that $W(\phi(z),u_+(z))$ cannot have a zero for $z\in\mathbb{C}\backslash\mathbb{R}$. Hence the first claim follows. The second claim is obvious by (3.11). □

Instead of $u_+(z,x)$ we will use

$$\psi(z,x) = \theta(z,x) + M(z)\phi(z,x). \tag{3.13}$$

Remark 3.8. *If we combine Corollary 3.3 and Corollary 3.5, we see that any system of real entire solutions $\tilde{\theta}(z,x)$ and $\tilde{\phi}(z,x)$ which satisfy $W(\tilde{\theta}(z),\tilde{\phi}(z)) = 1$ is related to the ones constructed in Lemma 3.2 and Lemma 3.4 by*

$$\tilde{\theta}(z,x) = \mathrm{e}^{-g(z)}\theta(z,x) - f(z)\phi(z,x) \qquad \text{and} \qquad \tilde{\phi}(z,x) = \mathrm{e}^{g(z)}\phi(z,x)$$

where $g(z)$ and $f(z)$ are real entire functions. If $\tilde{M}(z)$ is a singular Weyl function corresponding to the system $\tilde{\phi}(z,x)$ and $\tilde{\theta}(z,x)$, then it is related to $M(z)$ defined in (3.11) *via*

$$\tilde{M}(z) = \mathrm{e}^{-2g(z)}M(z) + \mathrm{e}^{-g(z)}f(z).$$

In particular, the maximal domain of holomorphy or the structure of the poles and singularities do not change.

Chapter 4

Spectral transformations

This chapter deals with spectral theory for our self-adjoint Dirac operator H. In particular, we extend [KST11, Section 3] to the case of one-dimensional Dirac operators. We start by observing that the singular Weyl function $M(z)$ defined in the previous chapter shares many properties with the Borel transform $m_f(z)$ of the spectral measure μ_f which will allow us to associate a measure with $M(z)$ by using the Stieltjes inversion formula. We are going to establish a spectral transformation which maps H to a multiplication operator. Furthermore, we will be able to read off the spectral types of H from the boundary behavior of the singular Weyl function $M(z)$. The chapter is concluded by a few observations concerning the Green function of H.

We start by setting

$$\hat{f}(z) = \int_a^b \left(\phi_1(z,x) f_1(x) + \phi_2(z,x) f_2(x)\right) dx \tag{4.1}$$

where

$$f(x) = \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} \in L^2_c((a,b),\mathbb{C}^2) \quad \text{and} \quad \phi(z,x) = \begin{pmatrix} \phi_1(z,x) \\ \phi_2(z,x) \end{pmatrix}$$

is the solution which lies in the domain of H near a constructed in Lemma 3.2. The function $\hat{f}(z)$ is entire and satisfies

$$\hat{f}(z^*)^* = \int_a^b \left(\phi_1(z,x) f_1(x)^* + \phi_2(z,x) f_2(x)^*\right) dx. \tag{4.2}$$

As we have seen in Chapter 2, for every $f \in L^2_c((a,b),\mathbb{C}^2)$ there is an associated spectral measure μ_f whose Borel transform is given by

$$m_f(z) = \langle f, (H-z)^{-1} f\rangle = \int_{\mathbb{R}} \frac{d\mu_f(\lambda)}{\lambda - z}. \tag{4.3}$$

Furthermore, for the resolvent we have

$$(H-z)^{-1} f(x) = \int_a^b G(z,x,y) f(y) dy \tag{4.4}$$

where

$$G(z,x,y) = \begin{cases} \psi(z,x) \otimes \phi(z,y), & y < x, \\ \phi(z,x) \otimes \psi(z,y), & y > x, \end{cases} \tag{4.5}$$

is the Green function of H. (4.5) is obtained from (1.23) as $\phi(z,.)$ is a solution which is in the domain of H near a, as $\psi(z,.)$ given by (3.13) is a solution which is in the domain of H near b and as the Wronskian satisfies

$$\begin{aligned} W(\psi(z),\phi(z)) &= W(\theta(z) + M(z)\phi(z), \theta(z)) \\ &= (\theta_1(z) + M(z)\phi_1(z))\,\phi_2(z) - (\theta_2(z) + M(z)\phi_2(z)) \\ &= \theta_1(z)\phi_2(z) - \theta_2(z)\phi_1(z) \\ &= W(\theta(z),\phi(z)) \\ &= 1. \end{aligned}$$

Explicitly, (4.5) reads

$$G(z,x,y) = \begin{cases} \begin{pmatrix} \psi_1(z,x)\phi_1(z,y) & \psi_1(z,x)\phi_2(z,y) \\ \psi_2(z,x)\phi_1(z,y) & \psi_2(z,x)\phi_2(z,y) \end{pmatrix}, & y < x, \\ \begin{pmatrix} \phi_1(z,x)\psi_1(z,y) & \phi_1(z,x)\psi_2(z,y) \\ \phi_2(z,x)\psi_1(z,y) & \phi_2(z,x)\psi_2(z,y) \end{pmatrix}, & y > x. \end{cases} \tag{4.6}$$

Now we link the singular Weyl function $M(z)$ to the Herglotz–Nevanlinna function $m_f(z)$ by a simple, but essential observation.

Lemma 4.1. *Let $\hat{f}(z)$ be given by* (4.1). *Then we have*

$$m_f(z) = E_f(z) + \hat{f}(z)\hat{f}(z^*)^* M(z) \tag{4.7}$$

for every $f \in L^2_c((a,b),\mathbb{C}^2)$. $E_f(z)$ is entire and satisfies $E_f(z^*)^* = E_f(z)$.

Proof. By plugging (4.5) into (4.4), we obtain

$$\begin{aligned} \langle f,(H-z)^{-1}f\rangle &= \int_a^b \left(f(x), \int_a^b G(z,x,y)f(y)\,dy \right) dx \\ &= \int_a^b \left(f(x), \int_a^x (\psi(z,x)\otimes\phi(z,y))f(y)\,dy + \int_x^b (\phi(z,x)\otimes\psi(z,y))f(y)\,dy \right) dx. \end{aligned}$$

Now we use (3.13) in order to get

$$\begin{aligned} &\langle f,(H-z)^{-1}f\rangle \\ &= \int_a^b \Bigg(f(x), \int_a^x (\theta(z,x)\otimes\phi(z,y) + M(z)\phi(z,x)\otimes\phi(z,y))f(y)\,dy \\ &\quad + \int_x^b (\phi(z,x)\otimes\theta(z,y) + M(z)\phi(z,x)\otimes\phi(z,y))f(y)\,dy \Bigg) dx \\ &= \int_a^b \Bigg(f(x), \int_a^x (\theta(z,x)\otimes\phi(z,y))f(y)\,dy + M(z)\int_a^x (\phi(z,x)\otimes\phi(z,y))f(y)\,dy \\ &\quad + \int_x^b (\phi(z,x)\otimes\theta(z,y))f(y)\,dy + M(z)\int_x^b (\phi(z,x)\otimes\phi(z,y))f(y)\,dy \Bigg) dx. \end{aligned}$$

If we set

$$E_f(z) = \int_a^b \left(f(x), \int_a^x (\theta(z,x) \otimes \phi(z,y)) f(y)\ dy + \int_x^b (\phi(z,x) \otimes \theta(z,y)) f(y)\ dy \right)\ dx,$$

we have

$$\begin{aligned}\langle f, (H-z)^{-1} f\rangle &= E_f(z) + \int_a^b \left(f(x), \int_a^b (\phi(z,x)\otimes\phi(z,y)) f(y)\ dy\right) dx \\ &= E_f(z) + M(z)\int_a^b \phi_1(z,x) f_1(x)^* + \phi_2(z,x) f_2(x)^*\ dx \int_a^b \phi_1(z,y) f_1(y) + \phi_2(z,y) f_2(y)\ dy \\ &= E_f(z) + \hat{f}(z)\hat{f}(z^*)^* M(z).\end{aligned}$$

Note that $E_f(z)$ defined above is entire and satisfies $E_f(z^*)^* = E_f(z)$. □

Now we fix some $\lambda_0 \in \mathbb{R}$ and choose

$$f(x) = \chi_{[c,d]}(x)\phi(\lambda_0, x) = \begin{pmatrix} \chi_{[c,d]}\phi_1(\lambda_0,x) \\ \chi_{[c,d]}\phi_2(\lambda_0,x)\end{pmatrix}.$$

Then we have $\hat{f}(\lambda_0) = \int_c^d (\phi_1(\lambda_0,x)^2 + \phi_2(\lambda_0,x)^2)\, dx > 0$ and obtain

$$M(z) = \frac{-E_f(z) + m_f(z)}{\hat{f}(z)^2} \tag{4.8}$$

for z in a neighborhood of λ_0. These considerations show that our singular Weyl function $M(z)$ shares many properties with the Herglotz–Nevanlinna function $m_f(z)$. Now the Stieltjes inversion formula (cf. Theorem B.5) comes into play. We can use it to associate a measure with $M(z)$ which will turn out to be equal to the spectral measure of f associated with the self-adjoint operator H up to multiplication with $|\hat{f}|^2$.

Lemma 4.2. *There is a unique Borel measure $d\rho$ defined via*

$$\frac{1}{2}\left(\rho\big((\lambda_0,\lambda_1)\big) + \rho\big([\lambda_0,\lambda_1]\big)\right) = \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} \mathrm{Im}\big(M(\lambda+\mathrm{i}\varepsilon)\big) d\lambda \tag{4.9}$$

such that

$$d\mu_f = |\hat{f}|^2 d\rho, \qquad f \in L^2_c((a,b),\mathbb{C}^2) \tag{4.10}$$

where $d\mu_f$ is the spectral measure of f defined in (4.3).

Proof. We fix $\lambda_0 < \lambda_1$ and some $f \in L^2_c((a,b),\mathbb{C}^2)$ such that $\hat{f}(\lambda) \neq 0$ holds for $\lambda \in [\lambda_0,\lambda_1]$. Then, for some function $w \in C[\lambda_1,\lambda_2]$, we have

$$\begin{aligned}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\big(M(\lambda+\mathrm{i}\varepsilon)\big)d\lambda &= \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\left(\frac{-E_f(\lambda+\mathrm{i}\varepsilon)+m_f(\lambda+\mathrm{i}\varepsilon)}{\hat{f}(\lambda+\mathrm{i}\varepsilon)\hat{f}(\lambda-\mathrm{i}\varepsilon)^*}\right)d\lambda \\ &= \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\left(\frac{-E_f(\lambda+\mathrm{i}\varepsilon)}{\hat{f}(\lambda+\mathrm{i}\varepsilon)\hat{f}(\lambda-\mathrm{i}\varepsilon)^*}\right)d\lambda \quad (4.11) \\ &+ \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\left(\frac{m_f(\lambda+\mathrm{i}\varepsilon)}{\hat{f}(\lambda+\mathrm{i}\varepsilon)\hat{f}(\lambda-\mathrm{i}\varepsilon)^*}\right)d\lambda. \quad (4.12)\end{aligned}$$

Note that the absolute value of the integrand of (4.11) is bounded since $w(\lambda)$ is continous in $[\lambda_0, \lambda_1]$ and thus bounded by the extreme value theorem, since $E_f(z)$ is entire and since we have chosen $f \in L^2_c((a,b), \mathbb{C}^2)$ such that $\hat{f}(\lambda) \neq 0$. Therefore we can use dominated convergence to obtain

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} w(\lambda) \mathrm{Im} \left(\frac{-E_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} \right) d\lambda = 0$$

as we have $E_f(z) = E_f(z^*)^*$ and thus $\mathrm{Im}(E_f(\lambda)) = 0$ for $\lambda \in \mathbb{R}$. Rewriting (4.12) yields

$$\begin{aligned}
&\lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} w(\lambda) \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} \right) d\lambda \\
&= \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} w(\lambda) \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2} \right) d\lambda \\
&\quad + \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} w(\lambda) \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{m_f(\lambda + \mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2} \right) d\lambda. \qquad (4.13)
\end{aligned}$$

We continue by estimating the integrand of (4.13).

$$\begin{aligned}
&\left| w(\lambda) \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{m_f(\lambda + \mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2} \right) \right| \\
&\leq |w(\lambda)| \, |m_f(\lambda + \mathrm{i}\varepsilon)| \left| \frac{1}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{1}{|\hat{f}(\lambda)|^2} \right|.
\end{aligned}$$

We have $|w(\lambda)| \leq C_1$ for some constant C_1 since $F(\lambda)$ is continous in $[\lambda_0, \lambda_1]$ again by the extreme value theorem. Furthermore, for $|m_f(\lambda + \mathrm{i}\varepsilon)|$ we have

$$|m_f(\lambda + \mathrm{i}\varepsilon)| = \left| \int_{\mathbb{R}} \frac{d\mu_f(t)}{t - (\lambda + \mathrm{i}\varepsilon)} \right| \leq \int_{\mathbb{R}} \frac{d\mu_f(\lambda)}{|\mathrm{i}\varepsilon|} = \frac{\mu_f(\mathbb{R})}{\varepsilon}.$$

Concerning the last expression, note that we can write $\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^* = |\hat{f}(\lambda)|^2 + O(\varepsilon)$ using Taylor series expansion. Thus we get

$$\left| \frac{1}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{1}{|\hat{f}(\lambda)|^2} \right| \leq C_2 \varepsilon$$

for some constant C_2. Combining these estimates yields

$$\left| w(\lambda) \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{m_f(\lambda + \mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2} \right) \right| \leq C_1 C_2 \mu_f(\mathbb{R})$$

which shows that the absolute value of the integrand of (4.13) is bounded. Using dominated convergence and the fact that

$$\lim_{\varepsilon \downarrow 0} \mathrm{Im} \left(\frac{m_f(\lambda + \mathrm{i}\varepsilon)}{\hat{f}(\lambda + \mathrm{i}\varepsilon)\hat{f}(\lambda - \mathrm{i}\varepsilon)^*} - \frac{m_f(\lambda + \mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2} \right) = 0$$

shows

$$\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\left(\frac{m_f(\lambda+\mathrm{i}\varepsilon)}{\hat{f}(\lambda+\mathrm{i}\varepsilon)\hat{f}(\lambda-\mathrm{i}\varepsilon)^*}-\frac{m_f(\lambda+\mathrm{i}\varepsilon)}{|\hat{f}(\lambda)|^2}\right)d\lambda = 0.$$

Altogether we have

$$\begin{aligned}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1} w(\lambda)\mathrm{Im}\big(M(\lambda+\mathrm{i}\varepsilon)\big)d\lambda &= \lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{\lambda_0}^{\lambda_1}\frac{w(\lambda)}{|\hat{f}(\lambda)|^2}\mathrm{Im}\left(m_f(\lambda+\mathrm{i}\varepsilon)\right)d\lambda\\ &= \int_{\lambda_0}^{\lambda_1}\frac{w(\lambda)}{|\hat{f}(\lambda)|^2}d\mu_f(\lambda)\end{aligned}$$

where the second equality follows from the Stieltjes inversion formula (Theorem B.5).
In order to get (4.9) we can choose $w(\lambda) = 1$ (if it is necessary, split the interval into smaller subintervals and use different functions f for the different subintervals). If we replace $w(\lambda)$ by $|\hat{f}(\lambda)|^2 w(\lambda)$, we obtain

$$\int_{\mathbb{R}} w|\hat{f}|^2 d\rho = \int_{\mathbb{R}} w d\mu_f$$

for every continuous function with compact support away from the real zeros of $\hat{f}(\lambda)$ which are discrete since $\hat{f}(z)$ is entire.
At every real zero λ_0 of $\hat{f}$ we have $\mu_f(\{\lambda_0\}) = 0$. Suppose $\mu_f(\{\lambda_0\}) > 0$. Then λ_0 must be an eigenvalue of H corresponding to the eigenfunction $\phi(\lambda_0, .)$. Then $0 < \mu_f(\{\lambda_0\}) = |\hat{f}(\lambda_0)|^2/\|\phi(\lambda_0)\|^2$ is a contradiction to $\hat{f}(\lambda_0) = 0$. Therefore we can remove the restriction "away from the real zeros of $\hat{f}(\lambda)$" which implies (4.10). □

Now we are ready to establish the main result of this chapter, that is, the spectral transformation which maps H to multiplication by λ.

