Math Phys Anal Geom (2011) 14:115–151
DOI 10.1007/s11040-011-9090-6

An Operator Theoretic Interpretation of the Generalized Titchmarsh-Weyl Coefficient for a Singular Sturm-Liouville Problem

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Received: 21 February 2008 / Accepted: 21 February 2011 / Published online: 12 March 2011

Abstract In this article an operator theoretic interpretation of the generalized Titchmarsh-Weyl coefficient for the Hydrogen atom differential expression is given. As a consequence we obtain a new expansion theorem in terms of singular generalized eigenfunctions.

Keywords Titchmarsh-Weyl coefficient · Singular differential operator · Generalized Nevanlinna function · Supersingular perturbation

Mathematics Subject Classifications (2010) 30H15 · 34L40 · 47E05 · 81Q10

The authors gratefully acknowledge support from the Swedish Research Council, Grant #50092501, and the Austrian Science Fund (FWF), grant numbers P15540-N05 and J2540-N13.

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1 Introduction

The main object in this paper is the ordinary differential expression

$$\ell(y) := -y''(x) + \left(\frac{q_0 + q_1 x}{x^2}\right) y(x), \qquad x \in (0, \infty), \tag{1}$$

with $q_0, q_1 \in \mathbb{R}$, which is known as the 'Hydrogen atom differential expression' (see [14], Section 39), since it appears after separation of variables in two- and three-dimensional Schrödinger equations with Coulomb potential. The corresponding differential equation

$$-y''(x) + \left(\frac{q_0 + q_1 x}{x^2}\right) y(x) = \lambda y(x), \tag{2}$$

is probably one of the most well studied equations in classical mathematical physics. Its solutions can be expressed in terms of Whittaker functions, or other confluent hypergeometric functions [1, 5]. However, we are going to make use of these special solutions only in the last part, starting with Section 4.1. Before that we actually only make use of asymptotic properties, since this approach will be used also in upcoming work for more general potentials.

The differential expression (1) has two singular endpoints. It is in limit point case at ∞ (in the terminology of H. Weyl [3, 26]). Due to the non integrability of the potential at the origin also the left endpoint is singular. The most important case for us is $q_0 \geqslant \frac{3}{4}$, where limit point case prevails also at 0.

Recall for a moment the case of a regular left endpoint. Then (usual) the Titchmarsh-Weyl coefficient, which plays a crucial role in the spectral analysis, is connected with the asymptotic behavior of the solutions to the differential equation (2). However, essentially the same function appears as Krein's Q-function in the denominator of the resolvent formula, which gives all possible self-adjoint realizations of the differential expression, described also by boundary conditions at the origin. Summing up one associates with the differential expression a Nevanlinna function which has a double nature: it appears both as Titchmarsh-Weyl coefficient and as Krein's Q-function.

For the singular differential expression (1), however these two approaches do not work directly. In Krein's approach the operator family is reduced to just one operator leaving no possibility for neither comparing resolvents of different operators nor imposing boundary conditions. Trying to follow the Titchmarsh-Weyl approach one finds that only one solution of (2) is regular at the origin. In [15, 16] it was suggested to overcome the latter problem by using also the singular solution in order to define a generalized Titchmarsh-Weyl coefficient, which in this case appeared to be a generalized Nevanlinna function with degree of non-positivity estimated in terms of the parameter q_0. See also [17], where generalized Titchmarsh-Weyl coefficients are studied also for a wider class of potentials.

It is the aim of this paper to give an operator interpretation for this generalized Titchmarsh-Weyl coefficient corresponding to the differential expression (1). Constructing the model we aimed to satisfy the following requirements:

- The operators should be self-adjoint in a Hilbert space of functions and act as the differential expression (1).
- The family of self-adjoint operators should be given by a Krein-type formula.

In order to meet these conditions we applied the theory of supersingular perturbations. In other words we obtain a family of self-adjoint operators acting in a new Hilbert space of (physically relevant but not necessarily square-integrable functions) and their domains are described by certain 'boundary conditions'. The main result, stated in Theorem 2, is that the generalized Nevanlinna function which describes this family coincides with the generalized Titchmarsh-Weyl coefficient up to a polynomial. Its degree is bounded in terms of the parameters, which also implies that the number of negative squares of the generalized Titchmarsh-Weyl coefficient equals $\left[\frac{1+\sqrt{\frac{1}{4}+q_0}}{2}\right]$.

This program has partially been carried out in the particular case of the Bessel operator, i.e. when $q_1 = 0$, in [12]. However, there a rather abstract Pontryagin space model for the generalized Nevanlinna function, which is obtained by analytic continuation from the Q-function of the limit circle case ($q_0 < \frac{3}{4}$), is constructed.

Finally we obtain a new kind of eigenfunction expansion involving not square integrable functions which may be interpreted as scattered waves. This expansion is proved using the model constructed in Section 3.

The paper is organized as follows. In the last part of this introduction, in Section 1.1, we shortly recall the situation for a Sturm-Liouville operator with one regular endpoint. Section 2 is devoted to the asymptotic behavior of certain solutions of (2).

In Section 3 the operator model is constructed explicitly. In Section 3.1 we first show that the perturbations we are interested in are indeed so-called supersingular perturbations and hence the corresponding theory can then be applied in Section 3.2. Section 3.3 contains the main result, which gives the connection between the generalized Titchmarsh-Weyl-coefficient and the denominator in the Krein-type formula describing the model.

Only in Section 4 we use classical results on the analytic behavior of solutions of (2). First we recall in Section 4.1 spectral properties of the classical Hydrogen atom operator and deduce from this corresponding results for the model operators. Finally in Section 4.2 we find a new kind of expansion in terms of functions which are not square integrable at the origin. In the appendix, finally, basic facts on the scale of Hilbert spaces are collected and a short discussion of the limit circle case, i.e. $-\frac{1}{4} < q_0 < \frac{3}{4}$, completes the picture.

Finally we want to mention that the Bessel operator (i.e. $q_1 = 0$) has recently also been investigated from completely different points of view. In [10] and [11] approximation by regular differential operators and corresponding models are discussed, and in [25] an indefinite canonical system is constructed.

1.1 Regular Case: Classical Theory

We briefly recall the situation in the case of a Sturm-Liouville-operator corresponding to the differential expression $\ell(y) := -y'' + qy$ on the half line $[0,\infty)$, which is regular at 0, that is for the real potential q it holds $q \in L^1_{loc}[0,\infty)$, and which is in limit point case at ∞. Under these assumptions for every $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the equation

$$\ell(y) = \lambda y \tag{3}$$

has exactly only one (up to a scalar multiple) solution which belongs to the space $L^2(0,\infty)$. Hence with the basic solutions y_1 and y_2 of (3), which are determined by the Cauchy data

$$\begin{aligned} y_1(0,\lambda) &= 0 \quad y_2(0,\lambda) = 1 \\ y_1'(0,\lambda) &= -1 y_2'(0,\lambda) = 0, \end{aligned}$$

the requirement

$$g(x,\lambda) := y_2(x,\lambda) - m(\lambda) y_1(x,\lambda) \in L^2(0,\infty)$$

defines $m(\lambda)$ uniquely. This function is usually called *Titchmarsh-Weyl coefficient* of the differential expression ℓ. It is a Nevanlinna function, $m \in \mathcal{N}_0$, that is, it is a symmetric function, i.e. $\overline{m(\lambda)} = m(\overline{\lambda})$, which maps the upper half plane $\mathbb{C}^+$ holomorphically into itself. Its analytic properties are closely connected with the spectrum of the self-adjoint realizations of ℓ. These realizations, or in other words, self-adjoint extensions of the corresponding minimal operator, which is defined on the domain $C_0^\infty\big((0,\infty)\big)$, are given as restrictions L_τ, $\tau \in \mathbb{R} \cup \{\infty\}$, of the differential expression ℓ to the domain

$$\operatorname{dom}(L_\tau) = \left\{ y \in L^2(0,\infty), \ell(y) \in L^2(0,\infty), y(0) - \tau y'(0) = 0 \right\}.$$

They are connected via

$$(L_\tau - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle g(x,\overline{\lambda}), \cdot \rangle}{m(\lambda) - \frac{1}{\tau}} g(x,\lambda), \tag{4}$$

where L_0 is the particular extension given by the Dirichlet boundary condition. Note that here and in the following we use the notation $\langle \cdot, \cdot \rangle$ for the inner product, such that it is linear in the second and conjugate linear in the first argument.

On the other side the same differential expression can also be considered using methods of classical perturbation theory. Define the element $\varphi := (L_0 - \lambda_0) g(\cdot, \lambda_0)$, which in general does not belong to $L^2(0,\infty)$, but rather $\varphi \in \mathcal{H}_{-2}(L_0)$ since $g \in L^2(0,\infty)$. For more details on the rigged spaces $\mathcal{H}_{-n}$

see Appendix A below, cf. also [2, 4]. Then by standard techniques with the singular perturbation

$$L_0 + t\langle \varphi, \,\cdot\, \rangle \varphi \qquad t \in \mathbb{R} \cup \{\infty\}$$

there is associated a whole family of self-adjoint operators in $L^2(0, \infty)$, which are given by

$$(L^\gamma - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle (L_0 - \overline{\lambda})^{-1}\varphi, \,\cdot\, \rangle}{Q(\lambda) + \gamma}(L_0 - \lambda)^{-1}\varphi, \qquad \gamma \in \mathbb{R} \cup \{\infty\}, \tag{5}$$

where in general the correspondence between t and γ is not fixed. Here Q is a Q-function corresponding to the symmetric operator S, which is defined as the restriction of L_0 to those elements y for which $\langle \varphi, y \rangle = 0$ and its self-adjoint extension L_0. Since $g(\,\cdot\,, \lambda) = (L_0 - \lambda)\varphi$ the formulas (5) and (4) describe the same family of self-adjoint extensions. Moreover, $Q(\lambda) - m(\lambda)$ is a real constant.

