

ASYMPTOTICS OF THE WEYL FUNCTION FOR SCHRÖDINGER OPERATORS WITH MEASURE-VALUED POTENTIALS

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ABSTRACT. We derive an asymptotic expansion for the Weyl function of a one-dimensional Schrödinger operator which generalizes the classical formula by Atkinson. Moreover, we show that the asymptotic formula can also be interpreted in the sense of distributions.

1. INTRODUCTION

The m -function or Weyl–Titchmarsh function introduced by Weyl in [31] plays a fundamental role in spectral theory for Sturm–Liouville operators. In particular, it is known that in the case of sufficiently ”nice” potentials q all information about the spectral properties of self-adjoint realizations of the differential expression

$$-\frac{d^2}{dx^2} + q(x), \quad (1.1)$$

acting in $L^2(0, \infty)$, are encoded in this function. In 1952 Marchenko proved (see [25, Theorem 2.2.1]) that the m -function corresponding to the Dirichlet boundary condition at $x = 0$ behaves asymptotically at infinity like the corresponding function of the unperturbed operator (corresponding to $q \equiv 0$), that is,

$$m(z) = -\sqrt{-z}(1 + o(1)), \quad (1.2)$$

as $z \rightarrow \infty$ in any nonreal sector in the open upper complex half-plane \mathbb{C}_+ (let us stress that the high-energy behavior of m can be deduced from the asymptotic behavior of the corresponding spectral function, see [24, Theorem II.4.3]). A simple proof of this formula was found by Levitan in [23] (a short self-contained proof of (1.2) can be found in, e.g., [30, Lemma 9.19]). Since then the high-energy asymptotics $z \rightarrow \infty$ of the m -function received enormous attention over the past three decades as can be inferred, for instance from [2], [4], [5], [6], [7], [12], [13], [14], [15]–[18], [19], [20], [21], [22], [27], [29] and the references therein.

Typically there are two directions which are of interest: If one assumes q to be smooth a full asymptotic expansion can be given. Otherwise, one tries to derive the leading asymptotic under minimal assumptions on q . One of the key improvements

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in this latter direction is due to Atkinson [2] who showed

$$m(z) = -\sqrt{-z} - \int_{[0, x_0)} e^{-2\sqrt{-z}y} q(y) dy + o(z^{-1/2}) \quad (1.3)$$

for arbitrary $x_0 \in (0, \infty)$. In particular, if 0 is a Lebesgue point of q this implies

$$m(z) = -\sqrt{-z} - \frac{q(0)}{2\sqrt{-z}} + o(z^{-1/2}). \quad (1.4)$$

On the other hand, the case of a locally integrable potential does not cover the case where q is a single Dirac δ one of the most popular toy models which can be found in any text book on quantum mechanics. Even though the case of delta potentials has a long tradition (see e.g. the monograph [1]) the case where q is replaced by an arbitrary measure got significant interest only recently and we refer to [3], [8]–[10], [11], [26], [28] and the literature therein.

Our question in the present paper is to what extent (1.3) remains valid when q is replaced by a measure. Moreover, we will also show that (1.4) remains true when interpreted in the sense of distributions.

2. SCHRÖDINGER OPERATORS WITH MEASURE-VALUED COEFFICIENTS

Our main object are one-dimensional Schrödinger operators in the Hilbert space $L^2(a, b)$, $-\infty < a < b \leq \infty$, associated with the differential expressions

$$\tau f = \left(-f' + \int f d\chi \right)', \quad (2.1)$$

where χ is a locally finite signed Borel measure on $[a, b)$. In particular, we assume that τ is regular at a , that is, $a \in \mathbb{R}$ and the total variation of χ is finite near a (i.e., $|\chi|([a, x_0)) < +\infty$ for every $x_0 \in (a, b)$).

The maximal domain of this differential expression is given as

$$\mathfrak{D}_\tau = \left\{ f \in AC_{\text{loc}}[a, b) \mid \left(x \mapsto -f'(x) + \int f d\chi \right) \in AC_{\text{loc}}[a, b) \right\},$$

which leads to a jump condition for $f'(x)$ at every point mass,

$$f'(x+) - f'(x-) = \chi(\{x\})f(x). \quad (2.2)$$

We fix $f'(x)$ to be left continuous. At $x = a$ the above condition has to be understood as the definition of the left limit.