Theorem 4.3. *The mapping*

$$U : L^2((a,b),\mathbb{C}^2) \to L^2(\mathbb{R}, d\rho), \qquad f \mapsto \hat{f} \tag{4.14}$$

where $\hat{f}$ is defined by

$$\hat{f}(\lambda) = \lim_{c\uparrow b}\int_a^c \phi_1(\lambda,x)f_1(x) + \phi_2(\lambda,x)f_2(x)\ dx \tag{4.15}$$

is unitary and its inverse

$$U^{-1} : L^2(\mathbb{R}, d\rho) \to L^2((a,b),\mathbb{C}^2), \qquad \hat{f} \mapsto f \tag{4.16}$$

is given by

$$f(x) = \lim_{r\to\infty}\int_{-r}^{r}\phi(\lambda,x)\hat{f}(\lambda)d\rho(\lambda) = \lim_{r\to\infty}\begin{pmatrix}\int_{-r}^{r}\phi_1(\lambda,x)\hat{f}(\lambda)\ d\rho(\lambda)\\ \int_{-r}^{r}\phi_2(\lambda,x)\hat{f}(\lambda)\ d\rho(\lambda)\end{pmatrix}. \tag{4.17}$$

Moreover, U maps H to multiplication by λ. Note that the right-hand sides of (4.15) *and* (4.17) *are to be understood as limits in in $L^2(\mathbb{R}, d\rho)$ and $L^2((a,b),\mathbb{C}^2)$, respectively.*

Proof. From (4.10) we obtain

$$\|f\|^2_{L^2((a,b),\mathbb{C}^2)} = \int_{\mathbb{R}} d\mu_f = \int_{\mathbb{R}} |\hat{f}|^2 d\rho = \|\hat{f}\|^2_{L^2(\mathbb{R},d\rho)}, \qquad f \in L^2_c((a,b),\mathbb{C}^2)$$

and conclude that the unique extension of this map to $L^2((a,b),\mathbb{C}^2)$ is isometric. (4.10) also implies

$$\langle f, F(H)f\rangle_{L^2((a,b),\mathbb{C}^2)} = \int_{\mathbb{R}} F d\mu_f = \int_{\mathbb{R}} F|\hat{f}|^2 d\rho = \langle \hat{f}, F\hat{f}\rangle_{L^2(\mathbb{R},d\rho)}, \qquad f \in L^2_c((a,b),\mathbb{C}^2)$$

for every bounded Borel function F. If we define $q_F(f) = \langle f, F(H)f\rangle_{L^2((a,b),\mathbb{C}^2)}$ and $q_F^\rho(\hat{f}) = \langle \hat{f}, F\hat{f}\rangle_{L^2(\mathbb{R},d\rho)}$, we can write this as $q_F(f) = q_F^\rho(\hat{f})$. Using the polarization identity yields

$$\begin{aligned}\langle f, F(H)g\rangle_{L^2((a,b),\mathbb{C}^2)} &= \frac{1}{4}\left(q_F(f+g) - q_F(f-g) + \mathrm{i}q_F(f-\mathrm{i}g) - \mathrm{i}q_F(f+\mathrm{i}g)\right)\\ &= \frac{1}{4}\Big(q_F^\rho(\hat{f}+\hat{g}) - q_F^\rho(\hat{f}-\hat{g}) + \mathrm{i}q_F^\rho(\hat{f}-\mathrm{i}\hat{g}) - \mathrm{i}q_F^\rho(\hat{f}+\mathrm{i}\hat{g})\Big)\\ &= \langle \hat{f}, F\hat{g}\rangle_{L^2(\mathbb{R},d\rho)}\end{aligned}$$

for $f, g \in L^2_c((a,b),\mathbb{C}^2)$ and every bounded Borel function F. By approximation we get

$$\langle f, F(H)g\rangle_{L^2((a,b),\mathbb{C}^2)} = \langle \hat{f}, F\hat{g}\rangle_{L^2(\mathbb{R},d\rho)}, \qquad f, g \in L^2((a,b),\mathbb{C}^2) \tag{4.18}$$

for every bounded Borel function F. Now consider $f, g \in L^2((a,b),\mathbb{C}^2)$ and two bounded Borel functions F, G. Set $h = F(H)g$. Then we have

$$\langle G(H)f, h - F(H)g\rangle_{L^2((a,b),\mathbb{C}^2)} = \langle G(H)f, h - h\rangle_{L^2((a,b),\mathbb{C}^2)} = 0$$

and, by (4.18), also

$$\langle G\hat{f}, \hat{h} - F\hat{g}\rangle_{L^2(\mathbb{R},d\rho)} = \int_{\mathbb{R}} G\hat{f}^*(\hat{h} - F\hat{g})\ d\rho = 0 \tag{4.19}$$

for every bounded Borel function G and thus $\hat{f}(\lambda)^*(\hat{h}(\lambda) - F\hat{g}(\lambda)) = 0$ for almost every λ with respect to the measure ρ. As we can find a function f such that $\hat{f}(\lambda_0) \neq 0$ holds for every λ_0, we even get $\hat{h} = F\hat{g}$ and conclude that $\mathrm{Ran}(U)$ contains, for example, all characteristic functions of intervals which implies $\mathrm{Ran}(U) = L^2(\mathbb{R}, d\rho)$. Altogether we see that U is unitary. This means that the inverse of U must be equal to the adjoint of U which we determine by the computation

$$\begin{aligned}\langle \hat{g}, Uf\rangle_{L^2(\mathbb{R},d\rho)} &= \int_{\mathbb{R}} \hat{g}(\lambda)^* \int_a^b \phi_1(\lambda,x)f_1(x) + \phi_2(\lambda,x)f_2(x)\ dx\ d\rho(\lambda)\\ &= \int_{\mathbb{R}}\int_a^b (\phi_1(\lambda,x)\hat{g}(\lambda)f_1(x)^* + \phi_2(\lambda,x)\hat{g}(\lambda)f_2(x)^*\ dx)^*\ d\rho(\lambda)\\ &= \int_a^b f_1(x)\left(\int_{\mathbb{R}}\phi_1(\lambda,x)\hat{g}(\lambda)d\rho(\lambda)\right)^* + f_2(x)\left(\int_{\mathbb{R}}\phi_2(\lambda,x)\hat{g}(\lambda)d\rho(\lambda)\right)^* dx\\ &= \left\langle \begin{pmatrix} \int_{\mathbb{R}}\phi_1(\lambda,x)\hat{g}(\lambda)d\rho(\lambda)\\ \int_{\mathbb{R}}\phi_2(\lambda,x)\hat{g}(\lambda)d\rho(\lambda)\end{pmatrix}, \begin{pmatrix} f_1(x)\\ f_2(x)\end{pmatrix}\right\rangle_{L^2((a,b),\mathbb{C}^2)}\\ &= \langle U^*g, f\rangle_{L^2((a,b),\mathbb{C}^2)} = \langle U^{-1}g, f\rangle_{L^2((a,b),\mathbb{C}^2)}.\end{aligned}$$

We have used Fubini's theorem to interchange the integrals in the third step and we have omited writing the limits of (4.15) and (4.17). This calculation shows that the inverse of U is indeed given by (4.17). □

We are now able to read off the spectral types from the boundary behaviour of the singular Weyl function $M(z)$ as usual.

Corollary 4.4. *The sets*

$$\begin{aligned}\Sigma_{ac} &= \{\lambda | 0 < \limsup_{\varepsilon\downarrow 0} \mathrm{Im}(M(\lambda + \mathrm{i}\varepsilon)) < \infty\},\\ \Sigma_{s} &= \{\lambda | \limsup_{\varepsilon\downarrow 0} \mathrm{Im}(M(\lambda + \mathrm{i}\varepsilon)) = \infty\}, \qquad (4.20)\\ \Sigma_{p} &= \{\lambda | \lim_{\varepsilon\downarrow 0} \varepsilon \mathrm{Im}(M(\lambda + \mathrm{i}\varepsilon)) > 0\},\\ \Sigma &= \Sigma_{ac} \cup \Sigma_{s} = \{\lambda | 0 < \limsup_{\varepsilon\downarrow 0} \mathrm{Im}(M(\lambda + \mathrm{i}\varepsilon))\} \qquad (4.21)\end{aligned}$$

are minimal supports for ρ_{ac}, ρ_s, ρ_{pp} and ρ, respectively. We could even restrict ourselves to values of λ where the lim sup *is a* lim *(finite or infinite).*
Moreover, the spectrum of H is given by the closure of Σ,

$$\sigma(H) = \overline{\Sigma}, \qquad (4.22)$$

the point spectrum (the set of eigenvalues) is given by Σ_p,

$$\sigma_p(H) = \Sigma_p, \qquad (4.23)$$

and the absolutely continuous spectrum of H is given by the essential closure of Σ_{ac},

$$\sigma(H_{ac}) = \overline{\Sigma}_{ac}^{ess}. \qquad (4.24)$$

Proof. It is sufficient to prove the claim restricted to sufficiently small intervals $[\lambda_0, \lambda_1]$. To this end, we choose $f \in L^2_c(a, b)$ such that we have $\hat{f}(\lambda) \neq 0$ for $\lambda \in [\lambda_0, \lambda_1]$ as in the proof of Lemma 4.2. Then, by Lemma 4.1, the above sets (restricted to $[\lambda_0, \lambda_1]$) remain unchanged if $M(z)$ is replaced by the Herglotz–Nevanlinna function $m_f(z)$. Moreover, the measures μ_f and ρ are mutually absolutely continuous on $[\lambda_0, \lambda_1]$. The claim then follows from the results in Section 2.2. □

Remark 4.5. *According to Remark 3.8, the singular Weyl function $M(z)$ is not unique. If we have given $\tilde{M}(z)$ as in Remark 3.8, then the spectral measures are related via*

$$d\tilde{\rho}(\lambda) = \mathrm{e}^{-2g(\lambda)} d\rho(\lambda).$$

Hence the measures are mutually absolutely continuous. The spectral transformation associated with $\tilde{M}(z)$ just differs by a simple rescaling with the function $\mathrm{e}^{-2g(\lambda)}$.

We conclude this chapter with a simple fact concerning the spectral transformation of the Green function of H which will turn out to be very useful later on.

Lemma 4.6. *Recall the Green function*

$$G(z,x,y) = \begin{pmatrix} G_{11}(z,x,y) & G_{12}(z,x,y) \\ G_{21}(z,x,y) & G_{22}(z,x,y) \end{pmatrix}$$

of H defined in (4.5)*. Then we have*

$$(UG_i(z,x,.))(\lambda) = \frac{\phi_i(\lambda,x)}{\lambda - z}, \qquad i{=}1,2 \tag{4.25}$$

for every $x \in (a,b)$ and every $z \in \mathbb{C} \setminus \sigma(H)$. Here $G_i(z,x,.)$ has to be interpreted as

$$G_i(z,x,.) = \begin{pmatrix} G_{i1}(z,x,.) \\ G_{i2}(z,x,.) \end{pmatrix}, \qquad i{=}1,2. \tag{4.26}$$

Proof. First we observe that, by (4.5), $G_i(z,x,.) \in L^2((a,b),\mathbb{C}^2)$, $i = 1,2$ for every $x \in (a,b)$ and every $z \in \mathbb{C} \setminus \sigma(H)$. Moreover, we have

$$(H-z)^{-1} f = U^{-1} \frac{1}{\lambda - z} U f \tag{4.27}$$

where the left hand side is given by (4.4) and the right hand side can be written as

$$\lim_{r\to\infty} \int_{-r}^{r} \frac{\phi(\lambda,x)}{\lambda - z} \hat{f}(\lambda) d\rho(\lambda).$$

Explicitly, (4.27) reads

$$\begin{pmatrix} \int_a^b G_{11}(z,x,.) f_1(y) + G_{12}(z,x,.) f_2(y)\ dy \\ \int_a^b G_{21}(z,x,.) f_1(y) + G_{22}(z,x,.) f_2(y)\ dy \end{pmatrix} = \begin{pmatrix} \int_{\mathbb{R}} \frac{\phi_1(\lambda,x)}{\lambda - z} \hat{f}(\lambda)\ d\rho(\lambda) \\ \int_{\mathbb{R}} \frac{\phi_2(\lambda,x)}{\lambda - z} \hat{f}(\lambda)\ d\rho(\lambda) \end{pmatrix}. \tag{4.28}$$

If we write the i-th component of (4.28) in terms of scalar products, we get

$$\left\langle \begin{pmatrix} f_1(y)^* \\ f_2(y)^* \end{pmatrix}, \begin{pmatrix} G_{i1}(z,x,.) \\ G_{i2}(z,x,.) \end{pmatrix} \right\rangle_{L^2((a,b),\mathbb{C}^2)} = \left\langle \hat{f}(\lambda)^*, \frac{\phi_i(\lambda,x)}{\lambda - z} \right\rangle_{L^2(\mathbb{R},d\rho)}, \quad i = 1,2. \tag{4.29}$$

Now we take advantage of the fact that U is unitary, that is, we have in particular $\langle f, f \rangle_{L^2((a,b),\mathbb{C}^2)} = \langle Uf, Uf \rangle_{L^2(\mathbb{R},d\rho)}$, and obtain

$$\langle \hat{f}(\lambda)^*, U(G_i(z,x,.)) \rangle_{L^2(\mathbb{R},d\rho)} = \left\langle \hat{f}(\lambda)^*, \frac{\phi_i(\lambda,x)}{\lambda - z} \right\rangle_{L^2(\mathbb{R},d\rho)} \qquad i = 1,2 \tag{4.30}$$

for every $f \in L^2((a,b),\mathbb{C}^2)$. Hence we obtain (4.25) for almost every x. If $\hat{f}$ has compact support, the left-hand side of (4.29) is continuous with respect to x and then, so is the right-hand side. Thus (4.25) follows by a density argument. □

We can even prove a stronger version of Lemma 4.6 if we differentiate with respect to z.

Corollary 4.7. *We even have*

$$(U\partial_z^k G_i(z,x,.))(\lambda) = \frac{k!\phi_i(\lambda,x)}{(\lambda-z)^{k+1}}, \qquad i{=}1{,}2 \tag{4.31}$$

for every $x \in (a,b)$, $k \in \mathbb{N}_0$ *and* $z \in \mathbb{C} \setminus \sigma(H)$.

Proof. We prove the claim by induction. For the case $k = 0$ (4.31) is just (4.25). For $k = 1$ we have

$$\partial_z(UG_i(z,x,.))(\lambda) = \partial_z\left(\frac{\phi_i(\lambda,x)}{\lambda-z}\right) = \frac{\phi_i(\lambda,x)}{(\lambda-z)^2}, \qquad i = 1,2 \tag{4.32}$$

where

$$\begin{aligned}\partial_z(UG_i(z,x,.))(\lambda) &= \partial_z\left(\lim_{c\uparrow b}\int_a^c \phi_1(\lambda,x)G_{i1}(z,x,.) + \phi_2(\lambda,x)G_{i2}(z,x,.)dx\right)\\ &= \lim_{c\uparrow b}\int_a^c \phi_1(\lambda,x)\partial_z G_{i1}(z,x,.) + \phi_2(\lambda,x)\partial_z G_{i2}(z,x,.)\ dx\\ &= (U\partial_z G_i(z,x,.))(\lambda), \qquad i = 1,2.\end{aligned} \tag{4.33}$$

Suppose (4.31) holds for $k = n$. Then we have

$$\partial_z(U\partial_z^n G_i(z,x,.))(\lambda) = \partial_z\left(\frac{n!\phi_i(\lambda,x)}{(\lambda-z)^{n+1}}\right) = \frac{(n+1)!\phi_i(\lambda,x)}{(\lambda-z)^{n+2}}, \qquad i = 1,2$$

where $\partial_z(U\partial_z^n G_i(z,x,.))(\lambda) = (U\partial_z^{n+1}G_i(z,x,.))(\lambda)$, $i = 1,2$ by performing the same computation as above with $U\partial_z^n G_i$ instead of UG_i. Thus we have verified (4.31) for every $k \in \mathbb{N}_0$. □

Chapter 5

Properties of singular Weyl functions

One of the most important properties of Herglotz–Nevanlinna functions is the existence of an integral representation. In this chapter we are going to establish such an integral representation for our singular Weyl function $M(z)$. As a consequence we will see that there is always a system of solutions such that the corresponding spectral measure is finite and that $M(z)$ is a Herglotz–Nevanlinna function. Furthermore, we will give a criterion when $M(z)$ is a generalized Nevanlinna function of the type N_κ^∞, that is, a generalized Nevanlinna function with no nonreal poles and the only generalized pole of nonpositive type at infinity. In particular, all results stated in [KST11, Section 4] remain true in the case of one-dimensional Dirac operators as well.

In order to prove the existence of an integral representation for $M(z)$, we need a result concerning the substitution rule for Lebesgue–Stieltjes integrals from [FT11].

Lemma 5.1 (cf. [FT11, (8) and (9)])**.** *Suppose μ, ν are nondecreasing functions on $\mathbb{R}$ and g is monotone. Then we have*

$$\int_{\mathbb{R}} (g \circ \mu)\, d(\nu \circ \mu) \le \int_{\mathrm{hull}(\mathrm{Ran}(\mu))} g\, d\nu \tag{5.1}$$

if μ is right continuous and g nonincreasing or μ left continuous and g nondecreasing. If μ is right continuous and g nondecreasing or μ left continuous and g nonincreasing, the inequality has to be reversed.

Theorem 5.2. *Suppose $M(z)$ is a singular Weyl function. Denote by ρ its associated spectral measure. Then there exists an entire function $g(z)$ which satisfies $g(\lambda) \ge 0$ for $\lambda \in \mathbb{R}$ and $\mathrm{e}^{-g(\lambda)} \in L^2(\mathbb{R}, d\rho)$.*
Moreover, for any entire function $\hat{g}(z)$ such that $\hat{g}(\lambda) > 0$ for $\lambda \in \mathbb{R}$ and $(1+\lambda^2)^{-1}\hat{g}(\lambda)^{-1} \in L^1(\mathbb{R}, d\rho)$ (e.g., $\hat{g}(z) = \mathrm{e}^{2g(z)}$) we have the integral representation

$$M(z) = E(z) + \hat{g}(z) \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \frac{d\rho(\lambda)}{\hat{g}(\lambda)}, \qquad z \in \mathbb{C}\backslash\sigma(H) \tag{5.2}$$

where $E(z)$ is a real entire function.