In what follows we are giving a corresponding connection for the singular differential expression (1).

2 Asymptotic Analysis and the Generalized Titchmarsh-Weyl Coefficient

In this section we study the solutions of the differential equation

$$-y''(x) + \left(\frac{q_0}{x^2} + \frac{q_1}{x}\right)y(x) = \lambda y(x) \qquad x \in (0, \infty),\ \lambda \in \mathbb{C}, \tag{6}$$

where $q_1 \in \mathbb{R}$ and $q_0 > -\frac{1}{4}$, with respect to their asymptotic behavior at the singular endpoints and introduce the generalized Titchmarsh-Weyl-coefficient. We want to point out that here we are making use of the asymptotic properties of equation (6) only, rather than using its explicit solutions.

2.1 Asymptotics at the Origin

We follow the lines of [15] but also extend the analysis there. Note that the equation (6) is of Fuchsian type with a weak singularity at the point $x = 0$. Hence Frobenius theory can be applied and the solutions can be obtained via the generalized power series Ansatz

$$y(x, \lambda) = x^\alpha \sum_{j=0}^{\infty} a_j(\lambda) x^j \qquad \text{with } a_0 \neq 0. \tag{7}$$

Then the corresponding index equation turns out to be

$$\alpha^2 - \alpha - q_0 = 0$$

which has the real solutions $\alpha_\pm := \frac{1}{2} \pm \sqrt{\frac{1}{4} + q_0}$, with $\alpha_- < \alpha_+$ and $\alpha_- + \alpha_+ = 1$. Two particular solutions $g_+(x, \lambda)$ and $g_-(x, \lambda)$ (the so-called 'regular' and 'singular' solutions) corresponding to the indices α_+ and α_-, respectively, will play an important role. The following lemma summarizes some of their asymptotic properties. Here and in the following $[x]$ denotes the integer part of x.

Lemma 1 *Set $\alpha_\pm = \frac{1}{2} \pm \sqrt{\frac{1}{4} + q_0}$. Then equation (6) has two linearly independent solutions satisfying*

$$g_+(x,\lambda) = \sum_{j=0}^{\infty} a_j(\lambda) x^{\alpha_+ + j}$$

$$g_-(x,\lambda) = \sum_{j=0}^{m_0-1} c_j(\lambda) x^{\alpha_- + j} + o\big(x^{\alpha_+ - 1}\big) \quad \textit{for } x \to 0+ \tag{8}$$

with $m_0 := [\alpha_+ - \alpha_-]$ and coefficients a_j and c_j given by the recursion

$$t_{j+2} = \frac{q_1 t_{j+1} - \lambda t_j}{(j+2)(2\alpha + j + 1)} \tag{9}$$

with $\alpha = \alpha_+$ and starting values $a_0 = 1$, $a_1 = \frac{q_1}{2\alpha_+}$ and with $\alpha = \alpha_-$ and starting values $c_0 = \frac{1}{\alpha_- - \alpha_+}$, $c_1 = \frac{q_1}{2\alpha_-} c_0$, respectively. Moreover the following holds:

- (i) *The functions $g_+(x,\lambda)$ and $g_-(x,\lambda)$ and their derivatives with respect to x are entire in λ for every $x \in (0,\infty)$ and*

$$g_\pm(\,\cdot\,, \overline{\lambda}) = \overline{g_\pm(\,\cdot\,, \lambda)} \quad \textit{and} \quad g'_\pm(\,\cdot\,, \overline{\lambda}) = \overline{g'_\pm(\,\cdot\,, \lambda)}.$$

- (ii) *With the notation W for the Wronskian*

$$W\big(y_1(x), y_2(x)\big) := y_1(x) y_2'(x) - y_1'(x) y_2(x)$$

it holds for all $\lambda, z \in \mathbb{C}$:

$$\begin{aligned} W\big(g_+(x,\lambda), g_-(x,\lambda)\big) &\equiv 1 \\ \lim_{x\to 0} W\big(g_+(x,\lambda), g_-(x,z)\big) &= 1 \\ \lim_{x\to 0} W\big(g_+(x,\lambda), g_+(x,z)\big) &= 0 \\ \lim_{x\to 0} W\big(g_-(x,\lambda), g_-(x,z)\big) &= \begin{cases} 0 & \textit{if } q_0 < \frac{3}{4} \\ \infty & \textit{if } q_0 \geqslant \frac{3}{4} \end{cases}. \end{aligned}$$

Note that with obvious adjustments the lemma also holds for $q_0 = -\frac{1}{4}$.

Throughout the whole paper we are going to write $\lim\limits_{x\to 0}$ instead of $\lim\limits_{x\to 0+}$, hoping that this will not lead to any missunderstanding since we always have $x > 0$.

Proof From (7) recursion (9) and hence also the expansion of g_+ follow directly. The classical theory shows that in order to obtain a second linear independent solution of (6) one has to distinguish two different cases. If $\alpha_+ - \alpha_- \notin \mathbb{N}$, then a ‘singular’ solution is of the form

$$g_-(x,\lambda) := \sum_{j=0}^{\infty} c_j(\lambda) x^{\alpha_- + j} \quad \text{with } c_0 = \frac{1}{\alpha_- - \alpha_+}, \tag{10}$$

where c_j satisfy the recursion (9) with $\alpha = \alpha_-$. Here the choice of c_0 is done such that the Wronskian in (ii) is normalized. If, however, $\alpha_+ - \alpha_- = m_0 \in \mathbb{N} \setminus \{0\}$ then the second solution is obtained by the Ansatz

$$g_-(x,\lambda) := \sum_{j=0}^{\infty} d_j(\lambda) x^{\alpha_- + j} + K(\lambda) \ln x \, g_+(x,\lambda), \tag{11}$$

where for normalization reasons we again choose $d_0 = \frac{1}{\alpha_- - \alpha_+}$, which immediately implies $d_1 = \frac{q_1}{2\alpha_-} d_0$. Then for $0 \leqslant j < m_0 - 2$ the Ansatz yields

$$d_{j+2} = \frac{q_1 d_{j+1} - \lambda d_j}{(j+2)(2\alpha_- + j + 1)}.$$

The coefficient d_{m_0} appears to be arbitrary, however, its choice does not effect (8). The corresponding equation yields

$$K(\lambda) = \frac{d_{m_0 - 1} q_1 - d_{m_0 - 2}}{m_0},$$

where we set $d_{-1} = 0$ in case $m_0 = 1$. For sake of completeness we also add that for $j > m_0 - 2$ the Ansatz (11) gives

$$d_{j+2} = -\frac{q_1 d_{j+1} - \lambda d_j}{(j+2)(m_0 - 2 - j)} + K(\lambda) a_{j+2-m_0} \frac{2j + 4 - m_0}{(j+2)(m_0 - 2 - j)}.$$

Summed up, this shows that in both cases the claimed expansion for g_- holds. The other statements follow then directly from the asymptotic expansions (8). For more details see also [15]. □

Note that in the above proof in the special case $\alpha_+ - \alpha_- \in \mathbb{N}$ there was no requirement on the coefficient d_{m_0} since then $\alpha_- + m_0 = \alpha_+$. However, it turns out to be possible to choose d_{m_0} such that the following further refinement of expansion (8) for g_- holds.

Corollary 1 *Equation (6) has a solution g_- which is of the form*

$$\begin{aligned} g_-(x,\lambda) = &\sum_{j=0}^{m_0} c_j(\lambda) x^{\alpha_- + j} + K(\lambda) x^{\alpha_+} \ln x \\ &+ x^{m_0 + \alpha_- + 1}\big(H_1(x,\lambda) + \ln x \, H_2(x,\lambda)\big), \end{aligned} \tag{12}$$

where $m_0 = [\alpha_+ - \alpha_-]$, the coefficients $c_j(\lambda)$ and $K(\lambda)$ are polynomials in λ of degree $\leqslant \left[\frac{m_0}{2}\right]$, and the functions H_1 and H_2 are both entire in λ and holomorphic at $x = 0$.

Proof We use the notations from the proof of the previous lemma. If $\alpha_+ - \alpha_- \notin \mathbb{N}$ then (10) gives directly $K(\lambda) = 0$ and $H_2(x) = 0$ and, indeed recursion (9) implies that $c_j(\lambda)$ is a polynomial in λ of degree $\left[\frac{j}{2}\right]$. If $\alpha_+ - \alpha_- \in \mathbb{N}$, then (12) follows immediately from (11), and here only $d_{m_0}(\lambda)$ has to be chosen as a polynomial in λ with degree $\leqslant \left[\frac{m_0}{2}\right]$. □

Remark 1 Let $q_0 > -\frac{1}{4}$. From Lemma 1 one sees that for all $\lambda \in \mathbb{C}$ and every fixed $x_0 \in \mathbb{R}^+$ it holds

$$\begin{aligned} &g_+(\,\cdot\,,\lambda) \in L^2(0,x_0),\\ &g_-(\,\cdot\,,\lambda) \in L^2(0,x_0) \text{ if and only if } -\tfrac{1}{4} < q_0 < \tfrac{3}{4}, \end{aligned}$$

Hence for the differential expression ℓ prevails limit point case at the singular endpoint 0 if and only if $q_0 \geqslant \frac{3}{4}$.

