

Commutation Methods for Schrödinger Operators with Strongly Singular Potentials

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COMMUTATION METHODS FOR SCHRÖDINGER OPERATORS WITH STRONGLY SINGULAR POTENTIALS

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ABSTRACT. We explore the connections between singular Weyl–Titchmarsh theory and the single and double commutation methods. In particular, we compute the singular Weyl function of the commuted operators in terms of the original operator. We apply the results to spherical Schrödinger operators (also known as Bessel operators). We also investigate the connections with the generalized Bäcklund–Darboux transformation.

1. INTRODUCTION

The present paper is concerned with spectral theory for one-dimensional Schrödinger operators

$$(1.1) \quad H = -\frac{d^2}{dx^2} + q(x), \quad x \in (a, b),$$

on the Hilbert space $L^2(a, b)$ with a real-valued potential $q \in L^1_{\text{loc}}(a, b)$. It has been shown recently by Gesztesy and Zinchenko [23], Fulton and Langer [14], [15], Kurasov and Luger [33] that, for a large class of singularities at a , it is still possible to define a singular Weyl function at the basepoint a . Furthermore, in previous work we have shown that this singular Weyl function shares many properties with the classical Weyl function [30] and established the connection with super singular perturbations for the special case of spherical Schrödinger operators

$$(1.2) \quad H = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + q(x), \quad x \in (0, \infty),$$

(also known as Bessel operators) [28].

On the other hand, commutation methods have played an important role in the theory of one-dimensional Schrödinger operators both as a method for inserting eigenvalues as well as for constructing solutions of the (modified) Korteweg–de Vries equation (see, e.g., [18] and the references therein). Historically, these methods of inserting eigenvalues go back to Jacobi [26] and Darboux [8] with decisive later contributions by Crum [7], Krein [31], Schmincke [39], and Deift [9]. Two particular methods turned out to be of special importance: The single commutation method, also called the Crum–Darboux method [7], [8] (actually going back at least to Jacobi [26]) and the double commutation method, to be found, e.g., in the seminal work of Gel’fand and Levitan [16]. For recent extensions of these methods we refer to [17], [20], [21], [40].

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Krein [31] was the first to realize the connection between inverse spectral problems and Crum's results. Namely, in [31], the connection between the spectral measures of the original and transformed operators was established and then exploited to characterize the spectral measures of Bessel operators in the case $l \in \mathbb{N}$ (see also [13]). This idea has been subsequently used by many authors: see, for instance, [2, 5, 9, 13, 24] and references therein.

The purpose of our present paper is to continue the work of Krein and establish the connection between the singular Weyl functions (and hence between the spectral measures) of the original and transformed operators for both the single and double commutation method. In particular, we will obtain an independent proof for the fact that the singular Weyl function of perturbed Bessel operators is a generalized Nevanlinna function. In addition, we investigate the connections with the generalized Bäcklund–Darboux transformation (GBDT) for a particular example. This method is a generalization of the double commutation method which it contains as a special case (cf. Subsection 5.1).

2. SINGULAR WEYL–TITCHMASH THEORY

We begin by recalling a few facts from [30]. To set the stage, we will consider one-dimensional Schrödinger operators on $L^2(a, b)$ with $-\infty \leq a < b \leq \infty$ of the form

$$(2.1) \quad \tau = -\frac{d^2}{dx^2} + q,$$

where the potential q is real-valued and satisfies

$$(2.2) \quad q \in L^1_{loc}(a, b).$$

We will use τ to denote the formal differential expression and H to denote a corresponding self-adjoint operator given by τ with separated boundary conditions at a and/or b .

If a (resp. b) is finite and q is in addition integrable near a (resp. b), we will say a (resp. b) is a *regular* endpoint. We will say τ , respectively H , is *regular* if both a and b are regular.

We will choose a point $c \in (a, b)$ and also consider the operators $H^D_{(a,c)}$, $H^D_{(c,b)}$ which are obtained by restricting H to (a, c) , (c, b) with a Dirichlet boundary condition at c , respectively. The corresponding operators with a Neumann boundary condition will be denoted by $H^N_{(a,c)}$ and $H^N_{(c,b)}$.

Moreover, let $c(z, x)$, $s(z, x)$ be the solutions of $\tau u = zu$ corresponding to the initial conditions $c(z, c) = 1$, $c'(z, c) = 0$ and $s(z, c) = 0$, $s'(z, c) = 1$.

Define the Weyl m -functions (corresponding to the base point c) such that

$$(2.3) \quad \begin{aligned} u_-(z, x) &= c(z, x) - m_-(z)s(z, x), & z \in \mathbb{C} \setminus \sigma(H^D_{(a,c)}), \\ u_+(z, x) &= c(z, x) + m_+(z)s(z, x), & z \in \mathbb{C} \setminus \sigma(H^D_{(c,b)}), \end{aligned}$$

are square integrable on (a, c) , (c, b) and satisfy the boundary condition of H at a , b (if any), respectively. The solutions $u_{\pm}(z, x)$ (as well as their multiples) are called Weyl solutions at a , b . For further background we refer to [42, Chap. 9] or [43].

To define an analogous singular Weyl m -function at the, in general singular, endpoint a we will first need an analog of the system of solutions $c(z, x)$ and $s(z, x)$. Hence our first goal is to find a system of real entire 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

$W(\theta(z), \phi(z)) = 1$. By a real entire function we mean an entire function which is real-valued on the real line. To this end we start with a hypothesis which will turn out necessary and sufficient for such a system of solutions to exist.

Hypothesis 2.1. *Suppose that the spectrum of $H_{(a,c)}^D$ is purely discrete for one (and hence for all) $c \in (a, b)$.*

Note that this hypothesis is for example satisfied if $q(x) \rightarrow +\infty$ as $x \rightarrow a$ (cf. Problem 9.7 in [42]).

Lemma 2.2 ([30]). *Suppose Hypothesis 2.1 holds. Then there exists a fundamental system of solutions $\phi(z, x)$ and $\theta(z, x)$ of $\tau u = zu$ which are real entire with respect to z such that*

$$(2.4) \quad W(\theta(z), \phi(z)) = 1$$

and $\phi(z, \cdot)$ is in the domain of H near a . Here $W_x(u, v) = u(x)v'(x) - u'(x)v(x)$ is the usual Wronski determinant.

It is important to point out that such a system is not unique and any other such system is given by

$$\tilde{\theta}(z, x) = e^{-g(z)}\theta(z, x) - f(z)\phi(z, x), \quad \tilde{\phi}(z, x) = e^{g(z)}\phi(z, x),$$

where $g(z), f(z)$ are real entire functions.

Given a system of real entire solutions $\phi(z, x)$ and $\theta(z, x)$ as in the above lemma we can define the singular Weyl function

$$(2.5) \quad M(z) = -\frac{W(\theta(z), u_+(z))}{W(\phi(z), u_+(z))}$$

such that the solution which is in the domain of H near b (cf. (2.3)) is given by

$$(2.6) \quad u_+(z, x) = a(z)(\theta(z, x) + M(z)\phi(z, x)),$$

where $a(z) = -W(\phi(z), u_+(z)) = \beta(z) - m_+(z)\alpha(z)$. By construction we obtain that the singular Weyl function $M(z)$ is analytic in $\mathbb{C} \setminus \mathbb{R}$ and satisfies $M(z) = M(z^*)^*$. Rather than $u_+(z, x)$ we will use

$$(2.7) \quad \psi(z, x) = \theta(z, x) + M(z)\phi(z, x).$$

Recall also from [30, Lem. 3.2] that associated with $M(z)$ is a corresponding spectral measure

$$(2.8) \quad \frac{1}{2}(\rho((x_0, x_1)) + \rho([x_0, x_1])) = \lim_{\varepsilon \downarrow 0} \frac{1}{\pi} \int_{x_0}^{x_1} \operatorname{Im}(M(x + i\varepsilon)) dx.$$

3. CONNECTION WITH THE SINGLE COMMUTATION METHOD

3.1. Preliminary basic results. We begin by recalling a few basic facts from the single commutation method. Let A be a densely defined closed operator and recall that $H = A^*A$ is a self-adjoint operator with $\ker(H) = \ker(A)$. Similarly, $\hat{H} = AA^*$ is a self-adjoint operator with $\ker(\hat{H}) = \ker(A^*)$. Then the key observation is the following well-known result (see e.g. [42, Thm. 8.6] for a short proof):

Theorem 3.1 ([9]). *Let A be a densely defined closed operator and introduce $H = A^*A$, $\hat{H} = AA^*$. Then the operators $H|_{\ker(H)^\perp}$ and $\hat{H}|_{\ker(\hat{H})^\perp}$ are unitarily equivalent.*

If $H\psi = \lambda\psi$, $\lambda \in \mathbb{R}$, $\psi \in \mathfrak{D}(H)$, then $\hat{\psi} = A\psi \in \mathfrak{D}(\hat{H})$ with $\hat{H}\hat{\psi} = \lambda\hat{\psi}$ and $\|\hat{\psi}\| = \sqrt{\lambda}\|\psi\|$. Moreover,

$$(3.1) \quad R_{\hat{H}}(z) \supseteq \frac{1}{z} (AR_H(z)A^* - \mathbb{1}), \quad R_H(z) \supseteq \frac{1}{z} (A^*R_{\hat{H}}(z)A - \mathbb{1}),$$

where $R_H(z) = (H - z)^{-1}$ denotes the resolvent of an operator H .