Proof. We first show that an entire function $\hat{g}$ with the required properties exists. We start by defining the function

$$R(\lambda) = \begin{cases} \int_{[-\lambda,\lambda]} d\rho, & \lambda \geq 0, \\ 0, & \lambda < 0, \end{cases} \tag{5.3}$$

and observe that it is nonnegative and nondecreasing for $\lambda > 0$. Then, by Corollary A.17, we can find an entire function $h(z) = \sum_{j=0}^{\infty} h_j z^j$ which satisfies $h(n^2) = R(n+1)$ for $n \in \mathbb{N}_0$. We choose

$$g(z) = \frac{1}{2}\sum_{j=0}^{\infty} |h_j| z^{2j}$$

and note that $g(\lambda) \geq 0$ for $\lambda \in \mathbb{R}$ is satisfied. By construction it follows

$$R(n+1) = h(n^2) = \sum_{j=0}^{\infty} h_j n^{2j} \leq \sum_{j=0}^{\infty} |h_j|\, n^{2j} = 2g(n)$$

and thus

$$R(\lambda) \leq 2g(\lambda) \text{ for } \lambda \geq 0. \tag{5.4}$$

Moreover, we have

$$\int_{\mathbb{R}} \mathrm{e}^{-2g(\lambda)} d\rho(\lambda) = \int_{[0,\infty)} \mathrm{e}^{-2g(\lambda)} dR(\lambda) \leq \int_{[0,\infty)} \mathrm{e}^{-R(\lambda)} dR(\lambda) \tag{5.5}$$

where the first step follows from the definition of $R(\lambda)$ in (5.3) and the second one from (5.4). Now, if we set $\nu(\lambda) = R(\lambda)$, $\mu(\lambda) = \lambda$ and $g(\lambda) = \mathrm{e}^{-\lambda}$, all assumptions of Lemma 5.1 are satisfied. Thus we have

$$\int_{[0,\infty)} \mathrm{e}^{-R(\lambda)} dR(\lambda) \leq \int_0^{\infty} \mathrm{e}^{-\lambda} d\lambda < \infty. \tag{5.6}$$

Combining (5.5) and (5.6) yields $\int_{\mathbb{R}} \mathrm{e}^{-2g(\lambda)} d\rho(\lambda) < \infty$ which means $\mathrm{e}^{-g(\lambda)} \in L^2(\mathbb{R}, d\rho)$.
It remains to verify the integral representation (5.2). To this end, let some $\hat{g}$ be given and set

$$\tilde{M}(z) = \hat{g}(z) \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \frac{d\rho(\lambda)}{\hat{g}(\lambda)}.$$

Note that $\tilde{M}(z)$ is holomorphic for $z \in \mathbb{C} \setminus \mathbb{R}$. Therefore we just need to show that $M(z) - \tilde{M}(z)$ is holomorphic near any point $\lambda_0 \in \mathbb{R}$. Fix $\lambda_0 \in \mathbb{R}$ and choose some real-valued function $f \in L^2_c((a,b),\mathbb{C}^2)$ such that $\hat{f}(z)$ defined in (4.1) does not vanish at λ_0.

Then, by virtue Lemma 4.1, we get

$$
\begin{aligned}
M(z) - \tilde{M}(z) &= -\frac{E_f(z)}{\hat{f}(z)^2} + \frac{m_f(z)}{\hat{f}(z)^2} - \tilde{M}(z) \\
&= -\frac{E_f(z)}{\hat{f}(z)^2} + \frac{1}{\hat{f}(z)^2}\int_{\mathbb{R}} \frac{d\mu_f(\lambda)}{\lambda - z} - \hat{g}(z)\int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\frac{d\rho(\lambda)}{\hat{g}(\lambda)} \\
&= -\frac{E_f(z)}{\hat{f}(z)^2} + \frac{1}{\hat{f}(z)^2}\int_{\mathbb{R}\setminus I} \frac{d\mu_f(\lambda)}{\lambda - z} - \hat{g}(z)\int_{\mathbb{R}\setminus I} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\frac{d\rho(\lambda)}{\hat{g}(\lambda)} \\
&\quad + \frac{1}{\hat{f}(z)^2}\int_{I} \frac{d\mu_f(\lambda)}{\lambda - z} - \hat{g}(z)\int_{I} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\frac{d\rho(\lambda)}{\hat{g}(\lambda)} \\
&= -\frac{E_f(z)}{\hat{f}(z)^2} + \frac{1}{\hat{f}(z)^2}\int_{\mathbb{R}\setminus I} \frac{d\mu_f(\lambda)}{\lambda - z} - \hat{g}(z)\int_{\mathbb{R}\setminus I} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\frac{d\rho(\lambda)}{\hat{g}(\lambda)} \\
&\quad + \hat{g}(z)\int_{I} \frac{\lambda}{1+\lambda^2}\frac{d\rho(\lambda)}{\hat{g}(\lambda)} + \int_{I} \frac{1}{\lambda - z}\left(\frac{\hat{f}(\lambda)^2}{\hat{f}(z)^2} - \frac{\hat{g}(z)}{\hat{g}(\lambda)}\right) d\rho(\lambda).
\end{aligned}
$$

Here I is some small interval which contains λ_0 such that $\hat{f}(z)$ does not vanish in a neighborhood of I. All terms in the above representation are holomorphic near λ_0. For the first four terms this is clear. Concerning the last term note that the integrand is holomorphic as a function of both variables in a neighborhood of (λ_0, λ_0). □

As a consequence, we can now show that there is always a system of solutions such that the corresponding spectral measure is finite and such that $M(z)$ is a Herglotz–Nevanlinna function. If we choose $\hat{g}(z) = \mathrm{e}^{2g(z)}$ in the previous theorem, we have

$$M(z) = E(z) + \mathrm{e}^{2g(z)} \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\frac{d\rho(\lambda)}{\mathrm{e}^{2g(\lambda)}} \tag{5.7}$$

which can be written as

$$M(z) = \tilde{E}(z) + \mathrm{e}^{2g(z)} \int_{\mathbb{R}} \frac{\mathrm{e}^{-2g(\lambda)} d\rho(\lambda)}{\lambda - z} \tag{5.8}$$

where

$$\tilde{E}(z) = E(z) - \mathrm{e}^{2g(z)} \int_{\mathbb{R}} \frac{\lambda \mathrm{e}^{-2g(\lambda)} d\rho(\lambda)}{1+\lambda^2}. \tag{5.9}$$

Setting $f(z) = -\mathrm{e}^{-g(z)}\tilde{E}(z)$ and switching to a new system of solutions as in Remark 3.8 yields

$$
\begin{aligned}
\tilde{M}(z) &= \mathrm{e}^{-2g(z)} M(z) + \mathrm{e}^{-g(z)}(-\mathrm{e}^{-g(z)}\tilde{E}(z)) = \mathrm{e}^{-2g(z)}(M(z) - \tilde{E}(z)) \\
&= \int_{\mathbb{R}} \frac{\mathrm{e}^{-2g(\lambda)} d\rho(\lambda)}{\lambda - z}.
\end{aligned}
$$

By Remark 4.5, the new measure is given by $d\tilde{\rho}(\lambda) = \mathrm{e}^{-2g(\lambda)} d\rho(\lambda)$. Note that $d\tilde{\rho}(\lambda)$ is a finite measure. In particular, we conclude that the new singular Weyl function is a Herglotz–Nevanlinna function as it can be written as the Borel transform of a finite measure.

Corollary 5.3. *There is always a system of real entire solutions $\tilde{\theta}(z,x)$ and $\tilde{\phi}(z,x)$ such that the associated spectral measure $\tilde{\rho}$ is finite and the associated singular Weyl function is a Herglotz–Nevanlinna function given by*

$$\tilde{M}(z) = \int_{\mathbb{R}} \frac{d\tilde{\rho}(\lambda)}{\lambda - z}. \tag{5.10}$$

In the case one does not want to rescale the measure too much, the entire function $\hat{g}(z) = \mathrm{e}^{-2g(z)}$ constructed in the proof of the previous theorem will not be optimal. In order to find a better $\hat{g}(z)$, note that $\phi_1(\lambda,x)^2 + \phi_2(\lambda,x)^2$ is positive for $\lambda \in \mathbb{R}$ and in $L^1(\mathbb{R},(1+\lambda^2)^{-1}d\rho)$.

Indeed, using the same notation as in (4.26), we have that $G_i(z,x,.) \in L^2((a,b),\mathbb{C}^2)$, $i = 1,2$ as already noted in the proof of Lemma 4.6. Then, by Theorem 4.3, we conclude $UG_i(z,x,.) \in L^2(\mathbb{R},d\rho)$, $i = 1,2$ which means

$$\int_{\mathbb{R}} |UG_i(z,x,.)|^2 d\rho(\lambda) < \infty, \qquad i = 1,2.$$

Plugging in (4.25), we obtain

$$\int_{\mathbb{R}} \frac{\phi_i(\lambda,x)^2}{|\lambda - z|^2} d\rho(\lambda) < \infty, \qquad i = 1,2$$

independently of the value of z. If we now choose $z = \mathrm{i}$, we obviously have $\phi_i(\lambda,x)^2 \in L^1(\mathbb{R},(1+\lambda^2)^{-1}d\rho)$, $i = 1,2$ which is then clearly true for every linear combination as well.

We will show in Chapter 6 that $M(z)$ is always a Herglotz–Nevanlinna function if one has the limit circle case at the endpoint a.

As another consequence of the established integral representation we get a criterion when our singular Weyl function $M(z)$ is a generalized Nevanlinna function with no nonreal poles and the only generalized pole of nonpositive type at infinity. We denote the set of all such functions by N_κ^∞. Further information concerning generalized Nevanlinna functions is provided in Appendix B.2.

Theorem 5.4. *Fix the solution $\phi(z,x)$. Then there is a corresponding solution $\theta(z,x)$ such that $M(z) \in N_\kappa^\infty$ for some $\kappa \le k$ if and only if $(1+\lambda^2)^{-k-1} \in L^1(\mathbb{R},d\rho)$. Moreover, $\kappa = k$ if $k = 0$ or $(1+\lambda^2)^{-k} \not\in L^1(\mathbb{R},d\rho)$.*

Proof. Suppose $(1+\lambda^2)^{-k-1} \in L^1(\mathbb{R},d\rho)$. Then we can choose $\hat{g}(z) = (1+z^2)^k$ and by Theorem 5.2 we have

$$M(z) = f(z) + (1+z^2)^k \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \frac{d\rho(\lambda)}{(1+\lambda^2)^k}$$

where $f(z)$ is an entire function. Now we invoke Remark 3.8 and set $\tilde{\theta}(z,x) = \theta(z,x) - f(z)\phi(z,x)$ (note that here we have chosen $g(z) \equiv 0$ in Remark 3.8). Then, our corresponding Weyl function reads

$$\tilde{M}(z) = M(z) - f(z) = (1+z^2)^k \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \frac{d\rho(\lambda)}{(1+\lambda^2)^k}. \tag{5.11}$$

As (5.11) coincides with (B.13) we have $M(z) \in N_\kappa^\infty$ for some $\kappa \leq k$ by Theorem B.9. Conversely, let $M(z) \in N_\kappa^\infty$ for some $\kappa \leq k$. Then, $M(z)$ admits the integral representation (B.13)–(B.14) where the measure $d\rho$ coincides with the one from Lemma 4.2. Thus, by (B.14), we get $(1+\lambda^2)^{-k-1} \in L^1(\mathbb{R}, d\rho)$. The last claim also follows from Theorem B.9. □

The condition $(1+\lambda^2)^{-k-1} \in L^1(\mathbb{R}, d\rho)$ is related to the growth of $M(z)$ along the imaginary axis (cf. Lemma B.10). One can try to bound λ^{-k} by a linear combination of $\phi_1(\lambda, x)^2$ and $\phi_2(\lambda, x)^2$ (which is in $L^1(\mathbb{R}, (1+\lambda^2)^{-1} d\rho)$) in order to identify possible values of k.

Chapter 6

The limit circle case

In this chapter we are going to extend [KST11, Appendix A] to the case of one-dimensional Dirac operators, that is, we show that the singular Weyl function is a Herglotz–Nevanlinna function whenever τ is limit circle at a. To this end, we start with a Hypothesis which will turn out to be equivalent to the claim that τ is limit circle at a.

Hypothesis 6.1. *Fix $\lambda_0 \in \mathbb{R}$. Suppose*

$$\phi_0(x) = \begin{pmatrix} \phi_{0,1}(x) \\ \phi_{0,2}(x) \end{pmatrix} \qquad \text{and} \qquad \theta_0(x) = \begin{pmatrix} \theta_{0,1}(x) \\ \theta_{0,2}(x) \end{pmatrix} \tag{6.1}$$

are two real-valued solutions of $\tau u = \lambda_0 u$ which satisfy $W(\theta_0, \phi_0) = 1$. Assume that the limits

$$\lim_{x \to a} W_x(\phi_0, u(z)) \qquad \text{and} \qquad \lim_{x \to a} W_x(\theta_0, u(z)) \tag{6.2}$$

exist for every solution $u(z, x)$ of $\tau u = zu$.

Remark 6.2. *Hypothesis 6.1 is independent of the choice of λ_0.*

Indeed, let $\phi_1(x)$ and $\theta_1(x)$ be two real-valued solutions of $\tau u = \lambda_1 u$ for some $\lambda_1 \in \mathbb{R}$, $\lambda_0 \neq \lambda_1$ which satisfy $W(\theta_1, \phi_1) = 1$. Setting $f_1 = \phi_0(x)$, $f_2 = \phi_1(x)$, $f_3 = \theta_0(x)$ and $f_4 = u(z, x)$ in the Plücker identity (1.11) and using $W(\theta_0, \phi_0) = 1$ yields

$$W_x(\phi_1, u(z)) = W_x(\phi_0, \phi_1) W_x(\theta_0, u(z)) - W_x(\phi_0, u(z)) W_x(\theta_0, \phi_1). \tag{6.3}$$

The Plücker identity (1.11) remains valid in the limit $x \to a$. If Hypothesis 6.1 holds, the limit $\lim_{x \to a} W_x(\phi_1, u(z))$ exists as then all limits on the right-hand side of (6.3) exist. To see that $\lim_{x \to a} W_x(\theta_1, u(z))$ exists as well, one needs just to replace $\phi_1(x)$ by $\theta_1(x)$ in the above calculation. Altogether we have shown that, if Hypothesis 6.1 holds for one $\lambda_0 \in \mathbb{R}$, it also holds for any other $\lambda_1 \in \mathbb{R}$, $\lambda_0 \neq \lambda_1$ which justifies Remark 6.2.

Lemma 6.3. *Suppose τ is limit circle at a. Then Hypothesis 6.1 holds. In this case, the limits* (6.2) *are holomorphic with respect to z whenever $u(z, x)$ is.*

Proof. For a solution $u(x)$ of $\tau u = zu$ and a solution $v(x)$ of $\tau v = \hat{z}v$ we have

$$(z-\hat{z})\int_c^x (u(y)^*, v(y))\ dy = W_x(u,v) - W_c(u,v). \tag{6.4}$$

First, we note that both sides of (6.4) are equal at $x = c$. Next, we compute the derivatives with respect to x of both sides of (6.4). For the right-hand side we get

$$\begin{aligned}(W_x(u,v) - W_c(u,v))' &= (u_1(x)v_2(x) - u_2(x)v_1(x))' \\ &= u_1'(x)v_2(x) + u_1(x)v_2'(x) - u_2'(x)v_1(x) - u_2(x)v_1'(x)\end{aligned}$$

whereas differentiating the left-hand side yields

$$\begin{aligned}\left((z-\hat{z})\int_c^x (u(y)^*, v(y))\,dy\right)' &= \left(\int_c^x z\,(u(y)^*, v(y)) + \hat{z}\,(u(y)^*, v(y))\,dy\right)' \\ &= \left(\int_c^x ((\tau u(y))^*, v(y)) + (u(y)^*, \tau v(y))\,dy\right)' \\ &= u_1'(x)v_2(x) + u_1(x)v_2'(x) - u_2'(x)v_1(x) - u_2(x)v_1'(x).\end{aligned}$$

As the derivatives coincide as well, (6.4) holds. In particular, this shows that we have

$$\lim_{x\to a} W_x(\phi_0, u(z)) = W_c(\phi_0, u(z)) - (\lambda_0 - z)\int_a^c (\phi_0(y), u(z,y))\,dy, \tag{6.5}$$

$$\lim_{x\to a} W_x(\theta_0, u(z)) = W_c(\theta_0, u(z)) - (\lambda_0 - z)\int_a^c (\theta_0(y), u(z,y))\,dy. \tag{6.6}$$

As τ is limit circle at a, all solutions of $\tau u = zu$ are square integrable near a for all $z \in \mathbb{C}$ and thus $\lim_{x\to a} W_x(\phi_0, u(z))$ and $\lim_{x\to a} W_x(\theta_0, u(z))$ exist.
In order to see that the limits (6.2) are holomorphic with respect to z whenever $u(z,x)$ is, we need to show that the integrals on the right-hand side of (6.5) and (6.6) are holomorphic if $u(z,x)$ is holomorphic in a neighborhood of z_0. To this end, we recall Lemma 1.7. We suppose $(\tau - z)u = 0$ and choose $c(z_0,x)$ and $s(z_0,x)$ as the fundamental system of $(\tau - z_0)u = 0$ which satisfies $W(c(z_0), s(z_0)) = 1$. Using $(\tau - z_0)u = (z - z_0)g$ and (1.10) we get

$$\begin{aligned}u(z,x) = {} & \alpha c(z_0,x) + \beta s(z_0,x) \\ & + (z-z_0)\int_c^x (s(z_0,x)\,(c(z_0,y)^*, u(z,y)) - c(z_0,x)\,(s(z_0,y)^*, u(z,y)))\,dy.\end{aligned} \tag{6.7}$$

Since $c \in L^2((c,b),\mathbb{C}^2)$ and $s \in L^2((c,b),\mathbb{C}^2)$, we can find a constant $M \geq 0$ such that

$$\int_c^b |c_j(z_0,y)|^2\ dy \leq M \quad \text{and} \quad \int_c^b |s_j(z_0,y)|^2\ dy \leq M \tag{6.8}$$

where $c_j(z_0,y)$ and $s_j(z_0,y)$ denote the j-th component of $c(z_0,y)$ and $s(z_0,y)$, respectively. We consider temporarily just

$$\int_c^x (s(z_0,x)\,(c(z_0,y)^*, u(z,y)) - c(z_0,x)\,(s(z_0,y)^*, u(z,y)))\,dy \tag{6.9}$$

and choose c close enough to b such that $|z - z_0|^2 M^2 \leq 1/24$ holds.