2.2 Asymptotics at ∞

The endpoint ∞ is—under our assumptions—always in limit point case. Thus for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ there is (up to a constant factor) exactly one linear combination of g_+ and g_- which is square integrable in a neighborhood of ∞:

$$g(\,\cdot\,,\lambda) := g_-(\,\cdot\,,\lambda) - m(\lambda) g_+(\,\cdot\,,\lambda) \in L^2(x_0,\infty) \quad \text{for } x_0 \in \mathbb{R}. \tag{13}$$

The function m, defined by (13), is called *generalized Titchmarsh-Weyl coefficient*. For the differential expression under consideration it has been introduced in [15] and further investigated in [16], see also [17]. Note that by classical arguments this definition can be extended also to $\lambda < 0$ except the eigenvalues of the Hydrogen atom operator.

Actually, m can be calculated even explicitly, see Section 4.1, where also further properties of the function g are deduced. However, for this more accurate analysis we are going to make use of the explicit form of the solutions of (6), which are not needed in the first part of this paper.

Remark 2 Note that the so defined function m heavily depends on the particular choice of $g_\pm$ as basic solutions, even if this basis seems to be natural for the problem. However, let us mention that for potentials where Frobenius theory is not available the choice of the basic solutions becomes a crucial question.

2.3 Regularizations

Locally at 0 the function g in (13) behaves as the singular solution g_-, that is, $g(x,\lambda) = O(x^{\alpha_-})$ as $x \to 0+$. However, the first two coefficients c_0 and c_1 in expansion (8) actually do not depend on the spectral parameter. Thus the difference $g(x,\mu_1) - g(x,\mu_2) = O(x^{\alpha_-+2})$ as $x \to 0+$, and hence is less singular at the origin. This gives rise to the following definition of higher order differences.

Here and in the following we use the notations

$$\mathbb{R}^- = (-\infty, 0), \qquad \mathbb{R}_0^- = (-\infty, 0],$$

and for $\mathbb{R}^+$ and $\mathbb{R}_0^+$ accordingly. Let $\mu_1, \ldots, \mu_k \in \mathbb{R}^-$ not be eigenvalues of the hydrogen atom operator and mutually different for $k \geqslant 1$, then define

$$g_k(x) := \sum_{i=1}^{k} A_i^{(k)} g(x, \mu_i) \tag{14}$$

with coefficients $A_i^{(k)}$ for $1 \leqslant i \leqslant k$ such that $A_1^{(1)} := 1$ and for $k > 1$

$$A_i^{(k)} := -\frac{1}{\mu_k - \mu_i} A_i^{(k-1)} \quad \text{for } i < k \quad \text{and} \quad A_k^{(k)} := -\sum_{i=1}^{k-1} A_i^{(k)}. \tag{15}$$

Remark 3 Note that it holds $(\ell - \mu_k)g_k = g_{k-1}$ for $k > 1$, and $(\ell - \mu_1)g_1 = 0$, where ℓ denotes the differential expression (6).

The next lemma shows that the regularity of these functions indeed increases with k. In Theorem 1 we will later also give an operator theoretic explanation for this fact. Let us first introduce the number

$$n := 2 + \left[\sqrt{\frac{1}{4} + q_0}\,\right],$$

which will play an important role in the following.

Lemma 2 *Assume* $q_0 \geqslant \frac{3}{4}$, *let* $k \leqslant n - 2 = \left[\sqrt{\frac{1}{4} + q_0}\,\right]$, *and* $m_0 = [\alpha_+ - \alpha_-]$. *Then the functions* $g_k(x)$ *(defined in* (14)*) have the asymptotic expansions*

$$g_k(x) = \sum_{j=2(k-1)}^{m_0-1} C_j^{(k)} x^{\alpha_- + j} + o(x^{\alpha_+ - 1}) \qquad \text{as } x \to 0+ \tag{16}$$

with some $C_j^{(k)} \in \mathbb{R}$, *where the first coefficient* $C_{2(k-1)}^{(k)} \neq 0$.

Proof Note first that under the above assumptions the sum in (16) is not empty. Using (8) we can write

$$g_k(x) = \sum_{j=0}^{m_0-1} C_j^{(k)} x^{\alpha_- + j} + o(x^{\alpha_+ - 1}) \qquad \text{as } x \to 0+$$

with $C_j^{(k)} := \sum_{i=1}^k A_i^{(k)} c_j(\mu_i)$, where the coefficients $A_i^{(k)}$ are given in (15) and c_j as in Lemma 1. We have to show that $C_j^{(k)} = 0$ for $j < 2(k-1)$. For $k = 1$ the above statement is already included in Lemma 1. Hence let us now assume $k > 1$. Since $c_0(\lambda)$ and $c_1(\lambda)$ do not depend on λ we have directly

$$C_j^{(k)} = c_j \sum_{i=1}^{k} A_i^{(k)} = 0 \quad \text{for } j = 0, 1 \text{ and } k > 1. \tag{17}$$

The defining recursion (15) for the $A_i^{(k)}$ gives

$$C_j^{(k)} = \sum_{i=1}^{k-1} \frac{A_i^{(k-1)}}{\mu_k - \mu_i} \big(c_j(\mu_k) - c_j(\mu_i)\big). \tag{18}$$

By using recursion (9) for the c_j for $j > 1$ and then again (18) we get

$$C_j^{(k)} = \frac{1}{j(2\alpha_- + j - 1)} \big(q_1 C_{j-1}^{(k)} - \mu_k C_{j-2}^{(k)} - C_{j-2}^{(k-1)}\big).$$

Going on like this one obtains in finitely many steps that $C_j^{(k)}$ is a linear combination of $C_0^{(i)}$ and $C_1^{(i)}$ with $i \leqslant k$. Here $i > 1$ as long as $j < 2(k-1)$ and hence $C_j^{(k)}$ equals zero by (17). However, for $j = 2(k-1)$ this implies furthermore $C_{2(k-1)}^{(k)} \neq 0$. □

Remark 4 For the first non-vanishing coefficients the following recursion relation holds

$$C_{2(k-1)}^{(k)} = -\frac{C_{2(k-2)}^{(k-1)}}{2(k-1)(2\alpha_- + 2k - 3)}.$$

3 Perturbations in the Limit Point Case

3.1 Recognizing the Perturbation as Supersingular

In what follows we concentrate on the case $q_0 \geqslant \frac{3}{4}$ only, that is ℓ is in limit point case at 0, or in other words, the maximal operator is self-adjoint:

$$\operatorname{dom} L_0 := \{y \in L^2(0,\infty) \,|\, y, y' \in AC_{loc}(0,\infty), \ell(y) \in L^2(0,\infty)\} \tag{19}$$

and

$$L_0 y := \ell(y).$$

Remark 5 Since in this case every $y \in \operatorname{dom} L_{\max}$ satisfies the boundary condition $\lim_{x\to 0} W(y(x), g_+(x,\lambda_0)) = 0$ the above notation is in accordance with the one used in the limit circle case, see also Appendix A.

Motivated from the regular case we are interested in perturbations formally given by

$$L_0 + t\langle \varphi, \,\cdot\,\rangle \varphi \qquad t \in \mathbb{R} \cup \{\infty\}$$

with $\varphi = (L_0 - \lambda_0) g(\,\cdot\,, \lambda_0)$, where $g(\,\cdot\,, \lambda_0)$ is the function given in (13). However, here $g(\,\cdot\,, \lambda_0)$ is not square integrable locally at 0, and hence we need some more considerations in order to make the definition of φ precise and identify it as an element from $\mathcal{H}_{-n}(L_0)$ for some $n \in \mathbb{N}$. As a first step the next lemma gives estimates for functions $f \in \operatorname{dom} L_0^k$.

Lemma 3 *For $f \in L^2(0, \infty)$ the resolvent of L_0 is given by*

$$\big((L_0 - \lambda)^{-1} f\big)(x) = -g(x, \lambda) \int_0^x g_+(s, \lambda) f(s)\, ds$$

$$-g_+(x, \lambda) \int_x^\infty g(s, \lambda) f(s)\, ds. \tag{20}$$

Let the integer k satisfy $k \leqslant \left[\frac{3+\sqrt{\frac{1}{4}+q_0}}{2}\right]$, then for every $f \in \operatorname{dom} L_0^k$ there exists a constant $C > 0$ such that for some fixed $x_0 > 0$ it holds for all $x \in (0, x_0)$:

$$|f(x)| \leqslant C x^{-\frac{1}{2}+2k} \quad \text{and} \quad |f'(x)| \leqslant C x^{-\frac{3}{2}+2k}. \tag{21}$$

Proof For λ in the resolvent set $\rho(L_0)$ denote by $R(\lambda) f$ the integral on the right side of (20), which is well defined for every $f \in L^2(0, \infty)$. We first prove equality (20) for $f \in C_0^\infty\big((0, \infty)\big)$. In particular, we have to show that $R(\lambda) f$ is square integrable locally at 0 and ∞, provided that f has compact support in the interval $(0, \infty)$. We choose positive real numbers a and b such that $\operatorname{supp} f \subset (a, b)$. Note that

$$\big(R(\lambda) f\big)(x) = -g_+(x, \lambda) \int\limits_{\operatorname{supp} f} g(s, \lambda) f(s)\, ds \qquad \text{for } x < a$$

and

$$\big(R(\lambda) f\big)(x) = -g(x, \lambda) \int\limits_{\operatorname{supp} f} g_+(s, \lambda) f(s)\, ds \qquad \text{for } x > b\,.$$

This also shows $R(\lambda) f\big|_{(0,a)} \in L^2(0, a)$ and $R(\lambda) f|_{(b,\infty)} \in L^2(b, \infty)$. Using Lemma 1 it is straight forward to see $\ell(R(\lambda) f) = \lambda R(\lambda) f$ and hence $R(\lambda) f = (L_0 - \lambda)^{-1} f$ for every $f \in C_0^\infty\big((0, \infty)\big)$.