3.2. Application to Schrödinger operators. In order to find such a factorization for a given Schrödinger operator H one requires a positive solution of the underlying differential equation. Existence of such a solution is equivalent to semi-boundedness of H and we will thus make the following assumption:

Hypothesis 3.2. *In addition to Hypothesis 2.1 assume that H is bounded from below and limit point at b . Let $\lambda \in \mathbb{R}$ be such that $H - \lambda \geq 0$.*

In particular, let $\phi(z, x)$, $\theta(z, x)$ be a fundamental system of solutions as in Lemma 2.2 and recall (cf. [42, Lem. 9.7]) that the Green's function of H is given by

$$(3.2) \quad G(z, x, y) = \begin{cases} \phi(z, x)\psi(z, y), & x \leq y, \\ \phi(z, y)\psi(z, x), & x \geq y. \end{cases}$$

Moreover, if $H - \lambda \geq 0$ we must have $\phi(\lambda, x) > 0$ (as well as $\psi(\lambda, x) > 0$) for $x \in (a, b)$ possibly after flipping signs by [19, Cor. 2.4].

Now consider the operator

$$(3.3) \quad A_\phi f = a_\phi f, \quad a_\phi = -\frac{d}{dx} + \frac{\phi'(\lambda, x)}{\phi(\lambda, x)},$$

$$\mathfrak{D}(A_\phi) = \{f \in L^2(a, b) \mid f \in AC_{loc}(a, b), a_\phi f \in L^2(a, b)\}.$$

Here we use A_ϕ and a_ϕ for the operator and differential expression, respectively. It is straightforward to check (cf. [42, Problem 9.3]) that A_ϕ is closed and that its adjoint is given by

$$(3.4) \quad A_\phi^* f = a_\phi^* f, \quad a_\phi^* = \frac{d}{dx} + \frac{\phi'(\lambda, x)}{\phi(\lambda, x)},$$

$$\mathfrak{D}(A_\phi^*) = \{f \in L^2(a, b) \mid f \in AC_{loc}(a, b), a_\phi^* f \in L^2(a, b),$$

$$\lim_{x \rightarrow a, b} f(x)g(x) = 0, \forall g \in \mathfrak{D}(A_\phi)\}.$$

If we also have $\theta(\lambda, x) > 0$ we can also define A_θ by using $\theta(\lambda, x)$ in place of $\phi(\lambda, x)$.

Lemma 3.3. *Assume Hypothesis 3.2 holds. Then $H - \lambda = A_\phi^* A_\phi$. If in addition $\theta(\lambda, x) > 0$ and τ is limit point at a , then we also have $H - \lambda = A_\theta^* A_\theta$.*

Proof. It is simple algebra to check that H and $A_\phi^* A_\phi$ agree on functions with compact support in (a, b) hence $A_\phi^* A_\phi$ is a self-adjoint extension of the minimal operator associated with τ and it remains to identify the boundary conditions. Since by assumption τ is limit point at b we only need to consider a . Moreover, since $\phi(\lambda, x)$ is in the domain of $A_\phi^* A_\phi$ near a by our choice of A_ϕ , both $A_\phi^* A_\phi$ and H are associated with the boundary condition generated by $\phi(\lambda, x)$ if τ is limit circle at a .

The case of A_θ is even simpler since by our limit point assumption there is no need to identify any boundary conditions. \square

The commuted operator $\hat{H} - \lambda = A_\phi A_\phi^*$ is associated with the potential

$$(3.5) \quad \hat{q}(x) = q(x) - 2 \frac{d}{dx} \frac{\phi'(\lambda, x)}{\phi(\lambda, x)}.$$

Moreover, it is straightforward to check that if $u(z)$ solves $\tau u = zu$ then

$$(3.6) \quad \hat{u}(z, x) = a_\phi u(z, x) = - \frac{W_x(\phi(\lambda), u(z))}{\phi(\lambda, x)}$$

solves $\hat{\tau} \hat{u} = z \hat{u}$ and given two solutions $u(z)$ and $v(z)$ we have

$$(3.7) \quad W(\hat{u}(z), \hat{v}(z)) = (z - \lambda)W(u(z), v(z)).$$

Similarly, $\check{H} - \lambda = A_\theta A_\theta^*$ is associated with the potential

$$(3.8) \quad \check{q}(x) = q(x) - 2 \frac{d}{dx} \frac{\theta'(\lambda, x)}{\theta(\lambda, x)}$$

and

$$(3.9) \quad \check{u}(z, x) = -a_\theta u(z, x) = \frac{W_x(\theta(\lambda), u(z))}{\theta(\lambda, x)}$$

solves $\check{\tau} \check{u} = z \check{u}$ and given two solutions $u(z)$ and $v(z)$ we have

$$(3.10) \quad W(\check{u}(z), \check{v}(z)) = (z - \lambda)W(u(z), v(z)).$$

Theorem 3.4. *Assume Hypothesis 3.2 holds. Then the operator $\hat{H} = A_\phi A_\phi^* + \lambda$ has an entire system of solutions*

$$(3.11) \quad \hat{\phi}(z, x) = \frac{1}{z - \lambda} a_\phi \phi(z, x) = - \frac{W_x(\phi(\lambda), \phi(z))}{(z - \lambda)\phi(\lambda, x)} = \frac{\int_a^x \phi(\lambda, y)\phi(z, y)dy}{\phi(\lambda, x)},$$

$$(3.12) \quad \hat{\theta}(z, x) = a_\phi \theta(z, x) = - \frac{W_x(\phi(\lambda), \theta(z))}{\phi(\lambda, x)},$$

which satisfy $W(\hat{\theta}(z), \hat{\phi}(z)) = 1$. In particular, \hat{H} satisfies again Hypothesis 2.1.

Furthermore, the Weyl solutions of \hat{H} are given by

$$(3.13) \quad \hat{\phi}(z, x), \quad \hat{\psi}(z, x) = a_\phi \psi(z, x) = - \frac{W_x(\phi(\lambda), \psi(z))}{\phi(\lambda, x)} = \hat{\theta}(z, x) + \hat{M}(z)\hat{\phi}(z, x),$$

where

$$(3.14) \quad \hat{M}(z) = (z - \lambda)M(z)$$

is the singular Weyl function of \hat{H} corresponding to the above system of solutions. Moreover, the associated spectral measures are related via

$$(3.15) \quad d\hat{\rho}(t) = (t - \lambda)d\rho(t).$$

Proof. The first part is easy to check using (3.7). To see

$$(3.16) \quad W_x(\phi(\lambda), \phi(z)) = (z - \lambda) \int_a^x \phi(\lambda, y)\phi(z, y)dy$$

note that both sides have the same derivative and are both equal 0 in the limit $x \rightarrow a$.

For the second part we set $\lambda = 0$ and fix $z \in \mathbb{C} \setminus \mathbb{R}$ without loss of generality. Moreover we will abbreviate $\phi(\lambda, x) = \phi_0(x)$, $\phi(z, x) = \phi(x)$, and $\psi(z, x) = \psi(x)$.