Estimating the first component of (6.9) using the inequality of Cauchy-Schwarz yields

$$\begin{aligned}
&\left| \int_c^x (s_1(z_0,x)\,(c(z_0,y)^*, u(z,y)) - c_1(z_0,x)\,(s(z_0,y)^*, u(z,y)))\,dy \right|^2 \\
&= \left| \int_c^x (s_1(z_0,x)c_1(z_0,y) - c_1(z_0,x)s_1(z_0,y))u_1(z,y)dy \right. \\
&\quad \left. + (s_1(z_0,x)c_2(z_0,y) - c_1(z_0,x)s_2(z_0,y))u_2(z,y)dy \right|^2 \\
&= \left| \int_c^x \left(\begin{pmatrix} (s_1(z_0,x)c_1(z_0,y) - c_1(z_0,x)s_1(z_0,y))^* \\ (s_1(z_0,x)c_2(z_0,y) - c_1(z_0,x)s_2(z_0,y))^* \end{pmatrix}, \begin{pmatrix} u_1(z,y) \\ u_2(z,y) \end{pmatrix} \right) dy \right|^2 \\
&\le \left(\int_c^x |s_1(z_0,x)c_1(z_0,y) - c_1(z_0,x)s_1(z_0,y)|^2 \right. \\
&\quad \left. + |s_1(z_0,x)c_2(z_0,y) - c_1(z_0,x)s_2(z_0,y)|^2 dy \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \\
&\le \left(|s_1(z_0,x)|^2 \int_c^x |s_1(z_0,y)|^2 dy + |c_1(z_0,x)|^2 \int_c^x |c_1(z_0,y)|^2 dy + |s_1(z_0,x)|^2 \int_c^x |c_2(z_0,y)|^2 dy \right. \\
&\quad \left. + |c_1(z_0,x)|^2 \int_c^x |s_2(z_0,y)|^2 dy \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \\
&\le 2M \left(|c_1(z_0,x)|^2 + |s_1(z_0,x)|^2 \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy.
\end{aligned}$$

By applying the same estimate to the second component of (6.9) we get

$$\begin{aligned}
&\left| \int_c^x (s_2(z_0,x)\,(c(z_0,y)^*, u(z,y)) - c_2(z_0,x)\,(s(z_0,y)^*, u(z,y)))\,dy \right|^2 \\
&\le 2M \left(|c_2(z_0,x)|^2 + |s_2(z_0,x)|^2 \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy.
\end{aligned}$$

Then we are able to conclude

$$\begin{aligned}
&\int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \\
&\le 3 \left(|\alpha|^2 \int_c^x |c_1(z_0,y)|^2 dy + |\beta|^2 \int_c^x |s_1(z_0,y)|^2 dy + \right. \\
&\quad + 2M|z-z_0|^2 \left(\int_c^x |c_1(z_0,y)|^2 dy + \int_c^x |s_1(z_0,y)|^2 dy \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \\
&\quad + |\alpha|^2 \int_c^x |c_2(z_0,y)|^2 dy + |\beta|^2 \int_c^x |s_2(z_0,y)|^2 dy + \\
&\quad \left. + 2M|z-z_0|^2 \left(\int_c^x |c_2(z_0,y)|^2 dy + \int_c^x |s_2(z_0,y)|^2 dy \right) \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \right) \\
&\le 6M(|\alpha|^2 + |\beta|^2) + 12M^2|z-z_0|^2 \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \\
&\le 6M(|\alpha|^2 + |\beta|^2) + \frac{1}{2} \int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy,
\end{aligned}$$

and thus we have

$$\int_c^x |u_1(z,y)|^2 + |u_2(z,y)|^2 dy \le 12M(|\alpha|^2 + |\beta|^2).$$

Plugging in this estimate, we get

$$\begin{aligned}
&\left| \int_c^x \left(s_1(z_0,x)\left(c(z_0,y)^*, u(z,y)\right) - c_1(z_0,x)\left(s(z_0,y)^*, u(z,y)\right)\right) dy \right| \\
&\le \sqrt{24}M(|\alpha| + |\beta|)(|c_1(z_0,x)| + |s_1(z_0,x)|), \\
&\left| \int_c^x \left(s_2(z_0,x)\left(c(z_0,y)^*, u(z,y)\right) - c_2(z_0,x)\left(s(z_0,y)^*, u(z,y)\right)\right) dy \right| \\
&\le \sqrt{24}M(|\alpha| + |\beta|)(|c_2(z_0,x)| + |s_2(z_0,x)|).
\end{aligned}$$

Altogether, for all z in a bounded neighborhood of z_0 we have

$$|u_1(z,x)| \le C_1|c_1(z_0,x)| + C_2|s_1(z_0,x)| \quad \text{and} \quad |u_2(z,x)| \le C_1|c_2(z_0,x)| + C_2|s_2(z_0,x)|$$

where $C_1 = |\alpha| + \sqrt{24}M(|\alpha| + |\beta|)$ and $C_2 = |\beta| + \sqrt{24}M(|\alpha| + |\beta|)$. Furthermore, we get

$$|u_1'(z,x)| \le C_3|c_1'(z_0,x)| + C_4|s_1'(z_0,x)| \quad \text{and} \quad |u_2'(z,x)| \le C_3|c_2'(z_0,x)| + C_4|s_2'(z_0,x)|$$

for some other constants C_3 and C_4. This shows that we have integrable bounds of the integrands independent of z in (6.5) and (6.6) and thus the limits (6.2) are holomorphic in the same domain as $u(z,x)$. □

Let now τ satisfy Hypothesis 6.1 and set

$$\phi(z,x) = W_a(c(z),\phi_0)s(z,x) - W_a(s(z),\phi_0)c(z,x), \tag{6.10}$$
$$\theta(z,x) = W_a(c(z),\theta_0)s(z,x) - W_a(s(z),\theta_0)c(z,x). \tag{6.11}$$

The solutions $s(z,x)$ and $c(z,x)$ are defined in the same way as in Section 1.5. Observe that we have $\phi(z,x)^* = \phi(z^*,x)$ and $\theta(z,x)^* = \theta(z^*,x)$. Moreover, an easy calculation shows $\phi(\lambda_0,x) = \phi_0(x)$ and $\theta(\lambda_0,x) = \theta_0(x)$.

Lemma 6.4. *Suppose Hypothesis 6.1. Then the solutions $\phi(z,x)$ and $\theta(z,x)$ defined in* (6.10) *and* (6.11) *satisfy the identities*

$$W(\theta(z),\phi(z)) = 1, \tag{6.12}$$
$$W_a(\theta(z),\phi(\hat{z})) = 1, \tag{6.13}$$
$$W_a(\phi(\hat{z}),\phi(z)) = W_a(\theta(\hat{z}),\theta(z)) = 0. \tag{6.14}$$

Proof. It suffices to show (6.13) and (6.14).

$$\begin{aligned}
W_a(\theta(z),\phi(\hat{z})) = &- W_a(c(\hat{z}),\phi_0)\left(W_a(c(z),\theta_0)W_a(s(\hat{z}),s(z)) - W_a(s(z),\theta_0)W_a(s(\hat{z}),c(z))\right) \\
&+ W_a(s(\hat{z}),\phi_0)\left(W_a(s(z),\theta_0)W_a(c(\hat{z}),s(z)) - W_a(s(z),\theta_0)W_a(c(\hat{z}),c(z))\right).
\end{aligned}$$

Choosing $f_1 = c(z)$, $f_2 = \theta_0$, $f_3 = c(\hat{z})$ and $f_4 = s(z)$ in (1.11) yields

$$W_x(s(\hat{z}), \theta_0) = W_x(c(z), \theta_0)W_x(s(\hat{z}), s(z)) - W_x(s(z), \theta_0)W_x(s(\hat{z}), c(z)),$$

and by replacing $c(\hat{z})$ by $s(\hat{z})$ we obtain

$$W_x(c(\hat{z}), \theta_0) = W_x(c(z), \theta_0)W_x(c(\hat{z}), s(z)) - W_x(s(z), \theta_0)W_x(c(\hat{z}), c(z)).$$

As the Plücker identity remains valid in the limit $x \to a$ we have

$$\begin{aligned} W_a(\theta(z), \phi(\hat{z})) = &-W_a(c(\hat{z}), \theta_0)W_a(s(\hat{z}), \theta_0) + W_a(s(\hat{z}, \theta_0)W_a(c(\hat{z}), \theta_0) \\ =&W_a(c(\hat{z}), s(\hat{z}))W_a(\theta_0, \phi_0) = 1 \end{aligned}$$

as stated. For $z = \hat{z}$ this is clearly (6.12), so it remains only to show (6.14).

$$\begin{aligned} W_a(\phi(\hat{z}), \phi(z)) =& W_a(c(\hat{z}), \phi_0)\left(W_a(c(z), \phi_0)W_a(s(\hat{z}), s(z)) - W_a(s(z), \phi_0)W_a(s(\hat{z}), c(z))\right) \\ &- W_a(s(\hat{z}), \phi_0)\left(W_a(c(z), \phi_0)W_a(c(\hat{z}, s(z)) - W_a(s(z), \phi_0)W_a(c(\hat{z}), c(z))\right) \end{aligned}$$

Now we choose $f_1 = c(z)$, $f_2 = \phi_0$, $f_3 = s(\hat{z})$ and $f_4 = s(z)$ in (1.11) to get

$$W_x(s(\hat{z}), \phi_0) = W_x(c(z), \phi_0)W_x(s(\hat{z}), s(z)) - W_x(s(z), \phi_0)W_x(s(\hat{z}), c(z))$$

and replace $s(\hat{z})$ by $c(\hat{z})$ to obtain

$$W_x(c(\hat{z}), \phi_0) = W_x(c(z), \phi_0)W_x(c(\hat{z}), s(z)) - W_x(s(z), \phi_0)W_x(c(\hat{z}), c(z)).$$

Again, by letting $x \to a$ and plugging in we get

$$W_a(\phi(\hat{z}), \phi(z)) = W_a(c(\hat{z}), \phi_0)W_a(s(\hat{z}), \phi_0) - W_a(s(\hat{z}), \phi_0)W_a(c(\hat{z}), \phi_0) = 0.$$

Replacing ϕ by θ in the above calculation shows $W_a(\phi(\hat{z}), \phi(z)) = 0$. ☐

Now we will prove that Hypothesis 6.1 is in fact equivalent to τ being limit circle at a.

Corollary 6.5. *If Hypothesis 6.1 holds, then τ is limit circle at a. Moreover, the solutions $\phi(z, x)$ and $\theta(z, x)$ defined in* (6.10) *and* (6.11) *satisfy*

$$W_c(\phi(z)^*, \phi(z)) = -2\mathrm{i}\mathrm{Im}(z)\int_a^c \|\phi(z, x)\|^2_{\mathbb{C}^2}\, dx, \tag{6.15}$$

$$W_c(\theta(z)^*, \theta(z)) = -2\mathrm{i}\mathrm{Im}(z)\int_a^c \|\theta(z, x)\|^2_{\mathbb{C}^2}\, dx \tag{6.16}$$

and are entire with respect to z.

Proof. We recall (6.4) and choose $u(y) = \phi(z, y)$ and $v(y) = \phi(z, y)^*$. Then we have

$$(z - z^*)\int_c^x (\phi(z, y)^*, \phi(z^*, y))\, dy = W_x(\phi(z), \phi(z^*)) - W_c(\phi(z), \phi(z^*))$$

which can be rewritten to

$$2\mathrm{iIm}(z)\int_c^x \|\phi(z,y)\|_{\mathbb{C}^2}^2\, dy = W_x(\phi(z),\phi(z^*)) - W_c(\phi(z),\phi(z)^*).$$

Letting $x \to a$ and using Lemma 6.4 proves (6.15). To obtain (6.16), just set $u(y) = \theta(z,y)$ and $v(y) = \theta(z,y)^*$ in (6.4) and perform the same calculation as above. As both integrals on the right hand sides of (6.15) and (6.16) are finite, $\phi(z,x)$ and $\theta(z,x)$ are square integrable near a and thus τ is limit circle at a. But then, by Lemma 6.3, we get that both solutions are entire. □

Lemma 6.6. *Suppose Hypothesis 6.1, let H be some self-adjoint operator associated with τ and let the boundary condition at a be induced by ϕ_0.*
Then $\phi(z,x)$ defined in (6.10) *lies in the domain of H near a. Moreover, we have*

$$m_-(z) = \frac{W_a(\phi_0, c(z))}{W_a(\phi_0, s(z))}. \tag{6.17}$$

Proof. In order to prove that $\phi(z,x)$ lies in the domain of H near a, one needs just to verify $W_a(\phi(z),\phi_0) = 0$ by a direct calculation using (6.10).
Now recall $u_-(z,x)$ defined in (1.28) and note that $u_-(z,x)$ and $\phi_0(x)$ are both in the domain of H near a, that is, $W_a(\phi_0, u(z)) = 0$. Using (1.29), we calculate $0 = W_a(\phi_0, c(z) - m_-(z)s(z)) = W_a(\phi_0, c(z)) - m_-(z)W_a(\phi_0, s(z))$ which shows (6.17). □

Now we are able to introduce the singular Weyl function $M(z)$ as in Chapter 3 such that

$$\psi(z,x) = \theta(z,x) + M(z)\phi(z,x) \in L^2((c,b),\mathbb{C}^2) \tag{6.18}$$

and $\psi(z,x)$ satisfies the boundary condition of H at b if τ is limit circle at b.

Now we are ready to prove the main result of this chapter.

Theorem 6.7. *Suppose Hypothesis 6.1. Let H be some self-adjoint operator associated with τ and let the boundary condition at a be induced by ϕ_0. Then the singular Weyl function defined in* (6.18) *is a Herglotz–Nevanlinna function and satisfies*

$$\mathrm{Im}(M(z)) = \mathrm{Im}(z)\int_a^b \|\psi(z,x)\|_{\mathbb{C}^2}^2\, dx. \tag{6.19}$$

Proof. Fixing z and setting $c = a$, $u(y) = \psi(z,y)$ and $v(y) = \psi(z,y)^*$ in (6.4) yields

$$(z - z^*)\int_a^x (\psi(z,y)^*, \psi(z,y)^*)\, dy = W_x(\psi(z),\psi(z)^*) - W_a(\psi(z),\psi(z)^*) \tag{6.20}$$

For the left-hand side we get

$$(z - z^*)\int_a^x (\psi(z,y)^*, \psi(z,y)^*)\, dy = 2\mathrm{iIm}(z)\int_a^x \|\psi(z,y)\|_{\mathbb{C}^2}^2\, dy.$$

Next, by a straightforward calculation using (6.18) and Lemma 6.4 we obtain

$$\begin{aligned} W_a(\psi(z),\psi(z)^*) &= W_a(\theta(z),\theta(z^*)) + M(z)^* W_a(\theta(z),\phi(z)^*) \\ &\quad + M(z) W_a(\phi(z),\theta(z^*)) + |M(z)|^2 W_a(\phi(z),\phi(z^*)) \\ &= M(z)^* - M(z) \\ &= -2\mathrm{i}\mathrm{Im}(M(z)). \end{aligned}$$

Altogether, we have

$$\mathrm{Im}(z) \int_a^x \|\psi(z,y)\|_{\mathbb{C}^2}^2 \, dy = -\frac{\mathrm{i}}{2} W_x(\psi(z),\psi(z^*)) + \mathrm{Im}(M(z)).$$

Letting $x \to b$ and observing that we have $W_b(\psi(z),\psi(z^*)) = 0$ as $\psi(z)$ and $\psi(z^*)$ are both in the domain of H near b proves (6.19). This formula shows that for $z \in \mathbb{C}_+$ we have $M(z) \in \mathbb{C}_+$ and thus $M(z)$ is indeed a Herglotz–Nevanlinna function. □

Lemma 6.8. *Suppose Hypothesis 6.1. Let H be some self-adjoint operator associated with τ and let the boundary condition at a be induced by ϕ_0. Denote by U the associated spectral transform from Chapter 4. Then we have*

$$(U\psi(z,.))(\lambda) = \frac{1}{\lambda - z} \tag{6.21}$$

for every $z \in \mathbb{C} \setminus \sigma(H)$. Differentiating with respect to z we even obtain

$$(U\partial_z^k \psi(z,.))(\lambda) = \frac{k!}{(\lambda - z)^{k+1}}. \tag{6.22}$$

Proof. Recall the Green function

$$G(z,x,y) = \begin{pmatrix} G_{11}(z,x,y) & G_{12}(z,x,y) \\ G_{21}(z,x,y) & G_{22}(z,x,y) \end{pmatrix}$$

of H given by (4.5). By $G_1(z,x,y)$ and $G_2(z,x,y)$ we denote the first and the second column of $G(z,x,y)$, respectively. By use of (6.18) we calculate

$$\begin{aligned} W_x(\theta(z), G_1(z,y)) &= \theta_1(z,x) G_{21}(z,x,y) - \theta_2(z,x) G_{11}(z,x,y) \\ &= \begin{cases} \theta_1(z,x)\psi_2(z,x)\phi_1(z,y) - \theta_2(z,x)\psi_1(z,x)\phi_1(z,y), & y < x, \\ \theta_1(z,x)\phi_2(z,x)\psi_1(z,y) - \theta_2(z,x)\phi_1(z,x)\psi_1(z,y), & y > x, \end{cases} \\ &= \begin{cases} W_x(\theta(z),\theta(z))\phi_1(z,y) + W_x(\theta(z),\phi(z)) M(z)\phi_1(z,y), & y < x, \\ W_x(\theta(z),\phi(z))\theta_1(z,y) + W_x(\theta(z),\phi(z)) M(z)\phi_1(z,y), & y > x, \end{cases} \\ &= \begin{cases} M(z)\phi_1(z,y), & y < x, \\ \theta_1(z,y) + M(z)\phi_1(z,y), & y > x. \end{cases} \end{aligned}$$

Analogously, we get

$$\begin{aligned} W_x(\theta(z), G_2(z,y)) &= \theta_1(z,x)G_{22}(z,x,y) - \theta_2(z,x)G_{12}(z,x,y) \\ &= \begin{cases} \theta_1(z,x)\psi_2(z,x)\phi_2(z,y) - \theta_2(z,x)\psi_1(z,x)\phi_2(z,y), & y < x, \\ \theta_1(z,x)\phi_2(z,x)\psi_2(z,y) - \theta_2(z,x)\phi_1(z,x)\psi_2(z,y), & y > x, \end{cases} \\ &= \begin{cases} W_x(\theta(z),\theta(z))\phi_2(z,y) + W_x(\theta(z),\phi(z))M(z)\phi_2(z,y), & y < x, \\ W_x(\theta(z),\phi(z))\theta_2(z,y) + W_x(\theta(z),\phi(z))M(z)\phi_2(z,y), & y > x, \end{cases} \\ &= \begin{cases} M(z)\phi_2(z,y), & y < x, \\ \theta_2(z,y) + M(z)\phi_2(z,y), & y > x. \end{cases} \end{aligned}$$

Next, we set

$$\tilde{\psi}(z,x,y) = \begin{pmatrix} W_x(\theta(z), G_1(z,y)) \\ W_x(\theta(z), G_2(z,y)) \end{pmatrix} = \begin{cases} M(z)\phi(z,y), & y < x, \\ \psi(z,y), & y > x. \end{cases} \tag{6.23}$$

Observe that we have

$$\lim_{x \to a} \tilde{\psi}(z,x,y) = \psi(z,y).$$

We will now derive the spectral transformation of $\tilde{\psi}$.

$$\begin{aligned} (U\tilde{\psi}(z,x,.))(\lambda) &= \lim_{c \uparrow b} \int_a^c \phi_1(\lambda,y)W_x(\theta(z),G_1(z,y)) + \phi_2(z,y)W_x(\theta(z),G_2(z,y))dy \\ &= \theta_1(z,x)\lim_{c \uparrow b} \int_a^c \phi_1(\lambda,y)G_{21}(z,x,y) + \phi_2(\lambda,y)G_{22}(z,x,y)dy \\ &\quad - \theta_2(z,x)\lim_{c \uparrow b} \int_a^c \phi_1(\lambda,y)G_{11}(z,x,y) + \phi_2(\lambda,y)G_{12}(z,x,y)dy \\ &= \theta_1(z,x)(UG_{2j}(z,x,.))(\lambda) - \theta_2(z,x)(UG_{1j}(z,x,.))(\lambda) \\ &= \theta_1(z,x)\frac{\phi_2(\lambda,x)}{\lambda - z} - \theta_2(z,x)\frac{\phi_1(\lambda,x)}{\lambda - z} \\ &= \frac{W_x(\theta(z),\phi(\lambda))}{\lambda - z}. \end{aligned}$$

Letting $x \to a$ and using Lemma 6.4 shows (6.21). (6.22) is proven by induction with respect to k which is done similar as in the proof of Corollary 4.7. □

We conclude this chapter by refining the integral representation of $M(z)$ which has been established in Theorem 5.2.