For each $f \in L^2(0,\infty)$ there exists then a sequence $f_n \in C_0^\infty\big((0,\infty)\big)$ such that $\|f - f_n\|_{L^2} \to 0$. Since the resolvent $(L_0-\lambda)^{-1}$ is a bounded operator it holds

$$(L_0-\lambda)^{-1} f = L^2\text{-}\lim_{n\to\infty} (L_0-\lambda)^{-1} f_n = L^2\text{-}\lim_{n\to\infty} R(\lambda) f_n.$$

For every $x \in (0,\infty)$, however, the continuous functions $\big(R(\lambda)f_n\big)(x)$ converge to the continuous function $\big(R(\lambda)f\big)(x)$, and hence this pointwise limit coincides with the L^2-limit, which finally gives

$$(L_0-\lambda)^{-1} f = R(\lambda) f \qquad \text{for every } f \in L^2(0,\infty).$$

In order to show (21) we use mathematical induction. The asymptotic expansion (8) for g_+ and Cauchy-Schwarz-inequality imply for every $x \in (0,x_0)$ with some fixed x_0

$$\begin{aligned}|g(x,\lambda)\int_0^x g_+(s,\lambda) f(s)\,ds| &\leqslant C_1 x^{\alpha_-}\int_0^x s^{\alpha_+}|f(s)|\,ds \\ &\leqslant C_2 x^{\alpha_-+\alpha_++\frac{1}{2}} = C_2 x^{\frac{3}{2}} \end{aligned} \tag{22}$$

and

$$\begin{aligned}|g_+(s,\lambda)\int_x^\infty g(s,\lambda) f(s)\,ds| &\leqslant C_3 x^{\alpha_+}\Big(\int_x^{x_0} s^{\alpha_-}|f(s)|\,ds + \int_{x_0}^\infty |g(s,\lambda) f(s)|\,ds\Big) \\ &\leqslant C_4 x^{\alpha_++\alpha_-+\frac{1}{2}} + C_5 x^{\alpha_+} \leqslant C_6 x^{\frac{3}{2}}, \end{aligned} \tag{23}$$

where we have used that if $q_0 \geqslant \frac{3}{4}$ then $\alpha_+ \geqslant \frac{3}{2}$. If $f \in \operatorname{dom} L_0^{k+1}$, that is $f = (L_0-\lambda)^{-1}h$ with some $h \in \operatorname{dom} L_0^k$ and $\lambda \in \mathbb{R}^-$. Then using (21) for h one obtains the corresponding estimate as in (22) and noting $-\frac{1}{2}+2k \leqslant \alpha_+$ also (23). This proves the first estimate in (21) for $k+1$. In the same way the second estimate can be shown. □

The following theorem establishes the connection between the operator L_0 and the functions $g(\,\cdot\,,\lambda)$ and g_k defined in (13) and (14), respectively. In particular, it makes the definition of $\varphi := (L_0-\lambda_0)g(\,\cdot\,,\lambda_0)$ precise.

Theorem 1 *Let g and g_k be given as above and $n = 2 + \left[\sqrt{\frac{1}{4}+q_0}\,\right]$. Then the element $\varphi := (L_0-\lambda_0)g(\,\cdot\,,\lambda_0)$ is independent of the particular choice of $\lambda_0 \in \mathbb{R}^-$ with $L_0-\lambda_0 > 0$ and*

$$\varphi \in \mathcal{H}_{-n}(L_0) \setminus \mathcal{H}_{-n+1}(L_0).$$

Furthermore, it holds

$$g_k = (L_0-\mu_k)^{-1}\ldots(L_0-\mu_1)^{-1}\varphi \tag{24}$$

and, in particular,

$$g_k \in H_{-n+2k}(L_0) \setminus \mathcal{H}_{-n+2k+1}(L_0).$$

Remark 6 In case $q_1 = 0$ and $\alpha_+ - \alpha_- \notin \mathbb{N}_{\text{even}}$ a modified Hankel transform was applied to the problem in [12], and then these statements become obvious. However, this transformation makes essential use of well known properties of Bessel functions and hence in the general case we prove the theorem differently.

Proof Since we consider the scale of Hilbert spaces corresponding only to the operator L_0, within this proof we are going to write simply $\mathcal{H}_s$ instead of $\mathcal{H}_s(L_0)$. Lemma 2 implies that for some large enough index m the function g_m belongs to $\mathcal{H}_0 \setminus \mathcal{H}_2$. In order to determine the number m note that the latter is equivalent to $g_m \in L^2(0, \infty)$ but $\ell(g_m) \notin L^2(0, \infty)$. Since $\ell(g_m) = \mu_m g_m + g_{m-1}$ the asymptotic expansion (16) implies that this is further equivalent to

$$2\big(\alpha_- + 2(m-1)\big) > 1 \quad \wedge \quad 2\big(\alpha_- + 2(m-1) - 2\big) \leqslant -1,$$

from which we can conclude

$$m = \left\lceil \frac{3 + \sqrt{\frac{1}{4} + q_0}}{2} \right\rceil. \tag{25}$$

In the next step we show that for $k = 1, \dots, m$ it holds

$$g_k \in \mathcal{H}_{-2(m-k)} \setminus \mathcal{H}_{-2(m-k)+2} \tag{26}$$

and

$$(L_0 - \mu_k) g_k = g_{k-1}. \tag{27}$$

Consider first $k = m$. Then we already have $g_m \in \mathcal{H}_0 \setminus \mathcal{H}_2$. Hence $(L_0 - \mu_m) g_m$ is an element from $\mathcal{H}_{-2}$ and we are going to show that, in fact, it coincides with the function g_{m-1}. To this end apply $(L_0 - \mu_m) g_m$ to an arbitrary $f \in \mathcal{H}_2$, that is

$$\begin{aligned}\langle f, (L_0 - \mu_m) g_m \rangle &= \int_0^\infty g_m(x) \overline{\big((L_0 - \mu_m) f\big)(x)}\, dx \\ &= \lim_{\varepsilon \to 0} \int_\varepsilon^\infty g_m(x) (\ell - \mu_m) \overline{f(x)}\, dx.\end{aligned}$$

Integrating by parts leads to

$$\lim_{\varepsilon \to 0} W\big(\overline{f(\varepsilon)}, g_m(\varepsilon)\big) + \int_\varepsilon^\infty (\ell - \mu_m) g_m(x) \overline{f(x)}\, dx.$$

Here the first limit exists according to Lemma 3 and equals 0. Using again Remark 3 finally gives

$$\langle f, (L_0 - \mu_m) g_m \rangle = \int_0^\infty g_{m-1}(x) \overline{f(x)}\, dx,$$

which is (27) for $k = m$. Next we reduce the number k step by step. Assume that the relations (26) and (27) already hold for some $k > 1$. Then (27), in particular, implies $g_{k-1} \in \mathcal{H}_{-2(m-k)-2} \setminus \mathcal{H}_{-2(m-k)}$. Take now an arbitrary function $f \in \mathcal{H}_{2(m-k)+2} = \operatorname{dom} L_0^{m-k+1}$ and consider $\langle f, (L_0 - \mu_{k-1})g_{k-1}\rangle$ as above. Then (27) for $k-1$ follows in the same way, where again the estimates (21) are essential and (24) is proved for $k \leqslant m$. We leave the details to the reader.

Since we know now that, in particular, $g(\,\cdot\,, \mu_1) \in \mathcal{H}_{-2m+2} \setminus \mathcal{H}_{-2m+4}$ the element $\varphi := (L_0 - \mu_1)g(\,\cdot\,, \mu_1)$ is well defined and belongs to $\mathcal{H}_{-n}$ for n either $2m-1$ or $2m$. In the next step of the proof we are going to determine n precisely. Obviously $\varphi \in \mathcal{H}_{-2m+1} \setminus \mathcal{H}_{-2m+2}$ exactly if $g_m \in \mathcal{H}_1 \setminus \mathcal{H}_2$, that is, g_m belongs to the domain of the quadratic form associated with the operator L_0 but not to the operator's domain, or in other words, this happens if and only if the following integral converges:

$$\int_0^\infty \left(|g_m'(x)|^2 + \frac{q_0 + q_1 x}{x^2}|g_m(x)|^2\right) dx,$$

but the integral $\int\limits_0^\infty |\ell(g_m(x))|^2\, dx$ diverges. By integration by parts the quadratic form becomes

$$\lim_{\varepsilon\to 0} -g_m'(\varepsilon)\overline{g_m(\varepsilon)} + \int_\varepsilon^\infty \ell(g_m(x))\overline{g_m(x)}\, dx. \tag{28}$$

From (16) it follows that both the boundary term and the integral term have an expansion starting with $\varepsilon^{2(\alpha_- + 2(m-1))-1}$. The only exception here is if $2(\alpha_- + 2(m-1)) - 1 = 0$, then the integral starts with a logarithmic term. Hence if $2(\alpha_- + 2(m-1)) - 1 > 0$ the limit (28) exists, if however $2(\alpha_- + 2(m-1)) - 1 < 0$ we have to investigate the leading coefficient, which equals

$$-(\alpha_- + 2(m-1))\left(C_{2(m-1)}^{(m)}\right)^2 - \frac{C_{2(m-2)}^{(m-1)}\, C_{2(m-1)}^{(m)}}{2(\alpha_- + 2(m-1)) - 1},$$