Now let f be some absolutely continuous function with compact support in (a, b) and $f' \in L^2$. Then invoking (3.1) one computes using (2.4), (3.11), (3.12), and integration by parts that

$$\begin{aligned}
R_{\hat{H}}(z)f(x) &= \frac{1}{z} \left(A_\phi \int_a^b G(z, x, y) A_\phi^* f(y) dy - f(x) \right) \\
&= \frac{1}{z} \left(a_\phi \left[\psi(x) \int_a^x \phi(y) (a_\phi^* f)(y) dy \right] + a_\phi \left[\phi(x) \int_x^b \psi(y) (a_\phi^* f)(y) dy \right] - f(x) \right) \\
&= \frac{1}{z} \left((a_\phi \psi)(x) \left(\phi(x) f(x) + \int_a^x f(y) (a_\phi \phi)(y) dy \right) \right. \\
&\quad \left. + (a_\phi \phi)(x) \left(-\psi(x) f(x) + \int_x^b f(y) (a_\phi \psi)(y) dy \right) - f(x) \right) \\
&= \frac{1}{z} \left(z \hat{\psi}(x) \int_a^x f(y) \hat{\phi}(y) dy + z \hat{\phi}(x) \int_x^b f(y) \hat{\psi}(y) dy \right. \\
&\quad \left. + \hat{\psi}(z) \phi(x) f(x) - z \hat{\phi}(x) \psi(x) f(x) - f(x) \right) \\
&= \hat{\psi}(x) \int_a^x \hat{\phi}(y) f(y) dy + \hat{\phi}(x) \int_x^b \hat{\psi}(y) f(y) dy = \int_a^b \hat{G}(z, x, y) f(y) dy,
\end{aligned}$$

which shows that

$$(3.17) \quad \hat{G}(z, x, y) = \begin{cases} \hat{\phi}(z, x) \hat{\psi}(z, y), & x \leq y, \\ \hat{\phi}(z, y) \hat{\psi}(z, x), & x \geq y, \end{cases}$$

is the Green's function of \hat{H} since the set of f under consideration is dense. Since the Green's function is unique, it follows that $\hat{\phi}(z, x)$ and $\hat{\psi}(z, x)$ are the Weyl solutions of \hat{H} . Finally, existence of the entire Weyl solution $\hat{\phi}(z, x)$ is equivalent to Hypothesis 2.1 by Lemma 2.2 in [29]. \square

Note

$$(3.18) \quad \hat{\phi}(\lambda, x) = -\frac{W_x(\phi(\lambda), \dot{\phi}(\lambda))}{\phi(\lambda, x)} = \frac{\int_a^x \phi(\lambda, y)^2 dy}{\phi(\lambda, x)}, \quad \hat{\theta}(\lambda, x) = \frac{1}{\phi(\lambda, x)},$$

where the dot denotes differentiation with respect to z .

Remark 3.5. *A few remarks are in order:*

- (i) *If τ is regular at a and $\theta(z, x)$, $\phi(z, x)$ are chosen to satisfy the boundary conditions*

$$\begin{aligned}
\theta(z, a) &= \cos(\alpha), \quad \theta'(z, a) = -\sin(\alpha), \\
\phi(z, a) &= \sin(\alpha), \quad \phi'(z, a) = \cos(\alpha),
\end{aligned}$$

then $\hat{\tau}$ will be again regular if and only if $\sin(\alpha) \neq 0$. Moreover, in this case we have

$$\begin{aligned}
\hat{\theta}(z, a) &= \sin(\alpha)^{-1}, \quad \hat{\theta}'(z, a) = \cos(\alpha) (z - \lambda - 1 - \cot(\alpha)^2), \\
\hat{\phi}(z, a) &= 0, \quad \hat{\phi}'(z, a) = \sin(\alpha).
\end{aligned}$$

(ii) If $\phi(\lambda, x)$ is the principal positive solution near a (i.e., if H is the Friedrich's extension of τ , see [34], [22]), that is,

$$(3.19) \quad \int_a^c \frac{dx}{\phi(\lambda, x)^2} = \infty,$$

then $\hat{\tau}$ will be limit point at a .

(iii) Note that \hat{H} has no eigenvalue at λ : $\sigma_p(\hat{H}) \cap \{\lambda\} = \emptyset$.

Recall that N_κ^∞ is the subclass of N_κ consisting of generalized Nevanlinna functions with κ negative squares and having no nonreal poles and the only generalized pole of nonpositive type at infinity. In particular, $M \in N_\kappa^\infty$ admits an integral representation

$$(3.20) \quad M(z) = (1+z^2)^k \int_{\mathbb{R}} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) \frac{d\rho(t)}{(1+t^2)^k} + \sum_{j=0}^l a_j z^j,$$

where $\lambda_0 = \inf \sigma(H)$, $k \leq \kappa$, $l \leq 2\kappa + 1$,

$$(3.21) \quad a_j \in \mathbb{R}, \quad \text{and} \quad \int_{\mathbb{R}} (1+t^2)^{-k-1} d\rho(t) < \infty.$$

Without loss of generality we can assume that the representation (3.20) is *irreducible*, that is, either $k = 0$ or $\int_{\mathbb{R}} (1+t^2)^{-k} d\rho(t) = \infty$. For further definitions and details we refer to, e.g., [32], [15, §2.2–2.3], [30, App. C].

Corollary 3.6. *Assume Hypothesis 3.2 holds. Assume also that the functions $M(z)$ and $\hat{M}(z)$ are connected by (3.14). Then $M \in N_\kappa^\infty$ for some $\kappa \in \mathbb{N}_0$ if and only if $\hat{M} \in N_{\tilde{\kappa}}^\infty$ with*

$$(3.22) \quad \tilde{\kappa} = \begin{cases} \kappa, & \lim_{y \uparrow \infty} \frac{M(iy)}{(iy)^{2\kappa}} \in [0, \infty), \\ \kappa + 1, & \lim_{y \uparrow \infty} \frac{\hat{M}(iy)}{(iy)^{2\kappa}} \in [-\infty, 0). \end{cases}$$

Proof. The proof is similar to the proof of Lemmas 5.1 and 5.2 from [27]. Assume that $M \in N_\kappa^\infty$ for some $\kappa \in \mathbb{N}_0$. Using an irreducible integral representation (3.20) we will show that

$$\begin{aligned} \hat{M}(z) &= (z - \lambda)M(z) \\ &= (z - \lambda)(1+z^2)^k \int_{\lambda_0}^{+\infty} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) \frac{d\rho(t)}{(1+t^2)^k} + (z - \lambda_0) \sum_{j=0}^l a_j z^j, \end{aligned}$$

where $\lambda_0 = \inf \sigma(H)$, lies in $N_{\tilde{\kappa}}^\infty$. Using

$$(z - \lambda) \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) = (z^2 + 1) \frac{1}{t-z} \frac{t-\lambda}{1+t^2} - \frac{z\lambda+1}{1+t^2}$$

we obtain

$$\hat{M}(z) = (1+z^2)^{k+1} \int_{\lambda_0}^{+\infty} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) \frac{d\hat{\rho}(t)}{(1+t^2)^{k+1}} + \sum_{j=0}^{l+1} \hat{a}_j z^j,$$

where $d\hat{\rho}$ given by (3.15) is positive since $\lambda \geq \lambda_0$ by Hypothesis 3.2.

The converse implication $\hat{M} \in N_{\tilde{\kappa}}^\infty \Rightarrow M \in N_\kappa^\infty$ can be established analogously.

Finally, the connection between κ and $\tilde{\kappa}$ is straightforward from the following characterization of N_κ^∞ -functions: Given a generalized Nevanlinna function M in N_κ^∞ , the corresponding κ is given by the multiplicity of the generalized pole at ∞

which is determined by the facts that the following limits exist and take values as indicated:

$$\lim_{y \uparrow \infty} -\frac{M(iy)}{(iy)^{2\kappa-1}} \in (0, \infty], \quad \lim_{y \uparrow \infty} \frac{M(iy)}{(iy)^{2\kappa+1}} \in [0, \infty).$$

□

Similarly, we obtain

Theorem 3.7. *Assume Hypothesis 3.2, τ is limit point at a , and let $\theta(\lambda, x) > 0$. The operator $\check{H} = A_\theta A_\theta^* - \lambda$ has an entire system of solutions*

$$(3.23) \quad \check{\phi}(z, x) = -a_\theta \phi(z, x) = \frac{W_x(\theta(\lambda), \phi(z))}{\theta(\lambda, x)},$$

$$(3.24) \quad \check{\theta}(z, x) = -\frac{1}{z-\lambda} a_\theta \theta(z, x) = \frac{W_x(\theta(\lambda), \theta(z))}{(z-\lambda)\theta(\lambda, x)},$$

which satisfy $W(\check{\theta}(z), \check{\phi}(z)) = 1$. In particular, \check{H} satisfies again Hypothesis 2.1.