In order to get a self-adjoint operator we look at the corresponding maximal operator associated with τ in $L^2(a, b)$ with the domain

$$\text{dom}(T_{\text{max}}) = \{f \in \mathfrak{D}_\tau \mid f, \tau f \in L^2(a, b)\}.$$

For $f, g \in \text{dom}(T_{\text{max}})$ we can define the Wronskian as usual

$$W_x(f, g) = f(x)g'(x) - f'(x)g(x) \quad (2.3)$$

and one can verify the Lagrange identity

$$\int_{[c, d)} (g\tau f - f\tau g) dx = W_d(f, g) - W_c(f, g) \quad (2.4)$$

where x, c, d include the interval endpoints as one-sided limits. In particular, the Wronskian is constant for two solutions of $\tau u = zu$.

We say τ is in the limit-circle (l.c.) case at b if all solutions of $\tau u = zu$ are square integrable near b and we say that τ is in the limit-point (l.p.) case at b otherwise.

To obtain a self-adjoint operator from T_{\max} we will choose appropriate boundary conditions. First of all we will choose a Dirichlet boundary condition at a . Then, if τ is in the l.p. case at b , no further boundary condition is needed and the corresponding operator

$$\text{dom}(S) = \{f \in \text{dom}(T_{\max}) \mid f(a) = 0\}$$

is a self-adjoint restriction of T_{\max} . Otherwise, if τ is in the l.c. case at b , we need an additional boundary condition at b in which case every restriction of T_{\max} with domain

$$\text{dom}(S) = \{f \in \text{dom}(T_{\max}) \mid f(a) = 0, W_b(f, w^*) = 0\},$$

where $w \in \text{dom}(T_{\max})$ satisfies $W_b(w, w^*) = 0$ and $W(h, w^*) \neq 0$ for some $h \in \text{dom}(T_{\max})$, is a self-adjoint operator.

We refer to [11] for background and general theory.

3. ASYMPTOTICS FOR THE WEYL FUNCTION

In this section we will assume that the left endpoint a is regular and without loss of generality we will assume $a = 0$. To simplify notation we denote

$$\chi(x) := \begin{cases} \chi([0, x]), & x \in (0, b), \\ 0, & x = 0. \end{cases}$$

In this case we have a basis of solutions $c(z, x)$, $s(z, x)$ of $\tau u = zu$ determined by the initial conditions

$$c(z, 0) = 1, c'(z, 0) = 0, \quad s(z, 0) = 0, s'(z, 0) = 1, \quad (3.1)$$

such that $W(c(z), s(z)) = 1$. Here and in what follows a prime will always denote a derivative with respect to the spatial coordinate x . They are given as the solutions of the following integral equations

$$c(z, x) = \cosh(\sqrt{-z}x) + \frac{1}{\sqrt{-z}} \int_{[0, x]} \sinh(\sqrt{-z}(x-y))c(z, y)d\chi(y), \quad (3.2)$$

$$s(z, x) = \frac{1}{\sqrt{-z}} \sinh(\sqrt{-z}x) + \frac{1}{\sqrt{-z}} \int_{[0, x]} \sinh(\sqrt{-z}(x-y))s(z, y)d\chi(y). \quad (3.3)$$

In fact, this can be verified using integration by parts, which also shows

$$c'(z, x) = \sqrt{-z} \sinh(\sqrt{-z}x) + \int_{[0, x]} \cosh(\sqrt{-z}(x-y))c(z, y)d\chi(y), \quad (3.4)$$

$$s'(z, x) = \cosh(\sqrt{-z}x) + \int_{[0, x]} \cosh(\sqrt{-z}(x-y))s(z, y)d\chi(y). \quad (3.5)$$

Here and in what follows $\sqrt{\cdot}$ will always denote the standard branch of the square root with branch cut along $(-\infty, 0)$.

We will need their high-energy asymptotics as $\text{Im}(z) \rightarrow \infty$.