Inserting the recursions for the coefficients from Remark 4 this further equals $\left(C_{2(m-1)}^{(m)}\right)^2 \frac{-(\alpha_-+2(m-1))(2(\alpha_-+2(m-1))-1)+2(m-1)(2\alpha_-+2m-3)}{2(\alpha_-+2(m-1))-1}$. The numerator can further be simplified to

$$-\left(\alpha_- + 2(m-1)\right)^2 - \alpha_-(\alpha_- - 1). \tag{29}$$

Since in this section we assumed limit circle case $\alpha_-(\alpha_- - 1) = q_0 > 0$ and thus (29) can not vanish. Hence the limit in (28), indeed, exists if and only if the inequality $2(\alpha_- + 2(m-1)) - 1 > 0$ holds. Inserting the formula (25) for m one easily finds that this inequality is satisfied if and only if $\left[\sqrt{\frac{1}{4} + q_0}\right]$ is an odd number. In this case $\varphi \in \mathcal{H}_{-2m+1} \setminus \mathcal{H}_{-2m+2}$ and $2m-1$ can be written as $2m - 1 = \left[\sqrt{\frac{1}{4} + q_0}\right] + 2$. In the other case, however, $\varphi \in \mathcal{H}_{-2m} \setminus \mathcal{H}_{-2m+1}$ and then $2m = \left[\sqrt{\frac{1}{4} + q_0}\right] + 2$. Hence in both cases it holds

$$\varphi \in \mathcal{H}_{-n} \setminus \mathcal{H}_{-n+1} \qquad \text{for } n = \left[\sqrt{\frac{1}{4} + q_0}\right] + 2.$$

We show now that $\varphi := (L_0 - \mu_1)g(\,\cdot\,, \mu_1)$ is independent of the particular choice of μ_1. To this end apply φ to $f \in \mathcal{H}_n$. Integration by parts gives

$$\begin{aligned}\langle \varphi, f\rangle &= \langle g(\,\cdot\,, \mu_1), (L_0 - \mu_1) f\rangle = \int_0^\infty g(x, \mu_1)(\ell - \mu_1) f(x)\, dx \\ &= \lim_{\varepsilon \to 0} W(g(\varepsilon, \mu_1), f(\varepsilon)).\end{aligned}$$

Since the asymptotic expansions

$$g(\varepsilon, \mu_1) = \frac{1}{\alpha_- - \alpha_+}\varepsilon^{\alpha_-} + O(\varepsilon^{\alpha_- + 1}), \quad g'(\varepsilon, \mu_1) = \frac{\alpha_-}{\alpha_- - \alpha_+}\varepsilon^{\alpha_- - 1} + O(\varepsilon^{\alpha_-})$$

hold for $\varepsilon \to 0$, Lemma 3 implies

$$\lim_{\varepsilon \to 0} W(g(\varepsilon, \mu_1), f(\varepsilon)) = \frac{1}{\alpha_- - \alpha_+} \lim_{\varepsilon \to 0} W(\varepsilon^{\alpha_-}, f(\varepsilon)),$$

which indeed is independent of the point μ_1. Finally (27), or equivalently

$$(L_0 - \mu_k)^{-1} g_{k-1} = g_k$$

follows also for $k > m$ directly by using the defining relation (14) for the functions g_{k-1} and applying the resolvent equation to the expression $(L_0 - \mu_k)^{-1}(L_0 - \mu_i)^{-1}\varphi$. □

Remark 7 Recall that the elements g_i are actually usual functions, but not necessarily square integrable locally at 0. However, the element φ is a singular distribution with support at the point $x = 0$ only:

$$\langle \varphi, f\rangle = \frac{1}{\alpha_- - \alpha_+} \lim_{x \to 0} W(x^{\alpha_-}, f(x)) \qquad \text{for } f \in \mathcal{H}_n(L_0).$$

Theorem 1 enables us now to give a meaning to the formal expression $L_0 + t\langle \varphi, \,\cdot\,\rangle \varphi$ by using the concept of supersingular perturbations.

3.2 Operator Model

Consider the formal expression

$$L_0 + t\langle \varphi, \,\cdot\,\rangle \varphi, \qquad t \in \mathbb{R}, \tag{30}$$

where L_0 is a self-adjoint semi-bounded linear operator acting in a Hilbert space $\mathcal{H}$ and $\varphi \in \mathcal{H}_{-n}(L_0) \setminus \mathcal{H}_{-n+1}(L_0)$ is a singular element. We are going to describe a family of model operators developed in the series of papers [20, 21, 23, 24] and modified in [6, 22]. We mention that an alternative approach using Pontryagin spaces was carried out in [8, 28, 30].

Motivated by the regular situation one might be intended to consider (non-trivial) self-adjoint extensions of the symmetric restriction $L_0 \,|_{\{\psi : \langle \varphi, \psi\rangle = 0\}}$.

However, in case $n \geqslant 3$, when the perturbation is called *supersingular*, observe the following two facts:

- The restriction $L_0 \mid_{\{\psi \in \operatorname{dom}(L_0) : \langle \varphi, \psi \rangle = 0\}}$ is essentially self-adjoint in $\mathcal{H}$ (and hence has only trivial self-adjoint extensions). However, considered as an operator in the Hilbert space $\mathcal{H}_{n-2}(L_0)$ with domain in $\mathcal{H}_n(L_0)$ it becomes symmetric with defect (1, 1).
- Since the Krein type formula for the resolvents should be kept, elements of the form $(L_0 - \mu)^{-1}\varphi \in \mathcal{H}_{-n+2}(L_0) \setminus \mathcal{H}_{-n+3}(L_0)$, which do not even belong to the space $\mathcal{H}_0$, have to be included.

These requirements lead to model operators acting in the restricted extended space

$$\mathbb{H} := \mathbb{C}^{n-2} \oplus \mathcal{H}_{n-2}(L_0). \tag{31}$$

Every element $\mathbf{U} := (\mathbf{u}, U) \in \mathbb{H}$ can be identified with an element from $\mathcal{H}_{-n+2}(L_0)$ by the following natural embedding

$$\rho \mathbf{U} := \sum_{j=1}^{n-2} u_j g_j + U, \tag{32}$$

where again the notation $g_j = (L_0 - \mu_j)^{-1} \dots (L_0 - \mu_1)^{-1}\varphi$ is used with distinct points $\mu_i \in \mathbb{R} \cap \varrho(L_0)$. The vector space $\mathbb{H}$ is equipped with the scalar product

$$\langle \mathbf{U}, \mathbf{V} \rangle_{\mathbb{H}} := \langle \mathbf{u}, \Gamma \mathbf{v} \rangle_{\mathbb{C}^{n-2}} + \langle U, b_{n-2}(L_0) V \rangle_{\mathcal{H}_0}, \tag{33}$$

where $\mathbf{U} := (\mathbf{u}, U)$ and $\mathbf{V} := (\mathbf{v}, V)$, with $\mathbf{u}, \mathbf{v} \in \mathbb{C}^{n-2}$, and the functions $U, V \in \mathcal{H}_{n-2}(L_0)$. Here $\Gamma = \Gamma^*$ is a Gram matrix, and b_{n-2} denotes the regularizing polynomial, which is convenient to chose as

$$b_{n-2}(\lambda) := (\lambda - \mu_1)(\lambda - \mu_2)...(\lambda - \mu_{n-2}). \tag{34}$$

Note that the norm given by the inner product $\langle U, b_{n-2}(L_0) V \rangle_{\mathcal{H}_0}$ is equivalent to the standard norm in the space $\mathcal{H}_{n-2}(L_0)$ corresponding to $\langle U, (L_0 - \mu_1)^{n-2} V \rangle_{\mathcal{H}_0}$. In what follows we skip the index $\langle \cdot, \cdot \rangle_{\mathcal{H}_0}$ and simply write $\langle \cdot, \cdot \rangle$.

Let M denote the $(n-2) \times (n-2)$ matrix

$$M := \begin{pmatrix} \mu_1 & 1 & 0 & \dots & 0 & 0 \\ 0 & \mu_2 & 1 & \dots & 0 & 0 \\ 0 & 0 & \mu_3 & \dots & 0 & 0 \\ \dots & \dots & \dots & \ddots & \dots & \dots \\ 0 & 0 & 0 & \dots & \mu_{n-3} & 1 \\ 0 & 0 & 0 & \dots & 0 & \mu_{n-2} \end{pmatrix}.$$

In the following we assume that the Gram matrix Γ is positive definite and satisfies

$$\Gamma M - M^* \Gamma = 0, \tag{35}$$

i.e. the matrix M is Hermitian with respect to the scalar product given by the Gram matrix Γ. It has been shown in [6] that such a choice is possible exactly if the regularization points μ_i are mutually distinct.

Under these conditions the following proposition, which was proven in [6], describes the family of self-adjoint model operators.

Proposition 1 *Let* $\theta \in [0, \pi)$ *and* $\mathbf{e}_{n-2} := (0, ..., 0, 1)$. *Then the operator* $\mathbb{L}_\theta$ *defined on the domain*

$$\begin{aligned} \operatorname{dom}(\mathbb{L}_\theta) := \Big\{ & \mathbf{U} = (\mathbf{u}, U) \in \mathbb{H} : \\ & U = u_{n-1} g_{n-1} + U_r,\ u_{n-1} \in \mathbb{C},\ U_r \in \mathcal{H}_n(L_0), \\ & \cos\theta\ u_{n-1} + \sin\theta\,(\langle \varphi, U_r \rangle - \langle \mathbf{e}_{n-2}, \Gamma \mathbf{u} \rangle_{\mathbb{C}^{n-2}}) = 0 \Big\} \end{aligned} \tag{36}$$

acting as

$$\mathbb{L}_\theta \begin{pmatrix} \mathbf{u} \\ U \end{pmatrix} := \begin{pmatrix} M\mathbf{u} + u_{n-1}\mathbf{e}_{n-2} \\ L_0 U_r + \mu_{n-1} u_{n-1} g_{n-1} \end{pmatrix}$$

is self-adjoint in $\mathbb{H}$, *provided that* Γ *satisfies* (35).