Furthermore, the Weyl solutions of \check{H} are given by

$$(3.25) \quad \check{\phi}(z, x), \quad \check{\psi}(z, x) = -a_\theta \psi(z, x) = \frac{W_x(\theta(\lambda), \psi(z))}{(z-\lambda)\theta(\lambda, x)} = \check{\theta}(z, x) + \check{M}(z)\check{\phi}(z, x),$$

where

$$(3.26) \quad \check{M}(z) = (z-\lambda)^{-1}M(z)$$

is the singular Weyl function of \check{H} . The associated spectral measures are related via

$$(3.27) \quad d\check{\rho}(t) = (t-\lambda)^{-1}d\rho(t) - M(\lambda)d\Theta(t-\lambda),$$

where $\Theta(t) = 0$ for $t < 0$ and $\Theta(t) = 1$ for $t \geq 0$ is the usual step function. Here $M(\lambda) = \lim_{\varepsilon \downarrow 0} M(\lambda - \varepsilon)$.

Note

$$(3.28) \quad \check{\phi}(\lambda, x) = \frac{1}{\theta(\lambda, x)}, \quad \check{\theta}(\lambda, x) = \frac{W_x(\theta(\lambda), \dot{\theta}(\lambda))}{\theta(\lambda, x)}.$$

Remark 3.8. *Again a few remarks are in order:*

- (i) *If $\theta(\lambda, x)$ is the principal positive solution near b , that is,*

$$(3.29) \quad \int_c^b \frac{dx}{\theta(\lambda, x)^2} = \infty,$$

then $\check{\tau}$ will be limit point at b . (Note that the principal positive solution near a is $\phi(\lambda, x)$ since we assumed the limit point case at a .)

- (ii) *Note that \check{H} has an eigenvalue at λ unless $\theta(\lambda, x)$ is the principal positive solution near b .*
- (iii) *Note that factorizing \hat{H} using $\hat{\theta}(\lambda, x) = \phi(\lambda, x)^{-1}$ will transform \hat{H} back into H . In particular, $\check{\phi}(z, x) = \phi(z, x)$ and $\check{\theta}(z, x) = \theta(z, x)$.*
- (iv) *Clearly this procedure can be iterated and we refer (e.g.) to Appendix A of [20] for the well-known formulas.*

3.3. Example: The Coulomb Hamiltonian. We can apply the single commutation method to the Coulomb Hamiltonian

$$(3.30) \quad H_l = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} - \frac{\gamma}{x}, \quad l \in \mathbb{N}_0,$$

by setting

$$(3.31) \quad A_l f = -\frac{d}{dx} + \frac{l+1}{x} + \frac{\gamma}{2(l+1)}, \quad A_l^* f = \frac{d}{dx} + \frac{l+1}{x} + \frac{\gamma}{2(l+1)},$$

which gives ([42, Thm. 10.10])

$$(3.32) \quad H_l = A_l^* A_l - c_l^2, \quad H_{l+1} = A_l A_l^* - c_l^2,$$

where

$$(3.33) \quad c_l = \frac{\gamma}{2(l+1)}.$$

In particular, the singular Weyl function is given by

$$(3.34) \quad M_l(z) = M_0(z) \prod_{k=0}^{l-1} (z - c_k^2),$$

where the singular Weyl function $M_0(z)$ of H_0 is a Herglotz–Nevanlinna function since H_0 is limit circle at $a = 0$.

Remark 3.9. *The singular Weyl function for this case was explicitly computed in [15, eq. (5.11)]. Moreover, the fact that it can be reduced to the case $l = 0$ via the above product formula was also first observed in [15, Lemma 5.1]. In the special case $\gamma = 0$ we obtain $M_l(z) = \sqrt{-z}z^l$ as was first observed by [11] (see also Section 5 in [30]).*

3.4. Application to perturbed Bessel operators. Next we want to apply these results to perturbed spherical Schrödinger equations which have attracted considerable interest in the past [1], [5], [25] [29], [28]. In particular, we want to mention [2], where commutation techniques were used to transfer results for $l = 0$ to $l \in \mathbb{N}_0$.

Lemma 3.10. *Fix $l \geq -\frac{1}{2}$ and $p \in [1, \infty]$. Suppose*

$$(3.35) \quad H = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + q(x), \quad x \in (0, b),$$

where

$$(3.36) \quad \begin{cases} xq(x) \in L^p(0, c), & p \in (1, \infty], l \geq -\frac{1}{2}, \\ xq(x) \in L^1(0, c), & p = 1, l > -\frac{1}{2}, \\ x(1 - \log(x))q(x) \in L^1(0, c), & p = 1, l = -\frac{1}{2}, \end{cases}$$

for some $c \in (0, b)$. In addition, suppose H is bounded from below. If τ is limit circle at $a = 0$ we impose the usual boundary condition (corresponding to the Friedrichs extension; see also [4], [12])

$$(3.37) \quad \lim_{x \rightarrow 0} x^l((l+1)f(x) - xf'(x)) = 0, \quad l \in [-\frac{1}{2}, \frac{1}{2}).$$

Then

$$(3.38) \quad \hat{H} = -\frac{d^2}{dx^2} + \frac{(l+1)(l+2)}{x^2} + \hat{q}(x), \quad x\hat{q} \in L^p(0, c)$$

and if $l \geq \frac{1}{2}$ then

$$(3.39) \quad \check{H} = -\frac{d^2}{dx^2} + \frac{(l-1)l}{x^2} + \check{q}(x), \quad x\check{q} \in L^p(0, c).$$

Proof. It suffices to observe that by [28, Lem. 3.2, Cor. 3.4]

$$\phi(\lambda, x) = x^{l+1}u_1(\lambda, x),$$

where $u_1(\lambda, x)$, $xu_1'(\lambda, x) \in W^{1,p}(0, c)$, and $\lim_{x \rightarrow 0} xu_1'(\lambda, x) = 0$. Noting that $\phi(\lambda, x) > 0$ for all $x \in [0, b)$, by (3.5) we get

$$x\hat{q}(x) = xq(x) - 2x \frac{d}{dx} \frac{u_1'(\lambda, x)}{u_1(\lambda, x)} \in L^p(0, c).$$

Similarly, to prove (3.39) it suffices to note that

$$\theta(\lambda, x) = x^{-l}u_2(\lambda, x),$$

where $u_2(\lambda, x)$, $xu_2'(\lambda, x) \in W^{1,p}(0, c)$ and $\lim_{x \rightarrow 0} xu_2'(\lambda, x) = 0$. \square

Since H is limit circle at 0 for $l \in [-\frac{1}{2}, \frac{1}{2})$ and thus the singular Weyl function is a Herglotz–Nevanlinna function in this case (cf. [30, App. A]), we obtain by induction:

Corollary 3.11. *Suppose*

$$(3.40) \quad H = -\frac{d^2}{dx^2} + \frac{l(l+1)}{x^2} + q(x), \quad xq(x) \in L^p,$$

where $p \in [1, \infty]$ if $l + \frac{1}{2} \notin \mathbb{N}_0$ and $p \in (1, \infty]$ if $l + \frac{1}{2} \in \mathbb{N}_0$. Then there is a singular Weyl function of the form

$$(3.41) \quad M(z) = (z - \lambda)^{\lfloor l+1/2 \rfloor} M_0(z),$$

where $M_0(z)$ is a Herglotz–Nevanlinna function and $\lambda \leq \min \sigma(H)$. Here $\lfloor x \rfloor = \max\{n \in \mathbb{Z} | n \leq x\}$ is the usual floor function. The corresponding spectral measure is given by

$$(3.42) \quad d\rho(t) = (t - \lambda)^{\lfloor l+1/2 \rfloor} d\rho_0(t),$$

where the measure ρ_0 satisfies $\int_{\mathbb{R}} d\rho_0(t) = \infty$ and $\int_{\mathbb{R}} \frac{d\rho_0(t)}{1+t^2} < \infty$.

Corollary 3.12 ([30, 28]). *Assume the conditions of Corollary 3.11. Then there is a singular Weyl function from the class N_κ^∞ with $\kappa = \lfloor \frac{l}{2} + \frac{3}{4} \rfloor$.*

Proof. The inequality $\kappa \leq \lfloor \frac{l}{2} + \frac{3}{4} \rfloor$ follows after combining Corollary 3.11 with Theorem 4.2 from [30].