Corollary 6.9. *Suppose the same assumptions as in Theorem 6.7. Then we have*

$$M(z) = \mathrm{Re}(M(\mathrm{i})) + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) d\rho(\lambda), \tag{6.24}$$

where ρ (which is exactly the spectral measure from Chapter 4) satisfies $\int_{\mathbb{R}} d\rho = \infty$ and $\int_{\mathbb{R}} \frac{d\rho(\lambda)}{1+\lambda^2} < \infty$.

Proof. First, we rewrite (6.19) by using unitarity of $U : L^2((a,b),\mathbb{C}^2) \to L^2(\mathbb{R}, d\rho)$, that is, we have $\|U\psi\|_{L^2(\mathbb{R},d\rho)} = \|\psi\|_{L^2((a,b),\mathbb{C}^2)}$, and Lemma 6.8 to obtain

$$\begin{aligned}\operatorname{Im}(M(z)) &= \operatorname{Im}(z)\int_a^b \|\psi(z,x)\|^2_{\mathbb{C}^2}\,dx = \operatorname{Im}(z)\|\psi(z,x)\|^2_{L^2((a,b),\mathbb{C}^2)}\\ &= \operatorname{Im}(z)\|(U\psi(z,.))(\lambda)\|^2_{L^2(\mathbb{R},d\rho)} = \operatorname{Im}(z)\int_{\mathbb{R}}(U\psi(z,.))(\lambda)^2\,d\rho(\lambda)\\ &= \int_{\mathbb{R}}\frac{\operatorname{Im}(z)}{|\lambda-z|^2}d\rho(\lambda).\end{aligned}$$

The calculation

$$\begin{aligned}\operatorname{Im}(M(z)) &= \operatorname{Im}(\operatorname{Re}(M(\mathrm{i})) + \operatorname{Im}\left(\int_{\mathbb{R}}\left(\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\right)d\rho(\lambda)\right)\\ &= \int_{\mathbb{R}}\operatorname{Im}\left(\frac{1}{\lambda-z}-\frac{\lambda}{1+\lambda^2}\right)d\rho(\lambda)\\ &= \int_{\mathbb{R}}\frac{\operatorname{Im}(z)}{|\lambda-z|^2}d\rho(\lambda)\end{aligned}$$

shows that the imaginary part of the representation (6.24) coincides with the one of $M(z)$. Next, we consider the real part of (6.24) at $z = \mathrm{i}$. By

$$\begin{aligned}\operatorname{Re}\left(\int_{\mathbb{R}}\left(\frac{1}{\lambda-\mathrm{i}}-\frac{\lambda}{1+\lambda^2}\right)d\rho(\lambda)\right) &= \int_{\mathbb{R}}\left(\operatorname{Re}\left(\frac{1}{\lambda-\mathrm{i}}\right)-\operatorname{Re}\left(\frac{\lambda}{1+\lambda^2}\right)\right)d\rho(\lambda)\\ &= \int_{\mathbb{R}}\left(\operatorname{Re}\left(\frac{\lambda+\mathrm{i}}{1+\lambda^2}\right)-\operatorname{Re}\left(\frac{\lambda}{1+\lambda^2}\right)\right)d\rho(\lambda)\\ &= 0,\end{aligned}$$

the real parts of $M(z)$ and the right-hand side of (6.24) coincide at $z = \mathrm{i}$. As a holomorphic function is determined by its imaginary part up to a real constant, we have proved the integral representation (6.24).
Moreover, we have

$$\operatorname{Im}(M(\mathrm{i})) = \int_{\mathbb{R}}\frac{\operatorname{Im}(\mathrm{i})}{|\lambda-\mathrm{i}|^2}d\rho(\lambda) = \int_{\mathbb{R}}\frac{d\rho(\lambda)}{1+\lambda^2}$$

and

$$\operatorname{Im}(M(\mathrm{i})) = \int_a^b \|\psi(\mathrm{i},x)\|^2_{\mathbb{C}^2}dx$$

which shows $\int_{\mathbb{R}}\frac{1}{1+\lambda^2}d\rho(\lambda) < \infty$ as $\psi \in L^2((a,b),\mathbb{C}^2)$.
If $\int_{\mathbb{R}} d\rho < \infty$, we would have $(z-\lambda)(U\psi(z,.))(\lambda) \in L^2(\mathbb{R}, d\rho)$ by Lemma 6.21 and thus $(U\psi(z,.))(\lambda) \in \mathfrak{D}(U^{-1}HU)$ which implies $\psi \in \mathfrak{D}(H)$, a contradiction. Therefore we have $\int_{\mathbb{R}} d\rho = \infty$ as stated. □

Chapter 7

An example: the radial Dirac operator

In this chapter we provide a prototypical example of a Dirac operator with two singular endpoints, namely the radial Dirac operator with a Coulomb potential. We will use this explicit example to illustrate some results from the foregoing chapters. Concerning the derivation of the solutions presented below we follow [GTV07, Section 3]. We will modify the solutions constructed there if it is necessary. Additional information about the radial Dirac operator mentioned in this chapter can be found in [Th92].

The radial Dirac operator is a self-adjoint extension of the differential expression

$$\tau_r = \frac{1}{\mathrm{i}}\sigma_2 \frac{d}{dx} + \phi(x), \qquad x \in (0,\infty) \tag{7.1}$$

where the potential $\phi(x)$ is a symmetric matrix given by

$$\phi(x) = \begin{pmatrix} m + \phi_{\mathrm{sc}}(x) + \phi_{\mathrm{el}}(x) & \frac{\kappa}{x} + \phi_{\mathrm{am}}(x) \\ \frac{\kappa}{x} + \phi_{\mathrm{am}}(x) & -m - \phi_{\mathrm{sc}}(x) + \phi_{\mathrm{el}}(x) \end{pmatrix} \tag{7.2}$$

with $\phi_{\mathrm{sc}}, \phi_{\mathrm{el}}, \phi_{\mathrm{am}} \in L^1_{loc}((0,\infty),\mathbb{R})$. The endpoints of the Dirac differential expression are now explicitly given by $a = 0$ and $b = \infty$. Note that τ_r is singular at $a = 0$ as $\phi_{12} = \frac{\kappa}{x} + \phi_{\mathrm{am}}(x)$ is not integrable near this endpoint and singular at $b = \infty$ because the endpoint itself is not finite (cf. Definition 1.11). Therefore $\phi(x)$ is indeed a strongly singular potential.

We are interested in the case of a Coulomb potential which describes an electron in the field of a point nucleus. Then we have

$$\phi_{\mathrm{sc}} = \phi_{\mathrm{am}} = 0 \quad \text{and} \quad \phi_{\mathrm{el}}(x) = -\frac{\gamma}{x} \tag{7.3}$$

where $\gamma = e^2 Z/\hbar$ is a constant including the elementary charge e, the nuclear charge Z and the Planck constant $\hbar$. The minus sign in ϕ_{el} corresponds to an attractive Coulomb potential. Explicitly, (7.1) reads

$$\tau_r = \begin{pmatrix} m - \frac{\gamma}{x} & -\frac{d}{dx} + \frac{\kappa}{x} \\ \frac{d}{dx} + \frac{\kappa}{x} & -m - \frac{\gamma}{x} \end{pmatrix}. \tag{7.4}$$

Note that τ_r is always limit point at $x = \infty$ (cf. Definition 1.11). For $|\gamma| \leq \sqrt{\kappa^2 - 1/4}$ we are in the limit point case at $x = 0$ as well. If $|\gamma| > \sqrt{\kappa^2 - 1/4}$, then τ_r is limit circle at $x = 0$ (cf. [Th92, p211]). In this case we need to restrict the domain. A self-adjoint realization H_r of τ_r is given by (cf. (7.122) in [Th92])

$$\begin{array}{rlll} H_r : & \mathfrak{D}(H_r) & \rightarrow & L^2((a,b),\mathbb{C}^2), \\ & f & \mapsto & \tau_r f \end{array} \tag{7.5}$$

where

$$\mathfrak{D}(H_r) = \{f \in L^2((a,b),\mathbb{C}^2) | f \in AC_{loc}((a,b),\mathbb{C}^2), \tau f \in L^2((a,b),\mathbb{C}^2), \lim_{x\to 0} W_x(\phi_r, f) = 0\}.$$

Here $\phi_r(z,x)$ denotes the solution which will be defined in (7.43).

We are interested in solutions

$$u(z,x) = \begin{pmatrix} u_1(z,x) \\ u_2(z,x) \end{pmatrix} \tag{7.6}$$

of the equation

$$\tau_r u(z,x) = z u(z,x), \qquad z \in \mathbb{C}, \tag{7.7}$$

or, equivalently, of the system of equations

$$\frac{d}{dx}u_1(z,x) + \frac{\kappa}{x}u_1(z,x) - \left(m + \frac{\gamma}{x} + z\right) u_2(z,x) = 0, \tag{7.8}$$

$$\frac{d}{dx}u_2(z,x) - \frac{\kappa}{x}u_2(z,x) - \left(m - \frac{\gamma}{x} - z\right) u_1(z,x) = 0. \tag{7.9}$$

We call (7.8) and (7.9) the radial equations. We will now present the general solution of the radial equations and start to follow [GTV07, Section 3]. The aim to get a fundamental system of special solutions $\phi(z,x)$ and $\theta(z,x)$ such that $\phi(z,x)$ lies in the domain of H_r near $a = 0$ and such that $W(\theta(z),\phi(z)) = 1$ (cf. Chapter 3). If we have given such a system, we can explicitly write down the singular Weyl function $M(z)$.

To this end, we represent $u_1(z,x)$ and $u_2(z,x)$ as a linear combination of some functions $P(y)$ and $Q(y)$,

$$u_1(z,x) = y^{\Upsilon} \mathrm{e}^{-y/2} \left[P(y) + Q(y)\right], \tag{7.10}$$

$$u_2(z,x) = -\mathrm{i}\Lambda y^{\Upsilon} \mathrm{e}^{-y/2} \left[P(y) - Q(y)\right]. \tag{7.11}$$

The new variable y is given by $y = -2\mathrm{i}Kx$. The radial equations (7.8) and (7.9) are now equations with respect to the temporarily unknown functions $P(y)$ and $Q(y)$. The constants Υ, Λ and K are given by

$$\Upsilon^2 = \kappa^2 - \gamma^2, \qquad \Lambda = \sqrt{\frac{z-m}{z+m}} \qquad \text{and} \qquad K = \sqrt{z^2 - m^2},$$

respectively.

Choosing

$$a = \Upsilon - \mathrm{i}\frac{\gamma z}{K} \qquad \text{and} \qquad b = 1 + 2\Upsilon$$

allows us to reduce the radial equations (7.8) and (7.9) to the system

$$y\frac{d^2Q}{dy^2} + (b-y)\frac{dQ}{dy} - aQ = 0, \tag{7.12}$$

$$P = -\frac{1}{\kappa - \mathrm{i}(\gamma m/K)}(y\frac{d}{dy} + a)Q. \tag{7.13}$$

Note that (7.12) is Kummer's equation (cf. (13.1.1) in [AS72]) with respect to the function $Q(y)$. Fortunately, we know how the general solution of this differential equation looks like. In order to construct solutions for (7.8) and (7.9), we have to distinguish the cases $\Upsilon \neq \frac{n}{2}$, $\Upsilon = \frac{n}{2}$ where $n \in \mathbb{N}$ and $\Upsilon = 0$. First, let $\Upsilon \neq -\frac{n}{2}$, $n \in \mathbb{N}$. Then the general solution of (7.12) can be represented as

$$Q(y) = AM(a,b,y) + BU(a,b,y) \tag{7.14}$$

where A and B are arbitrary constants and $M(a,b,y)$ and $U(a,b,y)$ are the so-called Kummer functions given by

$$M(a,b,y) = \sum_{j=0}^{\infty} \frac{(a)_j}{(b)_j j!} y^j \tag{7.15}$$

and

$$U(a,b,y) = \frac{\pi}{\sin \pi b}\left(\frac{M(a,b,y)}{\Gamma(1+a-b)\Gamma(b)} - y^{1-b}\frac{M(1+a-b,2-b,y)}{\Gamma(a)\Gamma(2-b)}\right) \tag{7.16}$$

(cf. (13.1.2) and (13.1.3) in [AS72]) where

$$(a)_n = a(a+1)(a+2)\dots(a+n-1), \qquad (a)_0 = 1. \tag{7.17}$$

Note that the representation (7.14) only makes sense if $b = 1+2\Upsilon \neq n$, $n \in \mathbb{N}$ (cf. (13.1.11) in [AS72]). Let us now determine $P(y)$. By (7.13) we have

$$\begin{aligned} P(y) &= -\frac{1}{\kappa - \mathrm{i}\frac{\gamma m}{K}}(y\frac{d}{dy}Q(y) + \alpha Q(y)) \\ &= -\frac{1}{\kappa - \mathrm{i}\frac{\gamma m}{K}}\left(Ay\frac{d}{dy}M(a,b,y) + By\frac{d}{dy}U(a,b,y)\right) + AaM(a,b,y) + BaU(a,b,y). \end{aligned}$$

Using the differentiation formulas

$$\frac{d}{dy}M(a,b,y) = \frac{a}{b}M(a+1,b+1,y) \qquad \text{and} \qquad \frac{d}{dy}U(a,b,y) = -aU(a+1,b+1,y)$$

(cf. (13.4.8) and (13.4.21) in [AS72]) we obtain

$$\begin{aligned} P(y) = -\frac{1}{\kappa - \mathrm{i}\frac{\gamma m}{K}}\Big(&Aa\left(\frac{y}{b}M(a+1,b+1,y) + M(a,b,y)\right) \\ &+ Ba\left(U(a,b,y) - yU(a+1,b+1,y)\right)\Big). \end{aligned}$$

Invoking the relations

$$\begin{aligned} M(a+1,b,y) &= \frac{y}{b}M(a+1,b+1,y)+M(a,b,y), \\ (b-a-1)U(a+1,b,y) &= U(a,b,y)-yU(a+1,b+1,y), \end{aligned}$$

(cf. (13.4.4) and (13.4.18) in [AS72]) finally yields

$$P(y) = -\frac{1}{\kappa - \mathrm{i}\frac{\gamma m}{K}}\left(AM(a+1,b,y) - B(\Upsilon + \mathrm{i}\frac{\gamma z}{K})U(a+1,b,y)\right). \tag{7.18}$$

If we now plug (7.14) and (7.18) into (7.10) and (7.11), we obtain that the general solution of the radial equations (7.8) and (7.9) is given by

$$\begin{aligned} u_1(z,x) &= y^{\Upsilon}\mathrm{e}^{y/2}\left[A\left(M(a,b,y)-c_+M(a+1,b,y)\right]+B\left[U(a,b,y)+dU(a+1,b,y)\right]\right), \\ u_2(z,x) &= \mathrm{i}\Lambda y^{\Upsilon}\mathrm{e}^{y/2}\left[A\left(M(a,b,y)-c_+M(a+1,b,y)\right]+B\left[U(a,b,y)+dU(a+1,b,y)\right]\right), \end{aligned}$$

where the constants $c_\pm$ and d are given by

$$c_\pm = \frac{\pm\Upsilon K - \mathrm{i}\gamma z}{\kappa K - \mathrm{i}\gamma m} \qquad \text{and} \qquad d = \frac{\kappa K + \mathrm{i}\gamma m}{K},$$

respectively. If we use the Kummer transformation

$$M(a+1,b,-2\mathrm{i}Kx) = \mathrm{e}^{-2\mathrm{i}Kx}M(b-a-1,b,2\mathrm{i}Kx) \tag{7.19}$$