Remark 8 Note that—up to the embedding ϱ—such an operator acts as the differential expression ℓ, that is,

$$\ell \varrho \mathbf{U} = \varrho \mathbb{L}_\theta \mathbf{U},$$

restricted to certain elements satisfying the generalized ‘boundary condition’ (36).

It is a straight forward calculation to see that Krein’s formula here takes the following form

$$(\mathbb{L}_\theta - \lambda)^{-1} = (\mathbb{L}_0 - \lambda)^{-1} - \frac{\langle \Phi(\bar{\lambda}), \cdot \rangle_{\mathbb{H}}}{Q(\lambda) + \cot\theta} \Phi(\lambda), \tag{37}$$

where $\mathbb{L}_0$ is the operator corresponding to $\theta = 0$, that is, $\mathbb{L}_0 = M \oplus L_0$, the vector

$$\Phi(\lambda) := \begin{pmatrix} (M - \lambda)^{-1} \mathbf{e}_{n-2} \\ (L_0 - \lambda)^{-1} g_{n-2} \end{pmatrix} \in \mathbb{H} \tag{38}$$

denotes the corresponding defect element and the Q-function takes the form

$$\begin{aligned} Q(\lambda) := {} & (\lambda - \mu_{n-1}) \langle \Phi(\mu_{n-1}), \Phi(\lambda) \rangle_{\mathbb{H}} \\ & + \langle \mathbf{e}_{n-2}, \Gamma (M - \mu_{n-1})^{-1} \mathbf{e}_{n-2} \rangle_{\mathbb{C}^{n-2}} . \end{aligned} \tag{39}$$

From (37) also the restricted-embedded resolvent $\varrho(\mathbb{L}_\theta - \lambda)^{-1}|_{\mathcal{H}_{n-2}(L_0)}$ in the form of Krein’s formula can be deduced.

Proposition 2 *Let the operators L_0 and $\mathbb{L}_\theta$ and the function $Q(\lambda)$ be given as above, and the natural embedding $\varrho : \mathbb{H} \to \mathcal{H}_{-n+2}(L_0)$, defined in (32). Then it holds*

$$\rho(\mathbb{L}_\theta - \lambda)^{-1}|_{\mathcal{H}_{n-2}(L_0)} = (L_0 - \lambda)^{-1} - \frac{1}{b_{n-2}(\lambda)(Q(\lambda) + \cot\theta)} \times\langle (L_0 - \overline{\lambda})^{-1}\varphi, \,\cdot\,\rangle (L_0 - \lambda)^{-1}\varphi, \tag{40}$$

where the polynomial b_{n-2} is defined in (34).

The essential step in order to proof this theorem is to verify the embedding of the defect element

$$\varrho\Phi = \frac{1}{b_{n-2}(\lambda)}(L_0 - \lambda)^{-1}\varphi. \tag{41}$$

Remark 9 Note that in the resolvent formula (40) the function

$$d(\lambda) := b_{n-2}(\lambda)(Q(\lambda) + \cot\theta) \tag{42}$$

is a generalized Nevanlinna function, since Q as the Q-function for operators in a Hilbert space is a usual Nevanlinna function.

3.3 Titchmarsh-Weyl Coefficient and Q-function

One of the main results of this paper is the following link between the generalized Titchmarsh-Weyl coefficient m (in the analytic approach) and d (in the above singular perturbation approach).

Theorem 2 *Let d be the generalized Nevanlinna function in (42) and m be the generalized Titchmarsh-Weyl-coefficient in (13). Then it holds*

$$d(\lambda) - m(\lambda) = \delta(\lambda),$$

where δ is a polynomial of degree less or equal to $n - 2 = \left[\sqrt{\frac{1}{4} + q_0}\right]$.

Proof Expanding (39) we find that d can be written as

$$d(\lambda) = b_{n-2}(\lambda) Q_{L_0}(\lambda) + p_{n-2}(\lambda), \tag{43}$$

where $Q_{L_0}(\lambda) := (\lambda - \mu_{n-1})\langle \varphi, (L_0 - \lambda)^{-1} g_{n-1}\rangle$ and p_{n-2} denotes a polynomial of degree $\leqslant n-2$. By integrating by parts the first summand in (43) can be rewritten as

$$\begin{aligned} &b_{n-2}(\lambda)\langle(\lambda - \mu_{n-1})g(\,\cdot\,,\lambda), g_{n-1}(\,\cdot\,)\rangle \\ &\quad = \lim_{\varepsilon\to 0} b_{n-2}(\lambda)\int_\varepsilon^\infty g_{n-1}(x)\big(\ell - \mu_{n-1} - (\ell - \lambda)\big)g(x,\lambda)\,dx \\ &\quad = \lim_{\varepsilon\to 0}(\lambda - \mu_1)\dots(\lambda - \mu_{n-2})\Big[\big(-g_{n-1}(\,\cdot\,)g'(\,\cdot\,,\lambda) + g'_{n-1}(\,\cdot\,)g(\,\cdot\,,\lambda)\big)\Big|_\varepsilon^\infty \\ &\qquad\qquad + \int_\varepsilon^\infty g_{n-2}(x)g(x,\lambda)\,dx\Big], \end{aligned}$$

and repeating this calculation with each factor $(\lambda - \mu_i)$ leads to

$$= \lim_{\varepsilon\to 0} W\big(G(\varepsilon,\lambda), g(\varepsilon,\lambda)\big) \tag{44}$$

with $G(\,\cdot\,,\lambda) := \sum\limits_{k=1}^{n-1} b_{k-1}(\lambda)g_k(\,\cdot\,)$. Here $b_{k-1}(\lambda) := \prod\limits_{j=1}^{k-1}(\lambda - \mu_j)$ and $b_0(\lambda) := 1$. According to (14) the function G can be written as

$$G(\,\cdot\,,\lambda) = \sum_{k=1}^{n-1}\sum_{i=1}^{k} b_{k-1}(\lambda)A_i^{(k)}g(\,\cdot\,,\mu_i)$$

where the coefficients $A_i^{(k)}$ were defined in (15). Expanding (44) by using (13) gives

$$\begin{aligned} &\lim_{\varepsilon\to 0} W\big(G(\varepsilon,\lambda), g(\varepsilon,\lambda)\big) \\ &\quad = \lim_{\varepsilon\to 0} W\left(\sum_{k=1}^{n-1}\sum_{i=1}^{k} b_{k-1}(\lambda)A_i^{(k)}g_-(\varepsilon,\mu_i), g_-(\varepsilon,\lambda)\right) && (45) \\ &\qquad - \sum_{k=1}^{n-1}\sum_{i=1}^{k} m(\mu_i)\,b_{k-1}(\lambda)A_i^{(k)}\lim_{\varepsilon\to 0} W\big(g_+(\varepsilon,\mu_i), g_-(\varepsilon,\lambda)\big) && (46) \\ &\qquad - m(\lambda)\sum_{k=1}^{n-1}\sum_{i=1}^{k} b_{k-1}(\lambda)A_i^{(k)}\lim_{\varepsilon\to 0} W\big(g_-(\varepsilon,\mu_i), g_+(\varepsilon,\lambda)\big) && (47) \\ &\qquad + m(\lambda)\sum_{k=1}^{n-1}\sum_{i=1}^{k} m(\mu_i)\,b_{k-1}(\lambda)A_i^{(k)}\lim_{\varepsilon\to 0} W\big(g_+(\varepsilon,\mu_i), g_+(\varepsilon,\lambda)\big) && (48) \end{aligned}$$

According to Lemma 1 the limits in (46), (47), and (48) are 1, -1, and 0, respectively. Note that the remaining factor in (47) becomes

$$\sum_{k=1}^{n-1} b_{k-1}(\lambda) \sum_{i=1}^{k} A_i^{(k)} = b_0(\lambda) A_1^{(1)} + \sum_{k=2}^{n-1} b_{k-1}(\lambda) \sum_{i=1}^{k} A_i^{(k)} = 1.$$

In order to see that the limit in (45) vanishes we have a closer look at the asymptotic behavior of the function $\sum_{k=1}^{n-1} \sum_{i=1}^{k} b_{k-1}(\lambda) A_i^{(k)} g_-(\varepsilon, \mu_i)$. In fact we will show that the relevant terms in the expansion coincide with those of $g_-(\varepsilon, \lambda)$. To this end we need the following technical lemma, which will be shown just after the current proof.