Lemma 3.1. *The function $c(z, x)$ and its derivative $c'(z, x)$ can be written as*

$$\begin{aligned} c(z, x) &= \cosh(\sqrt{-z}x) + \frac{1}{2\sqrt{-z}} \sinh(\sqrt{-z}x)\chi(x) \\ &\quad + \frac{e^{\sqrt{-z}x}}{4\sqrt{-z}} \left(\int_{[0,x]} e^{-2\sqrt{-z}y} d\chi(y) - \int_{[0,x]} e^{-2\sqrt{-z}(x-y)} d\chi(y) \right) \\ &\quad - \frac{e^{\sqrt{-z}x}}{z} E_1(z, x), \end{aligned} \quad (3.6)$$

$$\begin{aligned} c'(z, x) &= \sqrt{-z} \sinh(\sqrt{-z}x) + \frac{1}{2} \cosh(\sqrt{-z}x)\chi(x) \\ &\quad + \frac{e^{\sqrt{-z}x}}{4} \left(\int_{[0,x]} e^{-2\sqrt{-z}y} d\chi(y) + \int_{[0,x]} e^{-2\sqrt{-z}(x-y)} d\chi(y) \right) \\ &\quad + \frac{e^{\sqrt{-z}x}}{\sqrt{-z}} E_2(z, x), \end{aligned} \quad (3.7)$$

with error functions $E_j(z, x)$ satisfying $|E_j(z, x)| \leq C|\chi|([0, x])$ and

$$E_j(z, x) = \frac{1}{8} \int_{(0,x)} (\chi(y) + \chi(\{0\})) d\chi(y) + o(1), \quad j = 1, 2, \quad (3.8)$$

as $\text{Im}(z) \rightarrow +\infty$.

Similarly, the function $s(z, x)$ and its derivative $s'(z, x)$ can be written as

$$\begin{aligned} s(z, x) &= \frac{1}{\sqrt{-z}} \sinh(\sqrt{-z}x) - \frac{1}{2z} \cosh(\sqrt{-z}x)\chi(x) \\ &\quad + \frac{e^{\sqrt{-z}x}}{4z} \left(\int_{[0,x]} e^{-2\sqrt{-z}y} d\chi(y) + \int_{[0,x]} e^{-2\sqrt{-z}(x-y)} d\chi(y) \right) \\ &\quad + \frac{e^{\sqrt{-z}x}}{\sqrt{-z}^3} E_3(z, x), \end{aligned} \quad (3.9)$$

$$\begin{aligned} s'(z, x) &= \cosh(\sqrt{-z}x) + \frac{1}{2\sqrt{-z}} \sinh(\sqrt{-z}x)\chi(x) \\ &\quad - \frac{e^{\sqrt{-z}x}}{4\sqrt{-z}} \left(\int_{[0,x]} e^{-2\sqrt{-z}y} d\chi(y) - \int_{[0,x]} e^{-2\sqrt{-z}(x-y)} d\chi(y) \right) \\ &\quad - \frac{e^{\sqrt{-z}x}}{z} E_4(z, x), \end{aligned} \quad (3.10)$$

with error functions $E_j(z, x)$ satisfying $|E_j(z, x)| \leq C|\chi|([0, x])$ and

$$E_j(z, x) = \frac{1}{8} \int_{(0,x)} (\chi(y) - \chi(\{0\})) d\chi(y) + o(1), \quad j = 3, 4, \quad (3.11)$$

as $\text{Im}(z) \rightarrow +\infty$.

Proof. Abbreviate $k = \sqrt{-z}$ and note $\text{Re}(k) \geq 0$. First of all, considering the function $\tilde{c}(z, x) = e^{-kx}c(z, x)$ we look at the corresponding integral equation

$$\tilde{c}(z, x) = \frac{1 + e^{-2kx}}{2} + \int_{[0,x]} \frac{1 - e^{-2k(x-y)}}{2k} \tilde{c}(z, y) d\chi(y)$$

from which it follows that there is a bounded solution satisfying

$$|\tilde{c}(z, x)| \leq \exp(|k|^{-1}|\chi|([0, x]))$$

by using the usual iteration scheme (cf. [11, Theorem A.2]). Now we use bootstrapping and insert this information into our integral equation. First the integral equation for $c(z, x)$ can be written as