(cf. (13.1.27) in [AS72]), we are able to represent the general solution of the radial equations (7.8) and (7.9) by the expression

$$u(z,x) = \begin{pmatrix} u_1(z,x) \\ u_2(z,x) \end{pmatrix} = AX(z,x,\Upsilon) + By^{\Upsilon}\mathrm{e}^{-y/2}[U(a,b,y)\vartheta_+ - dU(a+1,b,y)\vartheta_-] \tag{7.20}$$

where

$$\vartheta_\pm = \begin{pmatrix} \pm 1 \\ \mathrm{i}\Lambda \end{pmatrix} \tag{7.21}$$

and $X(z,x,\Upsilon)$ is given by

$$\begin{aligned} X(z,x,\Upsilon) &= \frac{(mx)^{\Upsilon}}{2}\left[M_+(z,x,\Upsilon) + M_-(z,x,\Upsilon)\begin{pmatrix} 0 & m+z \\ m-z & 0 \end{pmatrix}\right]\begin{pmatrix} 1 \\ \frac{\kappa+\Upsilon}{\gamma} \end{pmatrix}, \quad (7.22) \\ M_+(z,x,\Upsilon) &= \mathrm{e}^{\mathrm{i}Kx}M(\Upsilon+\frac{\gamma z}{\mathrm{i}K}, 1+2\Upsilon, -2\mathrm{i}Kx) + \mathrm{e}^{-\mathrm{i}Kx}M(\Upsilon-\frac{\gamma z}{\mathrm{i}K}, 1+2\Upsilon, 2\mathrm{i}Kx), \\ M_-(z,x,\Upsilon) &= \frac{1}{\mathrm{i}K}\Big[\mathrm{e}^{\mathrm{i}Kx}M(\Upsilon+\frac{\gamma z}{\mathrm{i}K}, 1+2\Upsilon, -2\mathrm{i}Kx) - \mathrm{e}^{-\mathrm{i}Kx}M(\Upsilon-\frac{\gamma z}{\mathrm{i}K}, 1+2\Upsilon, 2\mathrm{i}Kx)\Big]. \end{aligned}$$

Now we are going to present some special solutions of (7.7). First we choose $A = 1$, $B = 0$ and

$$\Upsilon_+ = \begin{cases} \sqrt{\kappa^2-\gamma^2}, & \text{if } \gamma \le |\kappa|, \\ \mathrm{i}\sqrt{\gamma^2-\kappa^2}, & \text{if } \gamma > |\kappa|. \end{cases} \tag{7.23}$$

In what follows, we set $\nu = \sqrt{\kappa^2 - \gamma^2}$ and $\iota = \sqrt{\gamma^2 - \kappa^2}$. We obtain a solution

$$\phi(z,x) = X(z,x,\Upsilon_+) \tag{7.24}$$

whose asymptotic behavior near the endpoint 0 is given by (cf. (13.5.5) in [AS72])

$$\phi(z,x) = (mx)^{\Upsilon_+} \begin{pmatrix} 1 \\ \frac{\kappa+\Upsilon_+}{\gamma} \end{pmatrix} + O(x^{\Upsilon_+ + 1}), \qquad x \to 0. \tag{7.25}$$

In the case $\Upsilon_+ \neq \frac{n}{2}$, $n \in \mathbb{N}$ we can use another solution,

$$\theta(z,x) = \frac{\gamma}{2\Upsilon_+} X(z,x,-\Upsilon_+) \tag{7.26}$$

whose asymptotic behavior near the endpoint 0 is given by

$$\theta(z,x) = \frac{\gamma}{2\Upsilon_+}\left((mx)^{-\Upsilon_+} \begin{pmatrix} 1 \\ \frac{\kappa-\Upsilon_+}{\gamma} \end{pmatrix} + O(x^{-\Upsilon_+ + 1})\right), \qquad x \to 0. \tag{7.27}$$

Note that $\phi(z,x)$ is in the domain of H_r near the endpoint 0. Furthermore, using (7.25) and (7.27), one can compute the Wronskian of $\theta(z,x)$ and $\phi(z,x)$ at $x = 0$ and infers $W(\theta(z), \phi(z)) = 1$. It follows from the standard representation of the Kummer function $M(a,b,y)$ that, for real Υ ($\Upsilon \neq \frac{n}{2}$, $n \in \mathbb{N}$), the functions M_- and M_+ are real-valued and entire functions. Therefore, $\theta(z,x)$ and $\phi(z,x)$ are real-valued entire functions for real $\Upsilon_+ = \sqrt{\kappa^2 - \gamma^2}$. If Υ_+ is purely imaginary, $\Upsilon_+ = \mathrm{i}\sqrt{\gamma^2 - \kappa^2}$, then $\theta(z,x)$ and $\phi(z,x)$ are entire in z and complex conjugate for real $z = \lambda$. Thus we have now explicitly given a system of solutions whose existence was shown in Chapter 3, at least if $\Upsilon_+ \neq \frac{n}{2}$, $n \in \mathbb{N}$.

In this case, another useful nontrivial solution is given by (7.20) with $A = 0$ and a special choice for B, namely

$$\psi(z,x) = M(z)\left(B(z)(mx)^{\Upsilon} + \mathrm{e}^{\mathrm{i}Kx}\big[U(a,b,y)\vartheta_+ - dU(a+1,b,y)\vartheta_-\big]\right) \tag{7.28}$$

where

$$B(z) = \frac{\Gamma(-\Upsilon_+ + \frac{\gamma z}{\mathrm{i}K})}{\Gamma(-2\Upsilon_+)(1-c_+)}$$

and $M(z)$ is determined in (7.30). As any solution, $\psi(z,x)$ is a special linear combination of $\theta(z,x)$ and $\phi(z,x)$,

$$\psi(z,x) = \theta(z,x) + M(z)\phi(z,x) \tag{7.29}$$

where

$$M(z) = -\frac{1}{W(\theta(z),\psi(z))} = \frac{\gamma\Gamma(-2\Upsilon_+)\Gamma(\Upsilon_+ + \frac{\gamma z}{\mathrm{i}K})(1-c_+)}{2\Upsilon_+\Gamma(2\Upsilon_+)\Gamma(-\Upsilon_+ + \frac{\gamma z}{\mathrm{i}K})(1-c_-)(2\mathrm{e}^{\mathrm{i}\pi/2}\frac{K}{m})^{-2\Upsilon_+}}. \tag{7.30}$$

Note that $\psi(z,x)$ lies in the domain of H_r near the endpoint $b = \infty$ as it decreases exponentially with polynomial accuracy (cf. (12.5.2) in [AS72] for the asymptotics of $U(a,b,y)$ as $y = -2\mathrm{i}Kx \to \infty$). For $\Upsilon \neq \frac{n}{2}$, $n \in \mathbb{N}$ we have thus given a singular Weyl function.

Next, we consider the case $\Upsilon = \frac{n}{2}$, $n \in \mathbb{N}$. Note first that $\theta(z,x)$ and $\psi(z,x)$ are solutions which are not linearly independent of $\phi(z,x)$ at the points $\Upsilon_+ = \frac{n}{2}$, $n \in \mathbb{N}$ because $\theta(z,x)$ is not defined while $\psi(z,x)$ vanishes in this case. We need the analogues of $\theta(z,x)$ and $\psi(z,x)$ defined at these points such that all the required properties are satisfied. Unfortunately, we are only able to construct such solutions in some neighborhood of an arbitrary, but fixed $n \in \mathbb{N}$.

The solution $\psi(z,x)$ tends to zero as $\nu \to \frac{n}{2}$. The solution $\theta(z,x)$ has a singularity at the point $\nu = \frac{n}{2}$ and can be represented in a neighborhood of this point as

$$\theta(z,x) = \frac{\gamma}{2\Upsilon_+}\left(\Gamma(-2\nu)A_{n/2}(z)\phi(z,x) + \frac{2\nu}{\gamma}\theta_{n/2}(z,x)\right) \tag{7.31}$$

where

$$A_{n/2}(z) = \left(\frac{2\nu}{\gamma}\frac{M(z)}{\Gamma(-2\Upsilon_+)}\right)_{\nu=\frac{n}{2}}. \tag{7.32}$$

The function $\theta_{n/2}(z,x)$ has a finite limit as $\nu \to \frac{n}{2}$ and moreover, it satisfies the radial equations (7.8) and (7.9). Using the identity $\Gamma(z) = z\Gamma(z+1)$ shows that $A_{n/2}(z)$ is a polynomial in z with real coefficients. As $\theta(z,x)$ and $\phi(z,x)$ are real-valued solutions which are entire with respect to z, we conclude that the function

$$\theta_{n/2}(z,x) = \frac{\gamma}{2\nu}\left(\frac{2\Upsilon_+}{\gamma}\theta(z,x) - \Gamma(-2\nu)A_{n/2}(z)\phi(z,x)\right) \tag{7.33}$$

is a solution of the radial equations which is defined in some neighborhood of the point $\nu = \frac{1}{2}$ and at that point itself. This solution is entire, linearly independent of $\theta(z,x)$ and moreover, we have the asymptotics

$$\theta_{n/2}(z,x) = \frac{\gamma}{2\nu}\left((mx)^{-\nu}\begin{pmatrix} 1 \\ \frac{\kappa-\nu}{\gamma}\end{pmatrix} + O(x^{-\nu+1})\right), \qquad x \to 0 \tag{7.34}$$

which are obtained from combining (7.25) and (7.27). Using (7.25) and (7.34) one can compute the Wronskian of $\theta_{n/2}(z,x)$ and $\phi(z,x)$ at $x=0$ which yields $W(\theta_{n/2}(z), \phi(z)) = 1$. Another solution $\psi_{n/2}(z,x)$ which is well defined in some neighborhood of $\nu = \frac{n}{2}$ and at that point itself is given by

$$\psi_{n/2}(z,x) = M(z)\psi(z,x) = \theta_{n/2}(z,x) + M_{n/2}(z,x)\phi(z,x) \tag{7.35}$$

where

$$M_{n/2}(z) = \frac{M(z)}{\Gamma(-2\Upsilon_+)}\left(\Gamma(-2\Upsilon_+) + \frac{\gamma}{2\nu}M(z)A_{n/2}(z)\right). \tag{7.36}$$

Note that both, the function $M_{n/2}(z)$ as well as the solution $\psi_{n/2}(z,x)$, are defined in some neighborhood of the point $\nu = \frac{n}{2}$ and at that point itself. Moreover, $\psi_{n/2}(z,x)$ decreases exponentially as $x \to \infty$ (as $\psi(z,x)$ does). The solutions $\phi_{n/2}(z,x)$ and $\psi_{n/2}(z,x)$ are therefore the required analogues of $\phi(z,x)$ and $\psi(z,x)$ defined in the neighborhood of the point $\nu = \frac{n}{2}$ and at that point itself.

Let us finally consider the special case $\Upsilon = 0$. Denote by $\theta_\nu(z,x)$, $\phi_\nu(z,x)$ and $\psi_\nu(z,x)$ the solutions $\theta(z,x)$, $\phi(z,x)$ and $\psi(z,x)$ where $\nu = 0$, respectively. From now on we write $\zeta = \frac{\kappa}{\gamma}$. If one differentiates the radial equations (7.8) and (7.9) with respect to ν at $\nu = 0$, one can check that the function

$$\left.\frac{\partial\phi(z,x)}{\partial\nu}\right|_{\nu=0} = \lim_{\nu\to 0}\frac{\phi_\nu(z,x) - \frac{2\Upsilon_+}{\gamma}\theta_\nu(z,x)}{2\nu} \tag{7.37}$$

is a solution of these equations with $\nu = 0$. As two linearly independent solutions of the radial equations with $\nu = 0$ we choose

$$\phi(z,x) = \phi(z,x)\big|_{\nu=0} \tag{7.38}$$

$$\theta_0(z,x) = -\gamma\left(\left.\frac{\partial\phi(z,x)}{\partial\nu}\right|_{\nu=0} - \frac{\zeta}{\gamma}\phi(z,x)|_{\nu=0}\right) \tag{7.39}$$

which are both entire. Note that (cf. (13.5.9) in [AS72] for the asymptotics of $\theta_0(z,x)$)

$$\phi(z,x)\big|_{\nu=0} = \begin{pmatrix} 1 + O(x) \\ \zeta + O(x) \end{pmatrix}, \qquad x \to 0, \tag{7.40}$$

$$\theta_0(z,x) = -\gamma\begin{pmatrix} \log(mx) - \frac{\zeta}{\gamma} + O(x\log(x)) \\ \zeta\log(mx) + O(x\log(x)) \end{pmatrix}, \qquad x \to 0. \tag{7.41}$$

Moreover, we have $W(\theta_0(z), \phi(z)) = 1$. Let $\mathcal{L}$ be a symbol for the logarithmic derivative of the Γ-function. As an analogue of $\psi(z,x)$ in the case $\nu = 0$, we take the function

$$\psi_0(z,x) = C_0 e^{iKx}\left[U\left(\frac{\gamma z}{iK}, 1, -2iKx\right)\mathbb{1} + \gamma\frac{\zeta K + im}{K}U\left(\frac{\gamma z}{iK} + 1, 1, -2iKx\right)\sigma_3\right]\begin{pmatrix} 1 \\ i\Lambda \end{pmatrix}.$$

where

$$C_0 = \frac{\Gamma(\frac{\gamma z}{iK})}{\gamma(1 - \frac{z}{m + i\zeta K})}.$$

We represent $\psi_0(z,x)$ in terms of $\theta(z,x)$ and $\phi_0(z,x)$ by

$$\psi_0(z,x) = \theta(z,x) + M_0(z)\phi_0(z,x)$$

where

$$M_0(z) = -\frac{1}{\gamma}\left[\log\left(2e^{-i\pi/2}\frac{K}{m}\right) + \mathcal{L}\left(-\frac{i\gamma}{K}\right) + \frac{\zeta(z-m) + iK}{2\gamma z} + 2\mathcal{L}(1)\right]. \tag{7.42}$$

The solution $\psi_0(z,x)$ decreases exponentially with polynomial accuracy (cf. (12.5.2) in [AS72] for the asymptotics of $U(a,b,y)$ as $y = -2iKx \to \infty$).

Altogether, we have found an entire system of linearly independent solutions

$$\phi_r(z,x) = X(z,x,\Upsilon_+) \tag{7.43}$$

and

$$\theta_r(z,x) = \begin{cases} \frac{\gamma}{2\Upsilon_+} X(z,x,-\Upsilon_+), & \Upsilon \neq \frac{n}{2},\ n \in \mathbb{N}, \\ \frac{\gamma}{2\nu}\left(X(z,x,-\Upsilon_+) - \Gamma(-2\nu)A_{n/2}(z)X(z,x,\Upsilon_+)\right), & \Upsilon = \frac{n}{2},\ n \in \mathbb{N}, \\ \gamma\left(\frac{\partial}{\partial\nu}X(z,x,\Upsilon_+)\big|_{\nu=0} - \frac{\zeta}{\gamma}X(z,x,\Upsilon_+)|_{\nu=0}\right), & \Upsilon = 0. \end{cases} \tag{7.44}$$

where $A_{n/2}(z)$ was defined in (7.32). The solution $\phi_r(z,x)$ is in the domain of H_r near the endpoint 0. Moreover, we have

$$W(\theta_r(z), \phi_r(z)) = 1. \tag{7.45}$$

In all three cases, a solution $\psi(z,x)$ which is in the domain of H_r at infinity can be written down by

$$\psi_r(z,x) = \theta_r(z,x) + M_r(z)\phi_r(z,x) \tag{7.46}$$

where the singular Weyl function $M_r(z)$ is given by

$$M_r(z) = \begin{cases} \frac{\gamma\Gamma(-2\Upsilon_+)\Gamma(\Upsilon_+ + \frac{\gamma z}{\mathrm{i}K})(1-c_+)}{2\Upsilon_+\Gamma(2\Upsilon_+)\Gamma(-\Upsilon_+ + \frac{\gamma z}{\mathrm{i}K})(1-c_-)(2\mathrm{e}^{\mathrm{i}\pi/2}\frac{K}{m})^{-2\Upsilon_+}}, & \Upsilon \neq \frac{n}{2},\ n \in \mathbb{N}, \\ \frac{M(z)}{\Gamma(-2\Upsilon_+)}\left(\Gamma(-2\Upsilon_+) + \frac{\gamma}{2\nu}M(z)A_{n/2}(z)\right), & \Upsilon = \frac{n}{2},\ n \in \mathbb{N}, \\ -\frac{1}{\gamma}\left[\log\left(2\mathrm{e}^{-\mathrm{i}\pi/2}\frac{K}{m}\right) + \mathcal{L}\left(-\frac{\mathrm{i}\gamma}{K}\right) + \frac{\zeta(z-m)+\mathrm{i}K}{2\gamma z} + 2\mathcal{L}(1)\right], & \Upsilon = 0, \end{cases} \tag{7.47}$$

where $M(z)$ was defined in (7.30).

Using Lemma 4.2, we obtain a measure $d\rho_r(\lambda)$ from $M_r(z)$ by virtue of the formula

$$d\rho_r(\lambda) = \lim_{\varepsilon\downarrow 0} M_r(\lambda + \mathrm{i}\varepsilon). \tag{7.48}$$

Furthermore, a spectral transformation U_r which maps H_r to multiplication with the identity function in $L^2(\mathbb{R}, d\rho)$ is given by

$$U_r : L^2((0,\infty), \mathbb{C}^2) \to L^2(\mathbb{R}, d\rho_r), \qquad f \mapsto \hat{f} \tag{7.49}$$

where

$$\hat{f}(\lambda) = \lim_{c\uparrow\infty} \int_0^c \phi_r(\lambda,x) f(x) dx \tag{7.50}$$

and $\phi_r(z,x) = X(z,x,\Upsilon_+)$ as in (7.43).

Appendix A

A short glimpse on Complex Analysis

The purpose of this appendix is to recall some standard terms and results from Complex Analysis which are used in this thesis. After having a short look at analytic functions and their Taylor series expansion we will introduce the concept of Laurent series. We are going to recall the types of singularities of functions of a complex variable and we will see how the type of a singularity of such functions can be read off from the corresponding Laurent series. Furthermore, we will recall the necessary basics of entire and meromorphic functions. The second and the third section are devoted to the theorems of Weierstrass and Mittag–Leffler concerning the construction of entire and meromorphic functions, respectively. All the material contained in this appendix is standard and taken from the classical book of Markushevish [Mar85]. Another good reference is [Jan93].