It remains to show $\kappa \geq \lfloor \frac{l}{2} + \frac{3}{4} \rfloor$. To this end denote by $M_0(z)$ the Weyl function of the operator H with $l \in [-1/2, 1/2)$. Then, since H is the Friedrichs extension of the minimal operator in this case, $M_0(z)$ satisfies (cf. [10, Proposition 4])

$$(3.43) \quad M_0(z) \rightarrow -\infty, \quad \text{as } z \rightarrow -\infty.$$

Moreover, by [30, Cor. A.9] and Hypothesis 3.2, $M_0(z)$ admits the following representation

$$M_0(z) = \operatorname{Re}(M_0(i)) + \int_\lambda^{+\infty} \left(\frac{1}{t-z} - \frac{t}{1+t^2} \right) d\rho_0(t), \quad z \notin [\lambda, +\infty),$$

where the measure satisfies $\int_{\lambda}^{+\infty} d\rho_0(t) = \infty$ and $\int_{\lambda}^{+\infty} (1+t^2)^{-1} d\rho_0(t) < \infty$. Hence, by (3.43) we conclude that

$$(3.44) \quad \int_{\lambda}^{+\infty} \frac{d\rho_0(t)}{1+|t|} = \infty.$$

Combining (3.44) with Corollary 3.11 and Theorem 4.2 from [30], we arrive at the desired inequality. \square

Remark 3.13. *Corollary 3.12 was first established by Fulton and Langer [15] in the case when the potential $q(x)$ is analytic in a neighborhood of $x = 0$ (see also [33]). In the general case, it was proven in [28] (see also [30]). Namely, by using high energy asymptotic of $\phi(z, x)$ it was shown in [30] that $\kappa \leq \lceil \frac{l+1}{2} \rceil$ (for the details see Section 8 in [30]). The equality $\kappa = \lfloor \frac{l}{2} + \frac{3}{4} \rfloor$ was proven in [28] with the help of theory of super singular perturbations and detailed analysis of solutions $\phi(z, x)$ and $\theta(z, x)$.*

4. CONNECTION WITH THE DOUBLE COMMUTATION METHOD

In this section we want to look at the effect of the double commutation method. We refer to [17], [21] for further background of this method. We will use the approach from [21] with the only difference that we include the limiting case $\gamma = \infty$ (we omit the necessary minor modifications of the proofs of [21], cf. [41, Sect. 11.6]).

Let H together with a fundamental system of solutions $\phi(z, x)$, $\theta(z, x)$ as in Lemma 2.2 be given.

Hypothesis 4.1. *Assume Hypothesis 2.1. Let $\gamma \in (0, \infty]$ and $\lambda \in \mathbb{R}$ such that $\phi(\lambda, x)$ satisfies the boundary condition at b if τ is limit circle at b (i.e., λ is an eigenvalue with eigenfunction $\phi(\lambda, x)$ if τ is limit circle at b).*

Introduce

$$(4.1) \quad \tilde{\phi}_{\gamma}(\lambda, x) = \frac{\phi(\lambda, x)}{\gamma^{-1} + \int_a^x \phi(\lambda, y)^2 dy}.$$

Denote by P and P_{γ} the orthogonal projections onto the one-dimensional spaces spanned by $\phi(\lambda, x)$ and $\tilde{\phi}_{\gamma}(\lambda, x)$, respectively. Here we set the projection equal to zero if the function is not in $L^2(a, b)$. Note that $\tilde{\phi}_{\gamma}(\lambda, \cdot) \in L^2(a, b)$ if and only if $\gamma < \infty$ ([21, Lem. 2.1]).

By [21, Lem. 2.1] the transformation

$$(4.2) \quad U_{\gamma} f(x) = f(x) - \tilde{\phi}_{\gamma}(\lambda, x) \int_a^x \phi(\lambda, y) f(y) dy$$

is a unitary map from $(1 - P)L^2(a, b)$ onto $(1 - P_{\gamma})L^2(a, b)$. Moreover, by [21, Thm. 3.2]

$$(4.3) \quad H_{\gamma}(1 - P_{\gamma}) = U_{\gamma} H U_{\gamma}^{-1}(1 - P),$$

where the operator H_{γ} is associated with the potential

$$(4.4) \quad q_{\gamma}(x) = q(x) - 2 \frac{d^2}{dx^2} \log \left(\gamma^{-1} + \int_a^x \phi(\lambda, y)^2 dy \right)$$

and boundary conditions (if any)

$$(4.5) \quad W_a(\tilde{\phi}_{\gamma}(\lambda), f) = W_b(\tilde{\phi}_{\gamma}(\lambda), f) = 0.$$

Note that for $\gamma < \infty$ the operator H_γ is limit circle at a if and only H is and that for $\gamma = \infty$ the operator H_∞ is always limit point at b .

Theorem 4.2. *Assume Hypothesis 4.1 and let $\gamma < \infty$. The operator H_γ has an entire system of solutions*

$$\begin{aligned} \phi_\gamma(z, x) &= \phi(z, x) - \tilde{\phi}_\gamma(\lambda, x) \int_a^x \phi(\lambda, y) \phi(z, y) dy \\ &= \phi(z, x) + \frac{1}{z - \lambda} \tilde{\phi}_\gamma(\lambda, x) W_x(\phi(\lambda), \phi(z)), \end{aligned} \quad (4.6)$$

$$\theta_\gamma(z, x) = \theta(z, x) + \frac{1}{z - \lambda} \left(\tilde{\phi}_\gamma(\lambda, x) W_x(\phi(\lambda), \theta(z)) + \gamma \phi_\gamma(z, x) \right). \quad (4.7)$$

which satisfy $W(\theta_\gamma(z), \phi_\gamma(z)) = 1$. In particular, H_γ satisfies again Hypothesis 2.1.

Furthermore, the Weyl solutions of H_γ are given by

$$\begin{aligned} \phi_\gamma(z, x), \quad \psi_\gamma(z, x) &= \psi(z, x) + \frac{1}{z - \lambda} \tilde{\phi}_\gamma(\lambda, x) W_x(\phi(\lambda), \psi(z)) \\ &= \theta_\gamma(z, x) + M_\gamma(z) \phi_\gamma(z, x), \end{aligned} \quad (4.8)$$

where

$$M_\gamma(z) = M(z) - \frac{\gamma}{z - \lambda}$$

is the singular Weyl function of H_γ . The associated spectral measures are related via

$$d\rho_\gamma(x) = d\rho(x) + \gamma d\Theta(x - \lambda). \quad (4.9)$$

Proof. It is straightforward to check that $\phi_\gamma(z, x)$, $\theta_\gamma(z, x)$ is an entire system of solutions whose Wronskian equals one (cf. [21, (3.14) and (3.16)]). The extra multiple of $\phi_\gamma(z, x)$ has been added to $\theta_\gamma(z, x)$ to remove the pole at $z = \lambda$ (cf. (4.12) below).

That ψ_γ is square integrable near b follows from (cf. [21, (3.15)])

$$|\psi_\gamma(z, x)|^2 = |\psi(z, x)|^2 - \frac{\gamma}{|z - \lambda|^2} \frac{d}{dx} \left(\frac{|W_x(\phi(\lambda), \psi(z))|^2}{1 + \gamma \int_a^x \phi(\lambda, y)^2 dy} \right) \quad (4.10)$$

using the Cauchy–Schwartz inequality since

$$W_x(\phi(\lambda), \psi(z)) = W_c(\phi(\lambda), \psi(z)) + (\lambda - z) \int_c^x \phi(\lambda, y) \psi(z, y) dy.$$

To show that $\psi_\gamma(z, x)$ satisfies the boundary condition at b if τ_γ is limit circle at b we use (cf. [21, (3.16)] plus (3.16))

$$W_x(\phi_\gamma(\lambda), \psi_\gamma(z)) = \frac{W_x(\phi(\lambda), \psi(z))}{1 + \gamma \int_a^x \phi(\lambda, y)^2 dy}. \quad (4.11)$$

□

Note

$$\phi_\gamma(\lambda, x) = \gamma^{-1} \tilde{\phi}_\gamma(\lambda, x), \quad \theta_\gamma(\lambda, x) = \theta(\lambda, x) + \tilde{\phi}_\gamma(\lambda, x) W_x(\phi(\lambda), \dot{\theta}(\lambda)). \quad (4.12)$$

Remark 4.3. *Again a few remarks are in order:*

- (i) *Clearly this procedure can be iterated and we refer to Section 4 of [21] for the corresponding formulas.*
- (ii) *If λ is an eigenvalue, one could even admit $\gamma \in [-\|\phi(\lambda)\|^{-2}, \infty)$.*

- (iii) *This procedure leaves operators of the type (3.35) invariant. In particular, it does not change l .*

Theorem 4.4. *Assume Hypothesis 4.1 and let $\gamma = \infty$. The operator H_∞ has an entire system of solutions*

$$(4.13) \quad \phi_\infty(z, x) = \frac{1}{z - \lambda} \left(\phi(z, x) - \tilde{\phi}_\infty(\lambda, x) \int_a^x \phi(\lambda, y) \phi(z, y) dy \right)$$

$$(4.14) \quad \theta_\infty(z, x) = (z - \lambda)\theta(z, x) + \tilde{\phi}_\infty(\lambda, x) W_x(\phi(\lambda), \theta(z)),$$

which satisfy $W(\theta_\infty(z), \phi_\infty(z)) = 1$. In particular, H_∞ satisfies again Hypothesis 2.1.