$$c(z, x) = \cosh(kx) + \frac{e^{kx}}{k} \tilde{E}_1(z, x), \quad (3.12)$$

with the error term

$$\tilde{E}_1(z, x) = \int_{[0, x)} \frac{1 - e^{-2k(x-y)}}{2} \tilde{c}(z, y) d\chi(y)$$

which is locally uniformly bounded in x by the above estimate for $\tilde{c}(z, x)$. Reinserting (3.12) into the integral equation for $c(z, x)$ leads to the desired representation of the solution $c(z, x)$, where the error term

$$E_1(z, x) = \int_{[0, x)} \frac{1 - e^{-2k(x-y)}}{2} \tilde{E}_1(z, y) d\chi(y)$$

is locally uniformly bounded in x .

To compute the desired estimate for the error term $E_1(z, x)$ we insert (3.12) into the definition of $\tilde{E}_1(z, x)$, which leads to

$$\tilde{E}_1(z, x) = \begin{cases} \frac{1}{4}(\chi(x) + \chi(\{0\})) + \mathcal{O}(\frac{1}{2k}), & x > 0, \\ 0, & x = 0, \end{cases}$$

by the dominated convergence theorem, where the estimate is locally uniform in x as $\text{Im}(z) \rightarrow +\infty$. Now inserting this estimate into the definition of $E_1(z, x)$ and applying the dominated convergence theorem again, leads to the desired estimate for the error term $E_1(z, x)$.

Similarly, considering $\tilde{s}(z, x) = ke^{-kx}s(z, x)$ we look at the corresponding integral equation

$$\tilde{s}(z, x) = \frac{1 - e^{-2kx}}{2} + \int_{[0, x)} \frac{1 - e^{-2k(x-y)}}{2k} \tilde{s}(z, y) d\chi(y)$$

and conclude that there is a bounded solution satisfying

$$|\tilde{s}(z, x)| \leq \exp(|k|^{-1}|\chi|([0, x])).$$

The rest follows as before. \square

Next we recall the Weyl function $m(z)$ defined such that

$$u(z, x) = c(z, x) + m(z)s(z, x), \quad z \in \mathbb{C} \setminus \mathbb{R}, \quad (3.13)$$

is square integrable near b and satisfies the boundary condition of our operator at b (if there is one). Following the original approach of Weyl we recall the Weyl circles with center, radius given by

$$q(z, x_0) = -\frac{W_{x_0}(c(z, \cdot), s(z, \cdot)^*)}{W_{x_0}(s(z, \cdot), s(z, \cdot)^*)}, \quad r(z, x_0) = \frac{1}{|W_{x_0}(s(z, \cdot), s(z, \cdot)^*)|}, \quad (3.14)$$

with $x_0 \in [0, b)$, respectively. By construction the solutions $c(z, x) + m s(z, x)$ with m on the Weyl circle are precisely the ones which satisfy a real boundary condition at x_0 :

$$\frac{c'(z, x_0) + m s'(z, x_0)}{c(z, x_0) + m s(z, x_0)} \in \mathbb{R} \cup \{\infty\}. \quad (3.15)$$

Taking $x_0 \nearrow b$ these circles are nested and hence converge to a circle (limit circle case) or to a point (limit point case). In the first case, the points on the circle correspond to the Weyl functions corresponding to different self-adjoint realizations and in the second case the point corresponds to the unique Weyl function of the unique self-adjoint realization.

Moreover, for $\text{Im}(z) > 0$, those where the quotient in (3.15) is in the upper, lower half-plane are those for which m is in the interior, exterior of the Weyl circle, respectively. Hence, if we find an m in the interior, the distance between m and $m(z)$ can be at most $2r(z, x_0)$. This is precisely the idea (due to [2]) of the following lemma:

Lemma 3.2. *For every $x_0 \in (0, b)$ we have*

$$m(z) = -\frac{c(z, x_0)\sqrt{-z} + c'(z, x_0)}{s'(z, x_0) + \sqrt{-z}s(z, x_0)} + \mathcal{O}(ze^{-2\sqrt{-z}x_0}), \quad (3.16)$$

as $\text{Im}(z) \rightarrow +\infty$, where the error depends only on the total variation $|\chi|([0, x_0))$. Moreover,

$$\frac{c(z, x)\sqrt{-z} + c'(z, x)}{s'(z, x) + \sqrt{-z}s(z, x)} = \sqrt{-z} \frac{1 + \frac{1}{\sqrt{-z}} \int_{[0, x)} \tilde{c}(z, y) d\chi(y)}{1 + \frac{1}{\sqrt{-z}} \int_{[0, x)} \tilde{s}(z, y) d\chi(y)} \quad (3.17)$$

where $\tilde{c}(z, x) = e^{-\sqrt{-z}x}c(z, x)$ and $\tilde{s}(z, x) = \sqrt{-z}e^{-\sqrt{-z}x}s(z, x)$.