Lemma 4 *Let the polynomials $b_{k-1}(\lambda)$ and the coefficients $A_i^{(k)}$ be given as above. Then for all $l \leqslant n-2$ it holds*

$$\sum_{k=1}^{n-1} \sum_{i=1}^{k} b_{k-1}(\lambda) A_i^{(k)} \mu_i^l = \lambda^l.$$

Since in expansion (12) of the function $g_-(\cdot, \lambda)$ the coefficients $c_j(\lambda)$ for $j = 0, \dots, m_0$ and $K(\lambda)$ are polynomials of degree $\leqslant \left[\frac{m_0}{2}\right] = n-2$ the above lemma implies

$$\begin{aligned} &W\left(\sum_{k=1}^{n-1} \sum_{i=1}^{k} b_{k-1}(\lambda) A_i^{(k)} g_-(\varepsilon, \mu_i), g_-(\varepsilon, \lambda) \right) \\ &\quad = W\left(\sum_{j=1}^{m_0} c_j(\lambda) \varepsilon^{\alpha_- + j} + K(\lambda) \varepsilon^{\alpha_+} + \varepsilon^{m_0 + \alpha_- + 1} (h_1(\varepsilon, \lambda) + \ln x \, h_2(\varepsilon, \lambda)), \right. \\ &\qquad \left. \sum_{j=1}^{m_0} c_j(\lambda) \varepsilon^{\alpha_- + j} + K(\lambda) \varepsilon^{\alpha_+} + \varepsilon^{m_0 + \alpha_- + 1} (h_3(\varepsilon, \lambda) + \ln x \, h_4(\varepsilon, \lambda)) \right). \end{aligned}$$

where h_i for $i = 1 \dots, 4$ are holomorphic at $\varepsilon = 0$. Since the singular terms of the two functions here coincide the limit for $\varepsilon \to 0$ is zero, and we finally obtain from (44)

$$d(\lambda) - m(\lambda) = p_{n-2}(\lambda) - \sum_{k=1}^{n-1} b_{k-1}(\lambda) \sum_{i=1}^{k} m(\mu_i) A_i^{(k)},$$

which, indeed, is a polynomial of degree $\leqslant n-2$. □

Proof of Lemma 4 We note first that the coefficients $A_i^{(k)}$, which were defined recursively in (15), can also be given explicitly by derivatives b_k' of the polynomials b_k

$$A_i^{(k)} = \frac{1}{b_k'(\mu_i)} \qquad \text{for } i = 1, \dots, k. \tag{49}$$

Indeed, it is easy to see that the sequence in (49) satisfies the recursion in (15) for $i \leqslant k-1$. The remaining equality $A_k^{(k)} = -\sum_{i=1}^{k-1} A_i^{(k)}$ can be seen by multiplying the identity

$$\frac{1}{b_k(\lambda)} = \sum_{i=1}^{k} \frac{1}{b'_k(\mu_i)} \frac{1}{\lambda - \mu_i}$$

with λ and then taking the limit $\lambda \to \infty$. Hence in order to complete the proof we have to show

$$\sum_{k=1}^{n-1} b_{k-1}(\lambda) \sum_{i=1}^{k} \frac{\mu_i^l}{b'_k(\mu_i)} = \lambda^l \qquad \text{for } l = 0, 1, \dots, n-2. \tag{50}$$

For $k \geqslant l+1$ the partial fractional decomposition

$$\frac{\lambda^l}{b_k(\lambda)} = \sum_{i=1}^{k} \frac{\mu_i^l}{b'_k(\mu_i)} \frac{1}{\lambda - \mu_i}$$

implies

$$\sum_{i=1}^{k} \frac{\mu_i^l}{b'_k(\mu_i)} = \begin{cases} 0 & k > l+1 \\ 1 & k = l+1 \end{cases}. \tag{51}$$

Hence the polynomial

$$P_l(\lambda) := -\lambda^l + \sum_{k=1}^{n-1} b_{k-1}(\lambda) \sum_{i=1}^{k} \frac{\mu_i^l}{b'_k(\mu_i)} \tag{52}$$

is of degree $\leqslant l-1$. We are calculating its values at the points $\mu_1, \dots, \mu_l$. Changing the order of summation in (52) and taking into account (51) we immediately obtain $P_l(\mu_1) = 0$ and

$$P_l(\mu_j) = \sum_{i=1}^{j-1} \mu_i^l \sum_{k=i}^{j} \frac{b_{k-1}(\mu_j)}{b'_k(\mu_i)} \qquad \text{for } j = 2, \dots, l. \tag{53}$$

Changing the indices to $j =: i + N - 1$ with $i \geqslant 1$ and $N \geqslant 2$ and introducing $\lambda_{m+1} := \mu_{i+m}$ the inner sums in (53) become

$$\sum_{k=i}^{j} \frac{b_{k-1}(\mu_j)}{b'_k(\mu_i)} = \frac{b_{i-1}(\lambda_N)}{b'_i(\lambda_1)} \cdot I_1^k,$$

where $I_k^N := 1 + \sum_{m=1}^{N-k-1} \prod_{m_1=1}^{m} \frac{\lambda_N - \lambda_{m_1}}{\lambda_1 - \lambda_{m_1+1}} - \prod_{m_2=1}^{N-k-1} \frac{\lambda_N - \lambda_{m_2+1}}{\lambda_1 - \lambda_{m_2+1}}$. It is easy to see that $I_k^N = I_{k+1}$ for $k \leqslant N-3$ and hence

$$I_1^N = I_{N-2}^N = 1 + \frac{\lambda_N - \lambda_1}{\lambda_1 - \lambda_2} - \frac{\lambda_N - \lambda_2}{\lambda_1 - \lambda_2} = 0.$$

Thus the summands in (53) vanish and the polynomial P_l with degree at most $l-1$ has l distinct zeros, and hence vanishes identically, which finally proves relation (50). □

In [16] it was shown that the generalized Titchmarsh-Weyl coefficient m is a generalized Nevanlinna function with negative index $\kappa = \left[\frac{n-1}{2}\right]$. As a corollary of Theorem 2 we obtain an independent proof for this fact.

Corollary 2 *The generalized Titchmarsh-Weyl-coefficient m, introduced in* (13)*, belongs to the generalized Nevanlinna class $\mathcal{N}_\kappa$ where*

$$\kappa = \left[\frac{n-1}{2}\right] = \left[\frac{1+\sqrt{\frac{1}{4}+q_0}}{2}\right].$$

Proof In [6, Sections 4.4 and 5.2] it was shown that the function d admits also a minimal representation in a certain Pontryagin space and hence belongs to the class $\mathcal{N}_\kappa$ with $\kappa = \left[\frac{n-1}{2}\right]$. In fact, it belongs even to the class $\mathcal{N}_\kappa^\infty$, see [7, 9], and hence it has an irreducible representation of the form

$$d(\lambda) = (\lambda^2+1)^\kappa d_0(\lambda) + p_{2\kappa-1}(\lambda), \tag{54}$$

where d_0 is a usual Nevanlinna function satisfying

$$\lim_{y\to\infty} \frac{\operatorname{Im} d_0(iy)}{y} = 0, \qquad \lim_{y\to\infty} y \operatorname{Im} d_0(iy) = \infty$$

and $p_{2\kappa-1}$ is a polynomial of degree $\leqslant 2\kappa-1$. According to Theorem 2 the difference between m and d is a polynomial of degree at most $n-2 \leqslant 2\kappa$. Hence the function m admits an irreducible representation of the form (54) as well, which, in particular, implies $m \in \mathcal{N}_\kappa$. □

4 Spectral Analysis

4.1 Spectral Properties

Here we are collecting some well known spectral properties of the classical Hydrogen atom operator L_0 and derive corresponding properties for the model operators $\mathbb{L}_\theta$. To this end recall the following facts for *Whittaker-functions*, see [31, Sections 16.1–16.4].

Let $W_{l,m}(z)$ be the Whittaker function of index (l, m), which is well defined (as a contour integral) for all values $l, m \in \mathbb{C}$. It is analytic for $z \in \mathbb{C} \setminus (-\infty, 0]$ and satisfies in the domain $|\arg z| < \pi$

$$W_{l,m}(z) = e^{-\frac{z}{2}} z^l \left(1 + O\left(\frac{1}{|z|}\right)\right) \tag{55}$$

as $z \to \infty$. The functions $W_{l,m}(z)$ and $W_{-l,m}(-z)$ form a fundamental system of solutions of the so-called *Whittaker-equation*:

$$\frac{d^2}{dz^2}W(z) + \left(-\frac{1}{4} + \frac{l}{z} + \frac{\frac{1}{4} - m^2}{z^2}\right)W(z) = 0. \tag{56}$$

The following result is well known (see eg. [29, Section 4.17], [14]), we are going to give only a sketch of the proof, as far as we will make use of the arguments later on.

Proposition 3 *Let the operator L_0 be the Hydrogen-atom operator with parameters $q_0 \geqslant \frac{3}{4}$ and $q_1 \in \mathbb{R}$, that is, on the domain (19) it acts as*

$$(L_0 y)(x) = -y''(x) + \Big(\frac{q_0}{x^2} + \frac{q_1}{x}\Big)y(x).$$

Then the following holds

$$\sigma_c(L_0) = [0, \infty)$$

and

$$\sigma_p(L_0) = \begin{cases} \emptyset & \text{if} \quad q_1 \geqslant 0 \\ \left\{\lambda_j := \dfrac{-q_1^2}{\left(2j - 1 + 2\sqrt{q_0 + \frac{1}{4}}\right)^2} \;\middle|\; j = 1, 2, \dots\right\} & \text{if} \quad q_1 < 0 \end{cases}$$

Remark 10 The spectrum is simple.