Furthermore, the Weyl solutions of H_∞ are given by

$$(4.15) \quad \begin{aligned} \phi_\infty(z, x), \quad \psi_\infty(z, x) &= (z - \lambda)\psi(z, x) + \tilde{\phi}_\infty(\lambda, x) W_x(\phi(\lambda), \psi(z)) \\ &= \theta_\infty(z, x) + M_\infty(z)\phi_\infty(z, x), \end{aligned}$$

where

$$(4.16) \quad M_\infty(z) = (z - \lambda)^2 M(z)$$

is the singular Weyl function of H_∞ . The associated spectral measures are related via

$$(4.17) \quad d\rho_\infty(t) = (t - \lambda)^2 d\rho(t).$$

Proof. In the limiting case $\gamma \rightarrow \infty$ the definition (4.6) from the previous theorem would give $\phi_\infty(\lambda, x) = 0$ and we simply need to remove this zero. The rest follows as in the previous theorem. \square

Note

$$(4.18) \quad \phi_\infty(\lambda, x) = \dot{\phi}(z, x) - \tilde{\phi}_\infty(\lambda, x) \int_a^x \phi(\lambda, y) \dot{\phi}(z, y) dy, \quad \theta_\infty(\lambda, x) = -\tilde{\phi}_\infty(\lambda, x)$$

Remark 4.5. (i) *Again this procedure can be iterated and we refer to Section 4 of [21] for the corresponding formulas.*

- (ii) *For operators of the type (3.35) this procedure changes l to $l + 2$.*

5. EXAMPLES BASED ON THE GENERALIZED BÄCKLUND–DARBOUX TRANSFORMATION

In this section we want to look at connections with the generalized Bäcklund–Darboux transformation (GBDT) approach (see [35, 37] and the references therein). This approach contains the double commutation method as a special case as we will show below and there are close relations with the binary Darboux transform (see, e.g., the comparative discussion in [6, Section 7.2]). Here we will use the GBDT to construct an explicit example with a generalized Weyl function which is rational with respect to \sqrt{z} and which has non-real zeros.

More specific, we want to apply the GBDT to the Schrödinger equation

$$(5.1) \quad \tau u = zu, \quad x \in (0, \infty).$$

This case was treated in Proposition 2.2 [36], see also [35].

To begin with we fix an integer $n \in \mathbb{N}$, two $n \times n$ matrices $A, S(0)$ and two vectors $\Lambda_1(0), \Lambda_2(0) \in \mathbb{C}^n$ such that

$$(5.2) \quad AS(0) - S(0)A^* = \Lambda(0)J\Lambda(0)^*, \quad S(0) = S(0)^*,$$

where we have set

$$(5.3) \quad \Lambda(0) = [\Lambda_1(0) \quad \Lambda_2(0)], \quad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}.$$

Taking $\Lambda(0)$ as initial condition we define the $n \times 2$ matrix function $\Lambda(x) = [\Lambda_1(x) \quad \Lambda_2(x)]$ as the solution of the linear system

$$(5.4) \quad \Lambda_1'(x) = A\Lambda_2(x) - \Lambda_2(x)q(x), \quad \Lambda_2'(x) = -\Lambda_1(x)$$

and $S(x)$ via the relation

$$(5.5) \quad S(x) = S(0) + \int_0^x \Lambda_2(t)\Lambda_2(t)^* dt.$$

Note that $S(x) = S(x)^*$ as well as the identity

$$(5.6) \quad AS(x) - S(x)A^* = \Lambda(x)J\Lambda(x)^*$$

which follows from (5.2), (5.4), and (5.5). Furthermore, we will assume that $S(x) > 0$ for $x > 0$.

Given these data we can construct the Darboux matrix using a transfer matrix function representation. To this end introduce

$$(5.7) \quad w_A(z, x) = I_2 + J\Lambda(x)^*S(x)^{-1}(zI_n - A)^{-1}\Lambda(x),$$

where I_n is the $n \times n$ identity matrix and the variable x is added into the transfer matrix function in Lev Sakhnovich form from [38]. Now one can check that (5.7) acts as a Darboux matrix, that is, for any given set of linearly independent solutions y_0, y_1 of (5.1) we obtain a set of linearly independent solutions $\tilde{y} = [\tilde{y}_0 \quad \tilde{y}_1]$ of a transformed Schrödinger equation $-u'' + \tilde{q}u = zu$, where the transformed potential \tilde{q} can be expressed explicitly in terms of Λ and S , by virtue of

$$(5.8) \quad \tilde{y}(z, x) = \begin{bmatrix} 1 & 0 \end{bmatrix} w_A(z, x) w(z, x), \quad w(z, x) = \begin{bmatrix} y_0(z, x) & y_1(z, x) \\ y_0'(z, x) & y_1'(z, x) \end{bmatrix}.$$

In the special case $n = 1$, observe that the function Λ_2 is a solution of the Schrödinger equation corresponding to the value A of the spectral parameter. Therefore, in the case $n > 1$, the matrix A is called a generalized matrix eigenvalue. Moreover, in the case $n = 1$ the GBDT contains the double commutation method considered in Section 4:

5.1. The double commutation method as a special case of the GBDT.

Let $n = 1$ (i.e., A is a scalar) and set

$$(5.9) \quad A = \lambda \in \mathbb{C}, \quad y(z, x) = [\phi(z, x) \quad \theta(z, x)], \quad \Lambda(x) = [-\phi'(\lambda, x) \quad \phi(\lambda, x)].$$

Thus, for ϕ_γ , which is given below, formulas (5.8) and (5.9) imply

$$(5.10) \quad \phi_\gamma(z, x) = \tilde{y}(z, x) \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} w_A(z, x) \begin{bmatrix} \phi(z, x) \\ \phi'(z, x) \end{bmatrix}.$$

In view of (5.7), rewrite (5.10) in the form

$$(5.11) \quad \begin{aligned} \phi_\gamma(z, x) &= \phi(z, x) + \frac{\bar{\phi}(\lambda, x)}{S(x)(z - \lambda)} \Lambda(x) \begin{bmatrix} \phi(z, x) \\ \phi'(z, x) \end{bmatrix} \\ &= \phi(z, x) + \frac{\bar{\phi}(\lambda, x)}{S(x)(z - \lambda)} W_x(\phi(\lambda), \phi(z)). \end{aligned}$$

By (5.2), (5.5), and (5.9) we get

$$(5.12) \quad S(x) = (\lambda - \bar{\lambda})^{-1} \Lambda(0) J \Lambda(0)^* + \int_0^x |\phi(\lambda, t)|^2 dt \quad \text{for } \lambda \neq \bar{\lambda}.$$

In the case of $\lambda = \bar{\lambda}$ and real ϕ treated in Section 4, identity (5.6) is fulfilled automatically. Hence, noting that $S(0) \geq 0$, equality (5.11) becomes

$$(5.13) \quad \phi_\gamma(z, x) = \phi_\gamma(z, x) + \frac{\tilde{\phi}_\gamma(\lambda, x)}{z - \lambda} W_x(\phi(\lambda), \phi(z)), \quad \gamma := S(0)^{-1} \in (0, \infty],$$

where

$$(5.14) \quad \tilde{\phi}_\gamma(\lambda, x) = \frac{\phi(\lambda, x)}{S(x)}, \quad S(x) = \gamma^{-1} + \int_0^x \phi(\lambda, t)^2 dt.$$

Hence, if $\lambda = \bar{\lambda}$ and $\phi(\lambda, x)$ is real, the expressions for ϕ_γ and $\tilde{\phi}_\gamma$ from above agree with (4.1) and (4.6), (4.13).