Proof. For $\text{Im}(z) > 0$ it follows that the solution defined via the initial condition

$$v(z, x_0) = 1, \quad v'(z, x_0) = -\sqrt{-z}$$

with $x_0 \in (0, b)$ corresponds to a point in the interior of the Weyl circle. Indeed we have

$$\frac{v'(z, 0)}{v(z, 0)} = \frac{W_0(c(z, \cdot), v(z, \cdot))}{W_0(v(z, \cdot), s(z, \cdot))}$$

and the constancy of the Wronskian implies

$$\frac{v'(z, 0)}{v(z, 0)} = \frac{W_{x_0}(c(z, \cdot), v(z, \cdot))}{W_{x_0}(v(z, \cdot), s(z, \cdot))} = -\frac{c(z, x_0)\sqrt{-z} + c'(z, x_0)}{s'(z, x_0) + \sqrt{-z}s(z, x_0)}. \quad (3.18)$$

Now an easy computation shows that

$$\frac{c'(z, x_0) + s'(z, x_0)\frac{v'(z, 0)}{v(z, 0)}}{c(z, x_0) + s(z, x_0)\frac{v'(z, 0)}{v(z, 0)}} = -\sqrt{-z} \in \mathbb{C}_+.$$

Hence the point $\frac{v'(z, 0)}{v(z, 0)}$ lies in the interior of the Weyl circle by the considerations prior to this lemma. As the same is true for the Weyl function $m(z)$ of our problem, we obtain

$$m(z) = \frac{v'(z, 0)}{v(z, 0)} + \mathcal{O}(r(z, x_0)) = \frac{v'(z, 0)}{v(z, 0)} + \mathcal{O}(ze^{-2\sqrt{-z}x_0})$$

as $\text{Im}(z) \rightarrow \infty$, where we have used Lemma 3.1 for the second identity.

The last part is a straightforward calculation using (3.2)–(3.5). \square

Combining this lemma with Lemma 3.1 gives our main result:

Theorem 3.3. *For every $x_0 \in (0, b)$ the Weyl m -function has the asymptotic behavior*

$$m(z) = -\sqrt{-z} - \int_{[0, x_0)} e^{-2\sqrt{-z}y} d\chi(y) + o(z^{-1/2}) \quad (3.19)$$

as $\text{Im}(z) \rightarrow \infty$. Moreover, the error satisfies an estimate of the type $|o(z^{-1/2})| \leq C|z|^{-1/2}$, where the constant depends only on the total variation $|\chi|([0, x_0))$.

Proof. By inserting Lemma 3.1 into the identity (3.18) a long but straightforward computation shows that

$$m(z) = -k - I_1 - \frac{1}{k}(E_1 + E_2 - E_3 - E_4) + \frac{1}{2k}(\chi(x_0)I_1 - I_1^2) + o\left(\frac{1}{k}\right)$$

as $\text{Im}(z) \rightarrow +\infty$, where we abbreviated $k = \sqrt{-z}$ and $I_1(z) = \int_{[0, x_0)} e^{-2ky} d\chi(y)$. Inserting the estimates for the error terms $E_j(z) = E_j(z, x_0)$ of Lemma 3.1 as well as the estimate

$$I_1(z) = \chi(\{0\}) + o(1)$$

as $\text{Im}(z) \rightarrow +\infty$, finally proves the theorem. \square

Remark 3.4. (i). We want to emphasize that in contradistinction to [2] our approach is more direct and avoids the use of Riccati equations for the Weyl function. In addition to being simpler this approach also retains a good control over the error with respect to the total variation of χ . This will turn out crucial for our following application which states that (1.4) continues to hold in the sense of distributions. A similar result (for Neumann boundary conditions) can be found in Lemma 5.1 of [3] with a weaker error term and again without the above mentioned control.