A.1 Basic knowledge

Definition A.1 (Complex differentiability, analyticity). *Suppose $f(z)$ is a function of a complex variable which is defined on a set $E \subseteq \mathbb{C}$ and let z_0 be any point of E which is a limit point.*

(i) We call the expression

$$\frac{f(z) - f(z_0)}{z - z_0} \tag{A.1}$$

the difference quotient of $f(z)$ with respect to z_0. Note that (A.1) *is a function of z which defined for any point $z \neq z_0$ of E.*

(ii) The limit of (A.1) *as $z \to z_0$, $z \in E$, provided it exists, is called the derivative of the function $f(z)$ at the point z_0 and denoted by $\partial_z f(z_0)$.*

(iii) A function $f(z)$ which is differentiable on a domain G, i.e., at every point of G, is said to be analytic (synonymously holomorphic) on G.

(iv) If $f(z)$ is analytic in a neigborhood of z_0, $f(z)$ is said to be analytic at z_0.

Theorem A.2 ([Mar85, Theorem I.16.7]). *Let $f(z)$ be an analytic function on a domain G, let z_0 be an arbitrary (finite) point of G, and let $d(z_0, \partial G)$ be the distance between z_0 and the boundary of G. Then there exists a power series*

$$f(z) = \sum_{n=0}^{\infty} a_n (z - z_0)^n \tag{A.2}$$

converging to $f(z)$ on the disk $B_{d(z_0,\partial G)}(z_0) = \{z \in \mathbb{C} : |z - z_0| < d(z_0, \partial G)\}$.

One can also consider series of a related type which involve arbitrary integer powers of $z - z_0$. These are series of the form

$$\sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \tag{A.3}$$

which are interpreted as the sum of the series

$$\sum_{n=0}^{\infty} a_n (z - z_0)^n \quad \text{and} \quad \sum_{m=1}^{\infty} a_{-m} (z - z_0)^{-m}. \tag{A.4}$$

Definition A.3 (Laurent series). *Series of the form* (A.3) *are called Laurent series and they are regarded as convergent if and only if both series in in* (A.4) *converge. In other words,*

$$\sum_{n=-\infty}^{\infty} a_n (z - z_0)^n = \lim_{\nu \to \infty} \sum_{n=0}^{\nu} a_n (z - z_0)^n + \lim_{\mu \to \infty} \sum_{m=1}^{\mu} a_{-m} (z - z_0)^{-m}.$$

The first and the second expression in (A.4) *are called the regular and the principal part of the Laurent series* (A.3)*, respectively.*

Theorem A.4 ([Mar85, Theorem I.1.3]). *Let $f(z)$ be an analytic function on an annulus $D_r^R(z_0) = \{z \in \mathbb{C} : r < |z - z_0| < R\}$. Then there exists a Laurent series*

$$f(z) = \sum_{n=-\infty}^{\infty} a_n (z - z_0)^n \tag{A.5}$$

converging to $f(z)$ on $D_r^R(z_0)$.

Recall that a deleted neighborhood $\mathcal{N}'(z_0)$ of z_0 is a disk around z_0 without z_0 itself.

Definition A.5 (Laurent series expansions, isolated singular points).

(i) A function $f(z)$ is said to have a Laurent series expansion at $z = z_0$ if $f(z)$ has a Laurent series expansion (in the variable $z - z_0$) in some deleted neighborhood of z_0.

(ii) If $f(z)$ is a function which is analytic in a deleted neighborhood of z_0, then z_0 is called an isolated singular point of $f(z)$.

Concerning the behavior of $f(z)$ at an isolated singular point there are three possibilities.

Definition A.6 (Poles, essential and removable singularities)**.** *An isolated singular point z_0 of a function $f(z)$ such that*

(i) $f(z) \to \infty$ as $z \to z_0$ is called a pole of $f(z)$.

(ii) $f(z)$ approaches no limit (finite or infinite) as $z \to z_0$ is called an essential singular point (or essential singularity) of $f(z)$.

(iii) $f(z)$ can be analytically extended to $\mathcal{N}'(z_0) \cup \{z_0\}$ is called removable singular point (or removable singularity) of $f(z)$.

The point z_0 is a pole of the function $f(z)$ if and only if it is a zero of $1/f(z)$ (cf. [Mar85, Theorem II.1.6]).

Definition A.7 (Order of a pole)**.** *We say that the point z_0 is a pole of order k ($k \geq 1$) of the function $f(z)$, if z_0 is a zero of order k of the function $1/f(z)$.*

We can read off the type of a singularity z_0 of $f(z)$ from the corresponding Laurent series (A.3) of $f(z)$ in z_0.

(i) The point z_0 is a pole of order k of the function $f(z)$ if and only if the Laurent series expansion of $f(z)$ at z_0 is of the form $\sum_{n=-k}^{\infty} a_n(z - z_0)^n$ where $a_{-k} \neq 0$.

(ii) The point z_0 is an essential singular point of $f(z)$ if and only if the Laurent series expansion of $f(z)$ at z_0 has infinitely many terms of the form $a_{-k}(z - z_0)^{-k}$ where $k > 0$, $a_{-k} \neq 0$.

(iii) The point z_0 is removable singular point if and only if the principal part of the Laurent series expansion of $f(z)$ at z_0 vanishes, that is, $a_k = 0$ for all negative integers k.

We conclude this section by a short glimpse on entire and meromorphic functions.

Definition A.8 (Entire functions)**.** *A function is called entire if it is analytic everywhere in the finite complex plane.*

Such a function has a Taylor series expansion $\sum_{n=0}^{\infty} a_n(z - z_0)^n$ (or, equivalently, a Laurent series expansion with vanishing principal part) for all z in the finite complex plane.

Definition A.9 (Meromorphic functions)**.** *A function $f(z)$ is called meromorphic if it can be written as a quotient*

$$f(z) = \frac{g(z)}{h(z)} \tag{A.6}$$

of two entire functions $g(z)$ and $h(z)$ where $h(z) \neq 0$.

Finally, we recall that there is an equivalent characterization of meromorphic functions.

Theorem A.10 ([Mar85, Theorem II.10.8])**.** *A single-valued function $f(z)$ is meromorphic if and only if its only singular points in the finite complex plane are poles.*

A.2 Weierstrass' theorem

This section is devoted to Weierstrass' theorem which gives a positive answer to the question if one can construct an entire function whose zeros coincide with the points of an arbitrary increasing sequence of nonzero complex numbers $\{\zeta_n\}$ converging to infinity. In order to prove this, we recall two important facts from [Mar85].

Theorem A.11 ([Mar85, Theorem I.15.6]). *If the series*

$$\sum_{n=1}^{\infty} f_n(z) = f(z) \tag{A.7}$$

is uniformly convergent on every compact subset of a domain G, and if every term $f_n(z)$ is analytic on G, then the sum $f(z)$ of the series is also analytic on G.
Moreover, the series (A.7) *can be differentiated term by term any number of times, i.e.,*

$$\sum_{n=1}^{\infty} \partial_z^k f_n(z) = \partial_z^k f(z), \qquad k \in \mathbb{N} \tag{A.8}$$

for all $z \in G$, and each differntiated series is uniformly convergent on every compact subset of G.

Theorem A.12 ([Mar85, Theorem I.15.8]). *If the sequence $\{f_n(z)\}$ is uniformly convergent on every compact subset of a domain G, and if every term $f_n(z)$ is analytic on G, then the limit function*

$$f(z) = \lim_{n\to\infty} f_n(z)$$

is also analytic on G. Moreover, as $n \to \infty$, each sequence of derivatives $\{\partial_z^k f_n(z)\}$, $k \in \mathbb{N}$ converges uniformly to $\partial_z^k f(z)$ on every compact subset of G.

Now we prove the famous product theorem which was found by Karl Weierstrass in 1876.

Theorem A.13 (Weierstrass' theorem, [Mar85, Theorem II.10.1]). *Given a nonnegative integer λ and an increasing sequence of nonzero complex numbers $\{\zeta_n\}$ converging to infinity, there exists an entire function $f(z)$ whose zeros coincide with the points*

$$\underbrace{0, \ldots, 0}_{\lambda \text{ times}}, \zeta_1, \ldots, \zeta_n, \ldots. \tag{A.9}$$

Proof. Consider the sequence of entire functions

$$f_m(z) = z^\lambda \prod_{n=1}^{m} \left(1 - \frac{z}{\zeta_n}\right) \mathrm{e}^{P_n(z)}, \qquad m \in \mathbb{N}$$

where the $P_n(z)$ are polynomials, to be suitably chosen later. Obviously, the zeros of $f_m(z)$ coincide with the first $m + \lambda$ points of the sequence (A.9). In general, $f_m(z)$ has multiple zeros, since (A.9) can contain the same point several times (this possibility is explicitly indicated for the point $z = 0$). The idea of the proof is to choose the polynomials $P_n(z)$ in such a way that the sequence $\{f_m(z)\}$ is uniformly convergent on every compact subset, since then we can invoke Theorem A.12 to deduce that the limit function

$$f(z) = \lim_{m\to\infty} f_m(z) \tag{A.10}$$

is entire. With this in mind, let $K_R = \{z \in \mathbb{C} : |z| < R\}$ and let $N(R)$ be the smallest integer such that $|\zeta_n| > 2R$ for all $n > N(R)$. Then, if $z \in K_R$ and $n > N(R)$, we can write $f_m(z)$ in the form

$$f_m(z) = f_{N(R)}(z) \prod_{n=N(R)+1}^{m} \left(1 - \frac{z}{\zeta_n}\right) \mathrm{e}^{P_n(z)} \tag{A.11}$$

$$= f_{N(R)}(z)\ \exp\left\{ \prod_{n=N(R)+1}^{m} \left[\ln\left(1 - \frac{z}{\zeta_n}\right) + P_n(z)\right] \right\} \tag{A.12}$$

where every logarithmic therm can be expanded as a power series

$$\ln\left(1 - \frac{z}{\zeta_n}\right) = -\frac{z}{\zeta_n} - \cdots - \frac{z^n}{n\zeta_n^n} - \frac{z^{n+1}}{(n+1)\zeta_n^{n+1}} - \ldots, \tag{A.13}$$

since $|\frac{z}{\zeta_n}| < \frac{1}{2}$ for all $z \in K_R$ and $n < N(R)$. Choosing $P_n(z)$ so as to cancel the first n terms of this series, i.e.,

$$P_n(z) = \frac{z}{\zeta_n} + \cdots + \frac{z^n}{n\zeta_n^n}, \tag{A.14}$$

we have

$$\ln\left(1 - \frac{z}{\zeta_n}\right) + P_n(z) = -\frac{z^{n+1}}{(n+1)\zeta_n^{n+1}} - \ldots \tag{A.15}$$

which implies

$$\left|\ln\left(1 - \frac{z}{\zeta_n}\right) + P_n(z)\right| \le \frac{1}{n+1}\left|\frac{z}{\zeta_n}\right|^{n+1} + \frac{1}{n+2}\left|\frac{z}{\zeta_n}\right|^{n+2} + \cdots < \frac{1}{2^{n+1}} + \frac{1}{2^{n+2}} + \cdots = \frac{1}{2^n}.$$

Then the series

$$\sum_{n=N(R)+1}^{\infty} \left[\ln\left(1 - \frac{z}{\zeta_n}\right) + P_n(z)\right] \tag{A.16}$$

is uniformly convergent on K_R since

$$\sum_{n=N(R)+1}^{\infty} \left|\ln\left(1 - \frac{z}{\zeta_n}\right) + P_n(z)\right| < \sum_{n=1}^{\infty} \frac{1}{2^n} = 1 < \infty.$$

Therefore (A.16) represents an analytic function $\chi_R(z)$ on K_R (cf. Theorem A.11). Comparing (A.10) and (A.11), and using the continuity of the exponential function, we find that

$$f(z) = f_{N(R)} \mathrm{e}^{\chi_R(z)}, \qquad z \in K_R. \tag{A.17}$$

This shows that $f(z)$ is analytic on K_R. Since the radius of the disk K_R can be arbitrarily large, $\{f_m(z)\}$ is uniformly convergent on every compact set, and hence the function $f(z)$ is analytic on the whole plane, i.e., $f(z)$ is entire. The fact that the zeros of $f(z)$ coincide with the points (A.9) is almost obvious, and follows from the representation (A.17) and the arbitrariness of R, since $\mathrm{e}^{\chi_R(z)}$ is nonvanishing, while, by construction, the zeros of $f_{N(R)}(z)$ in K_R are precisely those points of the sequence (A.9) which lie in K_R. Finally, we note that

$$f(z) = \lim_{m\to\infty} z^{\lambda} \prod_{n=1}^{m} \left(1 - \frac{z}{\zeta_n}\right) \mathrm{e}^{P_n(z)} \tag{A.18}$$

which follows just by recalling the definition of $f_m(z)$. □

A.3 Mittag-Leffler's theorem

Now we turn to Mittag-Leffler's theorem which shows that any increasing sequence of distinct complex numbers converging to infinity, together with any infinite sequence of rational functions of the a certain form, can serve as the poles and corresponding principal parts of a meromorphic function. In order to prove this, we have to recall the so-called M-test of Weierstrass from [Mar85].

Theorem A.14 (Weierstrass' M-test, [Mar85, Theorem I.15.2])**.** *Given a convergent series*

$$\sum_{n=1}^{\infty} M_n, \tag{A.19}$$

whose terms are nonnegative constants, suppose the functions $f_n(z)$, $n \in \mathbb{N}$ are such that

$$|f_n(z)| \le M_n \tag{A.20}$$

for all $z \in E$ and all n exceeding a certain integer $N > 0$. Then the series

$$\sum_{n=1}^{\infty} f_n(z) = f(z), \qquad z \in E \tag{A.21}$$

is uniformly convergent on E.

Now we are ready to prove Mittag-Leffler's theorem which is kind of an analogue of Weierstrass' theorem. It was published in 1884 by Magnus Gösta Mittag-Leffler.

Theorem A.15 (Mittag-Leffler's theorem, [Mar85, Theorem II.10.10])**.** *Let*

$$\zeta_0 = 0, \zeta_1, \dots, \zeta_n, \dots \tag{A.22}$$

be an increasing sequence of distinct complex numbers converging to infinity, and let

$$G_0(z), G_1(z), \dots, G_n(z), \dots$$

be a sequence of rational functions of the form

$$G_n(z) = \frac{a_{-\beta_n}^{(n)}}{(z-\zeta_n)^{\beta_n}} + \cdots + \frac{a_{-1}^{(n)}}{z-\zeta_n}, \tag{A.23}$$

where $\beta_n \neq 0$, $a_{-\beta_n}^{(n)} \neq 0$ *if* $n \neq 0$. *Then there exists a meromorphic function* $f(z)$ *whose poles coincide with the points* (A.22)*, and whose principal part at the pole* ζ_n *equals* $G_n(z)$*, for each* $n \in \mathbb{N}_0$.

Proof. It is now not really surprising that the proof bears a strong resemblance to the proof of Weierstrass' theorem (Theorem A.13). We start from the Taylor series expansion

$$G_n(z) = a_0^{(n)} + a_1^{(n)} z + \dots a_k^{(n)} z^k + \dots, \qquad n \in \mathbb{N}_0$$

which is convergent on the disk $D = \{z \in \mathbb{C} : |z| < |\zeta_m|\}$ and uniformly convergent on every smaller disk, in particular on $D_n = \{z \in \mathbb{C} : |z| < \frac{1}{2}|\zeta_n|\}$. Let $\{\varepsilon_n\}$ any sequence of positive numbers such that

$$\sum_{n=0}^{\infty} \varepsilon_n < \infty. \tag{A.24}$$

Then, choosing integers k_0, k_1, k_2, ... such that

$$\left| G_n(z) - \left(a_0^{(n)} + a_1^{(n)} z + \cdots + a_{k_n}^{(n)} z^{k_n} \right) \right| < \varepsilon_n, \qquad n \in \mathbb{N}_0 \tag{A.25}$$

for all $z \in D_n$, we introduce the polynomials

$$P_n(z) = -a_0^{(n)} - a_1^{(n)} z - \cdots - a_{k_n}^{(n)} z^{k_n}, \qquad n \in \mathbb{N}_0 \tag{A.26}$$

where $P_0(z) \equiv 0$ if $G_0(z) \equiv 0$. Given any disk $K_R = \{z \in \mathbb{C} : |z| < R\}$, let $N(R)$ be the smallest integer such that $\|\zeta_n\| > 2R$ for all $n > N(R)$. Consider the series

$$\sum_{n=N(R)+1}^{\infty} \left[G_n(z) + P_n(z) \right], \tag{A.27}$$

noting that $K_R \subset D_n$ for all $n > N(R)$, while K_R contains none of the points $\zeta_{N(R)+1}$, $\zeta_{N(R)+2}$, ... It follows from (A.25) and (A.26) that we have

$$\|G_n(z) + P_n(z)\| < \varepsilon_n$$

for all $n > N(R)$ and $z \in K_R$. Therefore, because of (A.24) and Weierstrass' M-test (Theorem A.14), the series (A.27) is uniformly convergent on K_R, and hence represents an analytic function $\omega_R(z)$ on K_R (Theorem A.11). Thus, if

$$f(z) = \sum_{n=0}^{\infty} \left[G_n(z) + P_n(z) \right], \tag{A.28}$$

we have the representation

$$f(z) = f_{N(R)}(z) + \omega_R(z), \qquad z \in K_R, \tag{A.29}$$

where $\omega_R(z)$ is analytic on K_R, and the partial sum

$$f_{N(R)}(z) = \sum_{n=0}^{N(R)} [G_n(z) + P_n(z)]$$

is a rational function whose poles in K_R are precisely those points of the sequence (A.22) which lie in K_R. Moreover, the principal part of $f_{N(R)}(z)$, and hence of $f(z)$, at any point $\zeta_n \in K_R$ is just $G_n(z)$. The theorem now follows at once from the observation that K_R can have arbitrarily large radius. □

Corollary A.16. *Let $f(z)$ be a meromorphic function whose poles are given by an increasing sequence of complex numbers $b_0 = 0, b_1, \ldots, b_n, \ldots$ with corresponding principal parts $G_0(z), G_1(z), \ldots, G_n(z), \ldots$. Then $f(z)$ can be represented in the form*

$$f(z) = g(z) + \sum_{n=0}^{\infty} [G_n(z) + P_n(z)], \tag{A.30}$$

where $g(z)$ is an entire function and the $P_n(z)$ are polynomials.