5.2. A generalized Weyl function with non-real zeros. For the remainder of this section we consider the case

$$(5.15) \quad q \equiv 0, \quad \Lambda(0) J \Lambda(0)^* = 0, \quad S(0) = 0.$$

Clearly, (5.2) holds for this choice of $\Lambda(0)$ and $S(0)$. For $q \equiv 0$ we have (see also [24], where the case $q \equiv 0$, $S(0) = I_n$ was treated):

$$(5.16) \quad \tilde{q}(x) = 2 \left((\Lambda_2(x)^* S(x)^{-1} \Lambda_2(x))^2 + \Lambda_1(x)^* S(x)^{-1} \Lambda_2(x) + \Lambda_2(x)^* S(x)^{-1} \Lambda_1(x) \right).$$

Moreover, for the case that $q \equiv 0$, one can set in (5.8):

$$(5.17) \quad w(z, x) = T(z) \begin{bmatrix} e^{i\sqrt{z}x} & 0 \\ 0 & e^{-i\sqrt{z}x} \end{bmatrix} T(z)^{-1}, \quad T(z) = \begin{bmatrix} 1 & 1 \\ i\sqrt{z} & -i\sqrt{z} \end{bmatrix}.$$

In some places below we will need the sign in the square root fixed, hence we chose the branch cut in \sqrt{z} along the negative real axis and assume that $\text{Im}(\sqrt{z}) > 0$. Later we will need the expression for \tilde{y}' (see [24, formula (1.30)]) as well:

$$(5.18) \quad \tilde{y}'(z, x) = \begin{bmatrix} -\Lambda_2(x)^* S(x)^{-1} \Lambda_2(x) & 1 \end{bmatrix} w_A(z, x) w(z, x).$$

If $n = 1$, without loss of generality we assume that

$$(5.19) \quad \Lambda(0) = \begin{bmatrix} v_1 & 1 \end{bmatrix}, \quad v_1 = \bar{v}_1,$$

and the second relation in (5.15) is immediate.

Lemma 5.1. [30] *Let $n = 1$ and the parameters $A \in \mathbb{C} \setminus \{0\}$ and $v_1 \in \mathbb{R}$ be fixed. Then the relation (5.16), where*

$$\begin{aligned} \Lambda_1(x) &= v_1 \cos(\sqrt{A}x) + \sqrt{A} \sin(\sqrt{A}x), \\ \Lambda_2(x) &= \cos(\sqrt{A}x) - v_1 \sin(\sqrt{A}x)/\sqrt{A}, \quad S(x) = \int_0^x |\Lambda_2(t)|^2 dt, \end{aligned}$$

explicitly determines a singular potential \tilde{q} satisfying $\tilde{q}(x) = 2x^{-2}(1 + O(x))$ for $x \rightarrow 0$.

The corresponding entire solutions $\tilde{\phi}(z, x)$ and $\tilde{\theta}(z, x)$, such that both solutions are real-valued on \mathbb{R} , $W(\tilde{\theta}(z), \tilde{\phi}(z)) = 1$ and $\tilde{\phi}(z, x)$ is nonsingular at $x = 0$, are given by

$$\tilde{\phi}(z, x) = (z - \bar{A})^{-1} \tilde{y}(z, x) \begin{bmatrix} 1 \\ -v_1 \end{bmatrix}, \quad \tilde{\theta}(z, x) = -(z - A) \tilde{y}(z, x) \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

The singular Weyl function corresponding to this problem has the form

$$(5.20) \quad \tilde{M}(z) = -(z - A)(z - \bar{A})(i\sqrt{z} + v_1)^{-1}.$$

Now, we turn to the case $n = 2$. To simplify calculations set

$$(5.21) \quad A = \begin{bmatrix} \mu & 1 \\ 0 & \mu \end{bmatrix}, \quad \mu \neq \bar{\mu}; \quad \Lambda(0) = [dv \quad v], \quad v = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad d = \bar{d}.$$

By (5.21) the second relation in (5.2) is true and we assume also $S(0)=0$. It is straightforward to check that (5.4) (with $q \equiv 0$) and (5.21) hold for

$$(5.22) \quad \Lambda_1(x) = \frac{i}{2} \mathcal{A} \left(e^{-\omega x} \begin{bmatrix} c_3 x + c_4 \\ c_1 \end{bmatrix} - e^{\omega x} \begin{bmatrix} c_5 x - c_4 \\ c_2 \end{bmatrix} \right),$$

$$(5.23) \quad \Lambda_2(x) = \frac{1}{2} \left(e^{-\omega x} \begin{bmatrix} c_3 x + c_4 \\ c_1 \end{bmatrix} + e^{\omega x} \begin{bmatrix} c_5 x - c_4 \\ c_2 \end{bmatrix} \right),$$

where $\omega = i\sqrt{\mu}$,

$$(5.24) \quad \mathcal{A} = -i\omega I_2 + \frac{i}{2\omega} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \mathcal{A}^2 = A, \quad c_1 = 1 + \frac{d}{\omega},$$

$$(5.25) \quad c_2 = 1 - \frac{d}{\omega}, \quad c_3 = \frac{c_1}{2\omega}, \quad c_4 = \frac{d}{2\omega^3}, \quad c_5 = -\frac{c_2}{2\omega}.$$

The 2×2 matrix function S is defined by the equality

$$(5.26) \quad S(x) = \int_0^x \Lambda_2(t) \Lambda_2(t)^* dt.$$

Lemma 5.2. *Let $n = 2$ and let A and $\Lambda(0)$ be fixed such that (5.21) holds. Then the relations (5.16) and (5.22)–(5.26) explicitly determine a singular potential \tilde{q} , such that*

$$(5.27) \quad \tilde{q}(x) = \frac{12}{x^2} (1 + O(x)), \quad x \geq 0, \quad x \rightarrow 0.$$

The corresponding entire real solutions $\tilde{\phi}(z, x)$ and $\tilde{\theta}(z, x)$, such that $\tilde{\phi}(z, x)$ is nonsingular at $x = 0$ and $W(\tilde{\theta}(z), \tilde{\phi}(z)) = 1$, are given by

$$(5.28) \quad \tilde{\phi}(z, x) = \frac{\tilde{y}(z, x)}{(z - \bar{\mu})^2} \begin{bmatrix} 1 \\ -d \end{bmatrix}, \quad \tilde{\theta}(z, x) = -(z - \mu)^2 \tilde{y}(z, x) \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

where \tilde{y} is constructed via (5.8), (5.7), and (5.17). Moreover, the corresponding singular Weyl function is given by

$$(5.29) \quad \tilde{M}(z) = -(z - \mu)^2 (z - \bar{\mu})^2 (i\sqrt{z} + d)^{-1}.$$

Proof. We begin by deriving some asymptotics at $x = 0$. Rewrite (5.17) as

$$(5.30) \quad w(z, x) = \cos(\sqrt{z}x) I_2 + \sin(\sqrt{z}x) \begin{bmatrix} 0 & 1/\sqrt{z} \\ -\sqrt{z} & 0 \end{bmatrix}$$

to see that w is an entire matrix function of z (which has real-valued entries on \mathbb{R}) and the asymptotics

$$(5.31) \quad w(z, x) = \left(1 - \frac{z}{2}x^2\right)I_2 + x \begin{bmatrix} 0 & 1 \\ -z & 0 \end{bmatrix} + O(x^3)$$

hold. Using (5.22)–(5.26), after some direct calculations, we get the asymptotics of $\Lambda(x)$ and $S(x)^{\pm 1}$ at $x = 0$. In particular, we derive

$$(5.32) \quad \det S(x) = \frac{x^6}{45}(1 + O(x)), \quad S(x)^{-1} = \frac{45}{x^6} \begin{bmatrix} x(1 + O(x)) & x^3(\frac{1}{6} + O(x)) \\ x^3(\frac{1}{6} + O(x)) & x^5(\frac{1}{20} + O(x)) \end{bmatrix}.$$

Note that because of (5.26) and the first equality in (5.32) we have $S(x) > 0$ for $x > 0$. Moreover, the asymptotics of Λ and formula (5.32) imply

$$(5.33) \quad \Lambda_2(x)^* S(x)^{-1} = - \left[15x^{-3}(1 + O(x)) \quad \frac{3}{2}x^{-1}(1 + O(x))\right].$$

Similarly, in view of (5.31), we get

$$(5.34) \quad \Lambda(x)w(z, x) = \begin{bmatrix} x - dx^2/2 + O(x^3) & x^2/2 + O(x^3) \\ d - (z - \mu)x + (z - \mu)dx^2/2 + O(x^3) & 1 - (z - \mu)x^2/2 + O(x^3) \end{bmatrix}.$$

Finally, by (5.16), the asymptotics of Λ , and (5.32) it is easy to show that (5.27) holds true.