(ii). It is also possible to allow for more general potentials. In fact, one could consider potentials in H_{loc}^{-1} , however, in this case Lemma 3.1 is expected to break down since $\chi(x)$ will be in L^2 and hence there are no point values. We refer to Theorem B.2 in [10], where the weaker result $m(z) = -\sqrt{-z} + o(\sqrt{-z})$ for in fact a slightly larger class than H_{loc}^{-1} is shown.

(iii). For an arbitrary left endpoint a equation (3.19) reads

$$m(z) = -\sqrt{-z} - \int_{[a, x_0)} e^{-2\sqrt{-z}(y-a)} d\chi(y) + o(z^{-1/2}).$$

(iv). Of course one can iterate this procedure to get further terms in the above expansion. For example using one more step one obtains:

$$\begin{aligned} m(z) = & -k - \int_{[0, x_0)} e^{-2ky} d\chi(y) \\ & - \frac{1}{2k} \int_{[0, x_0)} \left((1 - e^{-2k(x_0-y)}) \int_{[0, y)} e^{-2kr} d\chi(r) \right) d\chi(y) \\ & + \frac{1}{2k} \int_{[0, x_0)} (1 - e^{-2ky}) d\chi(y) \int_{[0, x_0)} e^{-2ky} d\chi(y) + \mathcal{O}(k^{-2}). \end{aligned}$$

Theorem 3.5. *Denote by $m(z, t)$ the Weyl function associated with our operator restricted to the interval (t, b) with a Dirichlet boundary condition at $t \in [a, b)$*

and keeping the boundary condition at b (if any) fixed. Then for any test function $\phi \in C_c^\infty(a, b)$ we have

$$\int_a^b m(z, t)\phi(t)dt = -\sqrt{-z} \int_a^b \phi(t)dt - \frac{1}{2\sqrt{-z}} \int_a^b \phi(s)d\chi(s) + o(z^{-1/2}). \quad (3.20)$$

Proof. All we have to do is multiply (3.19) with ϕ and integrate with respect to t . By our bound on the error term we can integrate the error term using dominated convergence and the rest follows by Fubini:

$$\begin{aligned} \int_a^b m(z, t)\phi(t)dt &= -\sqrt{-z}\Phi_0 - \int_{\mathbb{R}^2} \phi(t)\mathbb{1}_{[t, t+\varepsilon)}(s)e^{-2\sqrt{-z}(s-t)}d\chi(s)dt + o(z^{-1/2}) \\ &= -\sqrt{-z}\Phi_0 - \int_{\mathbb{R}^2} \phi(t)\mathbb{1}_{(s-\varepsilon, s]}(t)e^{2\sqrt{-z}(t-s)}dt d\chi(s) + o(z^{-1/2}) \\ &= -\sqrt{-z}\Phi_0 - \frac{1}{2\sqrt{-z}} \int_a^b \phi(s)d\chi(s) + o(z^{-1/2}), \end{aligned}$$

where we have abbreviated $\Phi_0 = \int_a^b \phi(t)dt$ and $\mathbb{1}_\Omega$ denotes the indicator function of a set Ω . Moreover, in the last step we have used

$$\int_{s-\varepsilon}^s \phi(t)e^{2\sqrt{-z}(t-s)}dt = \frac{1}{2\sqrt{-z}}\phi(s) + O(z^{-1}),$$

which follows from a simple integration by parts. \square

Finally, we look at the example

Example 3.6. Denote by δ_0 a single Dirac delta measure located at $x = 0$ and set

$$\chi = \alpha\delta_0, \quad \alpha \in \mathbb{R}. \quad (3.21)$$

In this case the solution $u(z, x)$ from (3.13) is given as $u(z, x) = e^{-\sqrt{-z}x}$ and thus $u(z, 0) = 1$ and $u'(z, 0) = u'(z, 0-) = -\sqrt{-z} - \alpha$ implying

$$m(z, 0) = -\sqrt{-z} - \alpha \quad (3.22)$$

in agreement with (3.19).

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