Proof. Use Mittag-Leffler's theorem (Theorem A.15) to construct a function

$$\varphi(z) = \sum_{n=0}^{\infty} [G_n(z) + P_n(z)]$$

with the same poles and principal parts as $f(z)$. Then $f(z) - \varphi(z)$ is analytic in the whole plane and hence equals an entire function which we denote by $g(z)$. □

Corollary A.17 ([Mar85, II., Section 51, Example 1])**.** *Given an increasing sequence $\{\zeta_n\}$ of distinct nonzero complex numbers converging to infinity, and an arbitrary complex sequence $\{A_n\}$, find an entire function $f(z)$ such that*

$$f(\zeta_n) = A_n, \qquad n \in \mathbb{N}. \tag{A.31}$$

Proof. We begin by using Theorem A.13 and Corollary A.16 in order to construct an entire function $g(z)$ with simple zeros at the points $\zeta_1, \zeta_2, \ldots$, i.e.,

$$g(z) = \prod_{n=1}^{\infty} \left(1 - \frac{z}{\zeta_n}\right) \mathrm{e}^{\left(\frac{z}{\zeta_n} + \cdots + \frac{z^n}{n\zeta_n^n}\right)}. \tag{A.32}$$

Then, we calculate the derivative $\partial_z g(z)$ at every point ζ_n, obtaining a sequence of nonzero complex numbers $\{\partial_z g(\zeta_n)\}$. Next, we use Mittag-Leffler's theorem to find a meromorphic function $\varphi(z)$ with simple poles at the points $\zeta_1, \zeta_2, \ldots$ and corresponding principal parts

$$\frac{A_n/\partial_z g(\zeta_n)}{z - \zeta_n} \qquad n \in \mathbb{N}. \tag{A.33}$$

Thus

$$\varphi(z) = \sum_{n=1}^{\infty} \left[\frac{A_n/\partial_z g(\zeta_n)}{z - \zeta_n} + P_n(z) \right]$$

where the $P_n(z)$ are suitably chosen polynomials. Then the function

$$f(z) = g(z)\varphi(z)$$

is obviously entire, and satisfies

$$\begin{aligned} f(\zeta_n) &= \lim_{z \to \zeta_n} g(z)\varphi(z) = \lim_{z \to \zeta_n} \left[\frac{g(z) - g(\zeta_n)}{z - \zeta_n} \varphi(z)(z - \zeta_n) \right] \\ &= \frac{\partial_z g(\zeta_n) A_n}{\partial_z g(\zeta_n)} = A_n, \qquad n \in \mathbb{N} \end{aligned}$$

as stated. □

Appendix B

Nevanlinna functions

This appendix provides some facts concerning Herglotz–Nevanlinna and generalized Nevanlinna functions. In particular, we will have a look at generalized Nevanlinna functions which have no nonreal poles and the only generalized pole of nonpositive type at infinity.

B.1 Herglotz–Nevanlinna functions

We are going to define Herglotz–Nevanlinna functions and list some of their properties. The content of this section is taken from [KST11], [Te09] and [Tim95].

Denote by $\mathbb{C}_\pm = \{z \in \mathbb{C} | \pm \operatorname{Im}(z) > 0\}$ the upper, respectively, lower half plane.

Definition B.1 (Herglotz–Nevanlinna functions)**.** *A function $F : \mathbb{C}_+ \to \mathbb{C}_+$ is called Herglotz–Nevanlinna function if F is analytic everywhere in $\mathbb{C}_+$. On $\mathbb{C}_-$ one defines F using $F(z^*) = F(z)^*$.*

Definition B.2 (Borel transform)**.** *We define the Borel transform F of the measure μ by*

$$F(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda). \tag{B.1}$$

Considering just the imaginary part of (B.1),

$$\operatorname{Im}(F(z)) = \operatorname{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|} d\mu(\lambda), \tag{B.2}$$

we infer that $F(z)$ is an analytic map from the upper half plane into itself and thus a Herglotz–Nevanlinna function. Furthermore, F satisfies a growth estimate.

Theorem B.3 ([Te09, Theorem 3.10])**.** *The Borel transform $F(z)$ of a finite Borel measure μ is a Herglotz–Nevanlinna function. It is analytic in $\mathbb{C} \setminus \sigma(\mu)$ and satisfies*

$$F(z^*) = F(z)^*, \qquad |F(z)| \leq \frac{\mu(\mathbb{R})}{\operatorname{Im}(z)}, \qquad z \in \mathbb{C}_+. \tag{B.3}$$

Here, $\sigma(\mu)$ denotes the spectrum of the measure μ defined in (2.33).

The converse of Theorem B.3 also holds, that is, if a Herglotz function F satisfies a growth estimate, then there exists a finite measure μ such that F is the Borel transform of μ.

Theorem B.4 ([Te09, Theorem 3.20]). *Suppose F is Herglotz function satisfying*

$$|F(z)| \leq \frac{M}{\mathrm{Im}(z)}, \qquad z \in \mathbb{C}_+. \tag{B.4}$$

Then there is a Borel measure μ satisfying $\mu(\mathbb{R}) \leq M$. Here, $M \geq 0$ is some constant such that F is the Borel transform of μ.

Furthermore, the so-called Stieltjes inversion formula shows that one can associate a measure with every Herglotz–Nevanlinna function.

Theorem B.5 (Stieltjes inversion formula, cf. [KST11, Lemma 3.2]). *Suppose $F(z)$ is the Borel transform of a finite measure $d\mu$,*

$$F(z) = \int_{\mathbb{R}} \frac{d\mu(\lambda)}{\lambda - z}, \tag{B.5}$$

then we have

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} w(\lambda) \mathrm{Im}\big(F(\lambda + \mathrm{i}\varepsilon)\big)\ d\lambda = \int_{\lambda_0}^{\lambda_1} w(\lambda)\ d\mu(\lambda) \tag{B.6}$$

for every $w \in C[\lambda_0, \lambda_1]$ where

$$\int_{\lambda_0}^{\lambda_1} w\ d\mu = \frac{1}{2}\left(\int_{(\lambda_0,\lambda_1)} w\ d\mu + \int_{[\lambda_0,\lambda_1]} w\ d\mu\right). \tag{B.7}$$

Another important property of Herglotz–Nevanlinna functions is the existence of an integral representation.

Theorem B.6 ([Tim95, Theorem B.1]). *A function F is a Herglotz–Nevanlinna function if and only if it admits the integral representation*

$$F(z) = a + bz + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{1}{1+\lambda}\right) d\mu(\lambda), \qquad z \in \mathbb{C}_+ \tag{B.8}$$

where $a = \mathrm{Re}(F(\mathrm{i}))$, $b \geq 0$, and μ is a measure on $\mathbb{R}$ which satisfies

$$\int_{\mathbb{R}} \frac{d\mu(\lambda)}{1+\lambda^2} < \infty. \tag{B.9}$$

The measure $\mu(\lambda)$ in the above representation is given by the Stieltjes inversion formula.

B.2 Generalized Nevanlinna functions

This section provides some information about the classes N_κ of generalized Nevanlinna functions and coincides with [KST11, Appendix C] apart from some slight modifications. More information on this topic can be found, e.g., in [KrL77] and [Lan86].

Definition B.7 (Generalized Nevanlinna functions). *We define the set of generalized Nevanlinna functions N_κ, $\kappa \in \mathbb{N}_0$ as the set of all functions $G(z)$ which are meromorphic in $\mathbb{C}_+ \cup \mathbb{C}_-$, satisfy the symmetry condition*

$$G(z) = G(z^*)^* \tag{B.10}$$

for all z in the domain $\mathcal{D}_G$ of holomorphy of $G(z)$, and for which the Nevanlinna kernel

$$\mathcal{N}_G(z,\zeta) = \frac{G(z) - G(\zeta)^*}{z - \zeta^*}, \quad z, \zeta \in \mathcal{D}_G, \quad z \neq \zeta^* \tag{B.11}$$

has κ negative squares.

The Nevanlinna kernel (B.11) has exactly κ negative squares if and only if the matrix

$$\{\mathcal{N}_G(z_j, z_k)\}_{1\le j,k\le n} \tag{B.12}$$

has at most κ negative eigenvalues for any choice of finitely many points $\{z_j\}_{j=1}^n \subset \mathcal{D}_G$ and exactly κ negative eigenvalues for some choice of $\{z_j\}_{j=1}^n$. Note that N_0 coincides with the class of Herglotz–Nevanlinna functions.

Definition B.8 (Generalized poles). *Suppose $G \in N_\kappa$, $\kappa \ge 1$.*

(i) A point $\lambda_0 \in \mathbb{R}$ is said to be a generalized pole of nonpositive type of G if either

$$\limsup_{\varepsilon\downarrow 0} \varepsilon|G(\lambda_0 + \mathrm{i}\varepsilon)| = \infty \qquad \text{or} \qquad \lim_{\varepsilon\downarrow 0}(-\mathrm{i}\varepsilon)G(\lambda_0 + \mathrm{i}\varepsilon)$$

exists and is finite and negative.

(ii) The point $\lambda_0 = \infty$ is said to be a generalized pole of nonpositive type of G if either

$$\limsup_{y\uparrow\infty} \frac{|G(\mathrm{i}y)|}{\mathrm{i}y} = \infty \qquad \text{or} \qquad \lim_{y\uparrow\infty} \frac{G(\mathrm{i}y)}{\mathrm{i}y}$$

exists and is finite and negative.

All limits can be replaced by nontangential limits.

We are interested in the special subclass $N_\kappa^\infty \subset N_\kappa$ of generalized Nevanlinna function with no nonreal poles and the only generalized pole of nonpositive type at infinity. A more general version of Theorem B.6 holds for this subclass. In particular, for every function in N_κ^∞, there exists an integral representation.

Theorem B.9 ([KST11, Theorem C.1]). *A function $G \in N_\kappa^\infty$ admits the representation*

$$G(z) = (1+z^2)^k \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \frac{d\rho(\lambda)}{(1+\lambda^2)^k} + \sum_{j=0}^{l} a_j z^j \tag{B.13}$$

where $k \le \kappa$, $l \le 2\kappa + 1$,

$$a_j \in \mathbb{R} \quad \text{and} \quad \int_{\mathbb{R}} (1+\lambda^2)^{-k-1} d\rho(\lambda) < \infty. \tag{B.14}$$

The measure ρ is given by the Stieltjes inversion formula (cf. Theorem B.5)

$$\frac{1}{2}\big(\rho\big((\lambda_0,\lambda_1)\big) + \rho\big([\lambda_0,\lambda_1]\big)\big) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0}^{\lambda_1} \mathrm{Im}\big(G(\lambda + \mathrm{i}\varepsilon)\big) d\lambda. \tag{B.15}$$

The representation (B.13) *is called irreducible if k is chosen minimal, that is, either $k = 0$ or $\int_{\mathbb{R}} (1+\lambda^2)^{-k} d\rho(\lambda) = \infty$.*
Conversely, if (B.14) *holds, then $G(z)$ defined via* (B.13) *is in N_κ^∞ for some κ. If k is minimal, κ is given by*

$$\kappa = \begin{cases} k, & l \le 2k, \\ \lfloor \frac{l}{2} \rfloor, & l \ge 2k+1, \ l \text{ even, or, } l \text{ odd and } a_l > 0, \\ \lfloor \frac{l}{2} \rfloor + 1, & l \ge 2k+1, \ l \text{ odd and } a_l < 0. \end{cases} \tag{B.16}$$

Given a generalized Nevanlinna function in N_κ^∞, the corresponding κ is equal to the multiplicity of the generalized pole at infinity which is determined by the fact that the limits

$$\lim_{y \uparrow \infty} -\frac{G(\mathrm{i}y)}{(\mathrm{i}y)^{2\kappa-1}} \in (0,\infty] \qquad \text{and} \qquad \lim_{y \uparrow \infty} \frac{G(\mathrm{i}y)}{(\mathrm{i}y)^{2\kappa+1}} \in [0,\infty)$$

exist and take values as indicated. Again, the limits can be replaced by nontangential ones. Note that, if $G(z) \in N_\kappa$, then $-G(z)^{-1}$, $-G(1/z)$ and $1/G(1/z)$ also belong to N_κ. Moreover, generalized zeros of $G(z)$ are generalized poles of $-G(z)^{-1}$ of the same multiplicity.

Lemma B.10 ([KST11, Lemma C.2]). *Let $G(z)$ be a generalized Nevanlinna function given by* (B.13) *and* (B.14) *where $l < 2k+1$. Then, for every $0 < \gamma < 2$, we have*

$$\int_{\mathbb{R}} \frac{d\rho(\lambda)}{1+|\lambda|^{2k+\gamma}} < \infty \quad \text{if and only if} \quad \int_1^\infty \frac{(-1)^k \mathrm{Im}(G(\mathrm{i}y))}{y^{2k+\gamma}} dy < \infty. \tag{B.17}$$

Concerning the case $\gamma = 0$, we have

$$\int_{\mathbb{R}} \frac{d\rho(\lambda)}{(1+\lambda^2)^k} = \lim_{y \to \infty} \frac{(-1)^k \mathrm{Im}(G(\mathrm{i}y))}{y^{2k-1}} \tag{B.18}$$

where the two sides are either both finite and equal or both infinite.

Appendix C

Glossary of notation

$AC_{loc}((a,b),\mathbb{C}^2)$	set of locally absolutely continuous functions from (a,b) to $\mathbb{C}^2$
$\mathfrak{B}$	Borel sigma algebra of $\mathbb{R}$
$\mathbb{C}$	set of complex numbers
$\mathbb{C}_\pm$	upper, respectively, lower complex half plane
$\chi_\Omega(.)$	characteristic function of the set Ω
$\mathfrak{D}(.)$	domain of an operator or a differential expression
det	determinant
e	exponential function, $\mathrm{e}^z = \exp(z)$
$G(z,x,y)$	Green function of the self-adjoint Dirac operator H
H	self-adjoint Dirac operator
H_r	self-adjoint radial Dirac operator
hull(.)	convex hull
$\mathfrak{H}$	a (complex and separable) Hilbert space
i	complex unity, $\mathrm{i}^2 = -1$
$\mathbb{1}$	identity operator
$\mathrm{Im}(z)$	imaginary part of a complex number z
$\mathfrak{L}(X)$	set of all bounded linear operators from the space X to itself
λ	a real number
$L^p(\mathbb{R}, d\rho)$	real-valued p-integrable functions with respect to the measure ρ
$L^1_{loc}((a,b),\mathbb{C}^2)$	set of locally integrable functions from (a,b) to $\mathbb{C}^2$
$L^2((a,b),\mathbb{C}^2)$	set of square integrable functions from (a,b) to $\mathbb{C}^2$
$m_\pm(z)$	Weyl m-functions
$M(z)$	singular Weyl function
μ_ψ	spectral measure associated with the function ψ
N_κ	set of generalized Nevanlinna functions
$\mathbb{N}$	set of positive integers
$\mathbb{N}_0$	$= \mathbb{N} \cup \{0\}$
$O(x)$	Landau symbol big-O
Ω	a Borel set
$P(\Omega)$	projection-valued measure
P_A	family of spectral projections of an operator A

q_A	quadratic form of A
$\mathfrak{Q}(A)$	form domain of A
$\mathrm{Re}(z)$	real part of a complex number z
$\mathbb{R}$	set of real numbers
R_A	resolvent of an operator A
$\mathrm{Ran}(A)$	range of A
$\rho(A)$	resolvent set of A
$\sigma(A)$	spectrum of A
$\sigma_{ac}(A)$	absolutely continuous spectrum of A
$\sigma_d(A)$	discrete spectrum of A
$\sigma_{ess}(A)$	essential spectrum of A
$\sigma_p(A)$	point spectrum of A
$\sigma_{pp}(A)$	pure point spectrum of A
$\sigma_{sc}(A)$	singularly continuous spectrum of A
σ_1, σ_2, σ_3	Pauli matrices
τ	Dirac differential expression
τ_r	radial Dirac differential expression
$u_\pm(z,x)$	Weyl solutions
$W_x(u,v)$	Wronski determinant of the functions u and v at x
z	a complex number

z^*	complex conjugation
A^*	adjoint of an operator A
∂_z	differentiation with respect to z
$\hat{f}$	spectral transform of f
f'	derivative of f with respect to x
$\|.\|_{\mathbb{C}^2}$	norm in $\mathbb{C}^2$
$\|.\|$	norm in the Hilbert space $\mathfrak{H}$
$\|.\|_{L^2((a,b),\mathbb{C}^2)}$	norm in the Hilbert space $L^2((a,b),\mathbb{C}^2)$
$\|.\|_{L^2(\mathbb{R},d\rho)}$	norm in the Hilbert space $L^2(\mathbb{R},d\rho)$
$\|.\|_\infty$	sup norm
$(.,.)$	inner product in $\mathbb{C}^2$
$\langle .,. \rangle$	inner product in the Hilbert space $\mathfrak{H}$
$\langle .,. \rangle_{L^2((a,b),\mathbb{C}^2)}$	inner product in the Hilbert space $L^2((a,b),\mathbb{C}^2)$
$\langle .,. \rangle_{L^2(\mathbb{R},d\rho)}$	inner product in the Hilbert space $L^2(\mathbb{R},d\rho)$
$\oplus$	orthogonal sum of linear spaces or operators
$\otimes$	tensor product in $\mathbb{C}^2$
$M^\perp$	orthogonal complement of the set M
$\overline{M}$	closure of M
(λ_1,λ_2)	$=\{\lambda\in\mathbb{R} \mid \lambda_1<\lambda<\lambda_2\}$, open interval
$[\lambda_1,\lambda_2]$	$=\{\lambda\in\mathbb{R} \mid \lambda_1\le\lambda\le\lambda_2\}$, closed interval

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