Now, consider

$$(5.35) \quad \tilde{\phi}_D(z, x) = \tilde{y}(z, x) \begin{bmatrix} 1 \\ -d \end{bmatrix}.$$

Clearly, $\tilde{\phi}_D$ satisfies $\tau\tilde{\phi}_D = z\tilde{\phi}_D$, where the potential is given by (5.16), since $\tau\tilde{y} = z\tilde{y}$. According to (5.8), (5.7), (5.21), and (5.30), $\tilde{\phi}_D$ is meromorphic in z with only possible pole at $z = \mu$. Moreover, we shall show that $\tilde{\phi}_D(z, x) \in L^2(0, c)$. For that purpose rewrite (5.8) as

$$(5.36) \quad \tilde{y}(z, x) = \begin{bmatrix} 1 & 0 \end{bmatrix} w(z, x) + \Lambda_2(x)^* S(x)^{-1} (zI_2 - A)^{-1} [\Lambda_1(x) \quad \Lambda_2(x)] w(z, x).$$

It follows from (5.34) and $(zI_2 - A)^{-1} = \frac{1}{(z - \mu)^2} \begin{bmatrix} z - \mu & 1 \\ 0 & z - \mu \end{bmatrix}$ that

$$(5.37) \quad (zI_2 - A)^{-1} \Lambda(x) w(z, x) = \frac{1}{(z - \mu)^2} \begin{bmatrix} d + O(x^3) & 1 + O(x^3) \\ d(z - \mu) + O(x) & z - \mu + O(x^2) \end{bmatrix}.$$

Relations (5.33) and (5.35)–(5.37) yield $\tilde{\phi}(z, x) \in L^2(0, c)$.

To show that $\tilde{\phi}_D$ is an entire function, consider again the resolvent

$$(5.38) \quad (zI_2 - A)^{-1} \Lambda(x) w(z, x) \begin{bmatrix} 1 \\ -d \end{bmatrix} = \frac{1}{(z - \mu)^2} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \Lambda(x) w(\mu, x) \begin{bmatrix} 1 \\ -d \end{bmatrix} \\ + \frac{1}{(z - \mu)} \left(\Lambda(x) w(\mu, x) + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \Lambda(x) w_z(\mu, x) \right) \begin{bmatrix} 1 \\ -d \end{bmatrix} + \Omega(z, x),$$

where $w_z(z, x) = \frac{\partial}{\partial z} w(z, x)$, and Ω is an entire vector function of z . In view of (5.22)–(5.25) and (5.30), direct calculations show that the vector coefficients at $(z - \mu)^{-2}$ and $(z - \mu)^{-1}$ on the right-hand side of (5.38) equal zero, that is, the left-hand side of (5.38) is an entire vector function. Therefore, by (5.35) and (5.36) one can see that $\tilde{\phi}_D(z, x)$ is an entire function too.

Let us consider another solution

$$(5.39) \quad \tilde{\theta}_D(z, x) = \tilde{y}(z, x) \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

According to (5.8), (5.17), (5.18), and (5.35) we have

$$(5.40) \quad W(\tilde{\theta}_D(z), \tilde{\phi}_D(z)) = -\det w_A(z, x).$$

Thus, $\det w_A(z, x)$ does not depend on x . Moreover, using (5.7) and (5.6) we get

$$(5.41) \quad w_A(\bar{z}, x)^* J w_A(z, x) = J,$$

that is, $|\det w_A(z, x)| = 1$. Taking into account the fact that $w_A(z, x)$ is a rational function of z with the only possible pole at $z = \mu$ (of order no greater than 2) and recalling that the relations $\mu \neq \bar{\mu}$,

$$|\det w_A(z, x)| = 1, \quad \lim_{z \rightarrow \infty} \det w_A(z, x) = 1$$

hold, we derive: $\det w_A(z, x) = (z - \bar{\mu})^k (z - \mu)^{-k}$ ($0 \leq k \leq 4$). Further calculations show that $k = 2$:

$$(5.42) \quad \det w_A(z, x) = (z - \bar{\mu})^2 (z - \mu)^{-2}.$$

To prove that $\tilde{\phi}$ and $\tilde{\theta}$ are entire and real, rewrite (5.41) as $w_A(\bar{z}, x)^* = J w_A(z, x)^{-1} J^*$. In view of (5.42) the last equality yields

$$\begin{bmatrix} \bar{w}_{11}(\bar{z}, x) & \bar{w}_{21}(\bar{z}, x) \\ \bar{w}_{12}(\bar{z}, x) & \bar{w}_{22}(\bar{z}, x) \end{bmatrix} = (z - \mu)^2 (z - \bar{\mu})^{-2} \begin{bmatrix} w_{11}(z, x) & w_{21}(z, x) \\ w_{12}(z, x) & w_{22}(z, x) \end{bmatrix},$$

where $w_A =: \{w_{ij}\}_{i,j=1}^2$. In other words, we get

$$(5.43) \quad (z - \bar{\mu})^{-2} w_A(z, x) = (z - \mu)^{-2} \bar{w}_A(\bar{z}, x).$$

Recall that $w(z, x) = \bar{w}(\bar{z}, x)$, that is, w is real. Thus, by (5.8) and (5.43) the vector function $(z - \bar{\mu})^{-2} \tilde{y}(z, x)$ is real for $\mu \neq \bar{\mu}$. So, the functions $\tilde{\phi}$ and $\tilde{\theta}$, which are given by (5.28), are real. Definitions (5.28), (5.35), and (5.39) yield also

$$(5.44) \quad \tilde{\phi}(z, x) = (z - \bar{\mu})^{-2} \tilde{\phi}_D(z, x), \quad \tilde{\theta}(z, x) = -(z - \mu)^2 \tilde{\theta}_D(z, x).$$

Since $\tilde{\phi}_D$ is an entire function, it follows from (5.44) that the real function $\tilde{\phi}$ may have only one pole at $z = \bar{\mu}$ ($\mu \neq \bar{\mu}$). Therefore, $\tilde{\phi}$ is an entire function. It follows from (5.44) that $\tilde{\theta}$ is an entire function too. Finally, (5.40), (5.42), and (5.44) imply that $W(\tilde{\theta}(z), \tilde{\phi}(z)) = 1$. Thus, the statements of our lemma regarding $\tilde{\phi}$ and $\tilde{\theta}$ are proved.

Now, using $\tilde{\phi}$ and $\tilde{\theta}$ we can construct explicitly a singular Weyl function \tilde{M} . Observe that (5.17) yields

$$(5.45) \quad w(z, x) \begin{bmatrix} 1 \\ i\sqrt{z} \end{bmatrix} = \begin{bmatrix} e^{i\sqrt{z}x} \\ i\sqrt{z}e^{i\sqrt{z}x} \end{bmatrix}.$$

In view of (5.23) and (5.26) we calculate that

$$\det S(x) \sim |c_2 c_5|^2 (4\operatorname{Re}(\omega))^{-4} e^{4\operatorname{Re}(\omega)x} \quad (x \rightarrow +\infty),$$

and so the transfer function $w_A(z, x)$ given by (5.7) behaves like $O(x^4)$. Hence, it follows from (5.8) and (5.45) that

$$(5.46) \quad \tilde{\psi}_D(z, x) = \tilde{y}(x, z) \begin{bmatrix} 1 \\ i\sqrt{z} \end{bmatrix} = \begin{bmatrix} 1 & 0 \end{bmatrix} w_A(z, x) \begin{bmatrix} e^{i\sqrt{z}x} \\ i\sqrt{z}e^{i\sqrt{z}x} \end{bmatrix} \in L^2(c, \infty).$$

Therefore, by (5.28), (5.29), and (5.46) we get

$$\tilde{\psi}(z, x) = \tilde{\theta}(z, x) + \tilde{M}(z)\tilde{\phi}(z, x) \in L^2(c, \infty),$$

that is, $\tilde{M}(z)$ given by (5.29) is a singular Weyl function of our system. \square

Remark 5.3. According to (5.27), the GBDT generated by a 2×2 matrix A of the form (5.21) transforms a Schrödinger operator with $l = 0$ into one with $l = 3$.

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