Proof Here and in the following the function $\sqrt{\cdot}$ has its branch cut on the negative half line. For $\lambda \neq 0$ substituting $z := -2\sqrt{-\lambda}\,x$ in the eigenvalue equation

$$(L_0 y)(x) = -y''(x) + \Big(\frac{q_0}{x^2} + \frac{q_1}{x}\Big)y(x) = \lambda y(x) \tag{57}$$

yields the Whittaker equation (56) with parameters $m = \sqrt{\frac{1}{4} + q_0}$ and $l = \frac{q_1}{2\sqrt{-\lambda}}$ and hence (57) has the linearly independent solutions

$$y_1(x, \lambda) := W_{\frac{q_1}{2\sqrt{-\lambda}}, \sqrt{\frac{1}{4} + q_0}}\big(-2\sqrt{-\lambda}\,x\big)$$

and

$$y_2(x, \lambda) := W_{-\frac{q_1}{2\sqrt{-\lambda}}, \sqrt{\frac{1}{4} + q_0}}\big(2\sqrt{-\lambda}\,x\big).$$

For $\lambda > 0$ the estimate (55) implies that neither y_1 nor y_2 vanish as $x \to \infty$. It is easy to see that the same holds true for all their linear combinations. Hence

$$\sigma_p(L_0) \cap \mathbb{R}^+ = \emptyset.$$

From the asymptotics at ∞ it also follows that for $\operatorname{Re}\lambda > 0$ the Weyl solution $g(\,\cdot\,,\lambda)$ is a multiple of either $y_1(\,\cdot\,,\lambda)$ or $y_2(\,\cdot\,,\lambda)$ depending on the sign of $\operatorname{Im}\lambda$. However, due to the fact that these functions have different asymptotics at ∞ it is easy to see that $g(\,\cdot\,,\lambda)$ has a (finite) jump as λ crosses the real line and hence

$$(0,\infty) \subset \sigma_c(L_0).$$

In the same way one sees that on the negative real line there are no jumps (with the possible exception of a discrete set of points) and hence there is no continuous spectrum in $(-\infty,0)$. Let us now consider $\lambda = 0$. For $q_1 \neq 0$ it is easy to check that every solution of (57) is given by

$$y(x) := \sqrt{x}\, H_\gamma(2i\sqrt{q_1}\sqrt{x}),$$

where the function $H_\gamma(z)$ is an arbitrary solution of the Bessel equation $\frac{d^2}{dz^2}H(z) + \frac{1}{z}\frac{d}{dz}H(z) + (1-\frac{\gamma^2}{z^2})H(z) = 0$ with $\gamma := 2\sqrt{\frac{1}{4}+q_0}$. Using the asymptotics of Bessel functions one can check that for $q_1 < 0$ no solution is square integrable at ∞, and for $q_1 > 0$ there exists a solution which is square integrable at ∞, however, not at $x = 0$. Furthermore, one can see directly that also for $q_1 = 0$ the solution of (57) which is square integrable at ∞ does not belong to $L_2(0,\infty)$ due to its singularity at the origin. Hence in any case

$$0 \notin \sigma_p(L_0).$$

Note that for $q_1 \geqslant 0$ the operator L_0 is non-negative and hence it holds $\mathbb{R}_- \subset \varrho(L_0)$. If $q_1 < 0$, however, there exists a sequence of negative eigenvalues, accumulating at $\lambda = 0$. See eg. [14, 18, 29] for how to determine this sequence explicitly. □

As a direct consequence of Proposition 3 we also describe the spectra of $\mathbb{L}_\theta$.

Theorem 3 *Let the operator $\mathbb{L}_\theta$ for $\theta \in [0,\pi)$ be given as in Section 3.3. Then*

$$\sigma_c(\mathbb{L}_\theta) = [0,\infty).$$

- *If $q_1 \geqslant 0$ then $\sigma_p(\mathbb{L}_\theta)$ consists of at most finitely many negative points. There exists exactly one exceptional parameter $\theta_0 \in (0,\pi)$ such that $0 \in \sigma_p(\mathbb{L}_{\theta_0})$.*
- *If $q_1 < 0$ then $\sigma_p(\mathbb{L}_\theta)$ consists of a sequence of negative points accumulating at 0, but $\lambda = 0$ is never an eigenvalue.*

Proof Since for each $\theta \in [0,\pi)$ the operator $\mathbb{L}_\theta$ is a finite rank perturbation (in the resolvent sense) of L_0 it follows from Proposition 3 that

$$\mathbb{R}^+ \subset \sigma_c(\mathbb{L}_\theta) \cup \sigma_p(\mathbb{L}_\theta)$$

and

$$\mathbb{R}^- \subset \varrho(\mathbb{L}_\theta) \cup \sigma_p(\mathbb{L}_\theta)$$

and, in particular, that for $q_1 \geqslant 0$ the number of negative eigenvalues has to be finite.

Assume now that $\lambda_0 > 0$ is an eigenvalue of some $\mathbb{L}_\theta$ with eigenelement $\mathbf{U}_0$. Then according to Remark 8 the embedding $\varrho(\mathbf{U}_0)$ satisfies equation (57). However, in the proof of Proposition 3 we have seen that none of these solutions are square integrable at ∞. Hence for each parameter $\theta \in [0, \pi)$ this implies $\mathbb{R}^+ \subset \sigma_c(\mathbb{L}_\theta)$.

Let us now consider the point $\lambda = 0$. As before for $q_1 < 0$ there is no solution of (57) which is square integrable at ∞. However, for $q_1 \geqslant 0$ there is such a solution u_0. Using Lemma 4 it is not hard to see that this function actually belongs to the range of $\varrho(\mathbb{H})$. Then obviously for exactly one value $\theta_0 \in (0, \pi)$ the boundary condition (36) is satisfied for $\mathbf{U}_0 := \varrho^{-1} u_0$. Hence the point $\lambda = 0$ is an eigenvalue exactly for the operator $\mathbb{L}_{\theta_0}$. □

The above considerations provide also more insight in the behavior of $m(\lambda)$ and $g(\,\cdot\,, \lambda)$ towards the positive real line.

Corollary 3 *The functions $m(\lambda)$ and $-\dfrac{1}{Q(\lambda) + \cot\theta}$, which are analytic in the upper half plane, can be continued analytically to every point $\lambda_0 \in \mathbb{R}^+$.*

Remark 11

- (i) Note, in particular, that for every fixed $x \in \mathbb{R}$ also $g(x, \lambda)$ has an analytic continuation across the positive real line.
- (ii) In general, these continuations will not be real valued on $\mathbb{R}^+$.
- (iii) On the lower half plane the continuation does in general not coincide with the original function.

Proof Since the function $y_1(x, \lambda)$ in the proof of Proposition 3 is a solution of (57) which is square integrable at ∞ for each λ with $\operatorname{Im}\lambda > 0$ it is proportional to $g(x, \lambda)$, i.e.

$$y_1(x, \lambda) = a(\lambda) g(x, \lambda) = a(\lambda)\big[g_-(x, \lambda) - m(\lambda) g_+(x, \lambda)\big]$$

holds with some factor $a(\lambda)$. Note that $y_1(x, \lambda)$ and $\frac{d}{dx} y_1(x, \lambda)$ are both holomorphic at least for $\lambda \in \mathbb{C} \setminus \mathbb{R}_0^-$. Since $g_+(x, \lambda)$ and $\frac{d}{dx} g_+(x, \lambda)$ are entire in λ it follows that $a(\lambda)$, which can be expressed via the Wronskian by

$$a(\lambda) = W\big(y_1(\,\cdot\,, \lambda), g_+(\,\cdot\,\lambda)\big),$$

can be continued holomorphically across $\mathbb{R}^+$. Hence, since obviously $a(\lambda) \neq 0$, also $g(x, \lambda) = \frac{y_+(x,\lambda)}{a(\lambda)}$ can be continued holomorphically across the positive real line. Note that for every $\lambda_0 \in \mathbb{R}^+$ there exists an $x_0 \in \mathbb{R}^+$ such that $g_+(x_0, \lambda_0) \neq 0$ and hence also

$$m(\lambda) = \frac{g_-(x_0, \lambda) - g(x_0, \lambda)}{g_+(x_0, \lambda)}$$

can be continued holomorphically to λ_0. Therefore by Theorem 2 also $Q(\lambda) + \cot\theta$ can be continued. However, note that this continuation cannot vanish in any $\lambda_0 \in \mathbb{R}^+$. Indeed, due to the analyticity then also the limit

$$\lim_{\lambda \to \lambda_0} \frac{Q(\lambda) + \cot\theta}{\lambda - \lambda_0}$$

would exist, i.e. λ_0 is a zero of the function $Q(\lambda) + \cot\theta$, which would imply $\lambda_0 \in \sigma_p(\mathbb{L}_\theta)$. Hence, finally, also $-\frac{1}{Q(\lambda)+\cot\theta}$ has an analytic continuation across $\mathbb{R}^+$. □

Alternatively to the Whittaker functions one can also use another set of linearly independent solutions of (56), the so-called *Kummer-functions*, which satisfy as $z \to 0$

$$M_{l,m}(z) = z^{\frac{1}{2}+m} e^{-\frac{z}{2}} \left(1 + \frac{\frac{1}{2}+m-l}{1!(2m+1)} z + \frac{\left(\frac{1}{2}+m-l\right)\left(\frac{3}{2}+m-l\right)}{2!(2m+1)(2m+2)} z^2 + \dots\right),$$

$$M_{l,-m}(z) = z^{\frac{1}{2}-m} e^{-\frac{z}{2}} \left(1 + \frac{\frac{1}{2}-m-l}{1!(-2m+1)} z + \frac{\left(\frac{1}{2}-m-l\right)\left(\frac{3}{2}-m-l\right)}{2!(-2m+1)(-2m+2)} z^2 + \dots\right).$$

If $2m \notin \mathbb{N}$ then the following relation holds

$$W_{l,m}(z) = \frac{\Gamma(-2m)}{\Gamma\left(\frac{1}{2}-m-l\right)} M_{l,m}(z) + \frac{\Gamma(2m)}{\Gamma\left(\frac{1}{2}+m-l\right)} M_{l,-m}(z), \tag{58}$$

where Γ denotes the Gamma function. This relation between solutions with known asymptotics at 0 and ∞, respectively, immediately implies the following explicit form of m.

Corollary 4 *For* $2\sqrt{\frac{1}{4}+q_0} = \alpha_+ - \alpha_- \notin \mathbb{N}$ *the generalized Titchmarsh Weyl coefficient* m *has the form*

$$m(\lambda) = \frac{1}{2\sqrt{\frac{1}{4}+q_0}} \cdot \frac{\Gamma\left(\frac{1}{2}+\sqrt{\frac{1}{4}+q_0} - \frac{q_1}{2\sqrt{-\lambda}}\right)}{\Gamma\left(\frac{1}{2}-\sqrt{\frac{1}{4}+q_0} - \frac{q_1}{2\sqrt{-\lambda}}\right)} \cdot \frac{\Gamma\left(-2\sqrt{\frac{1}{4}+q_0}\right)}{\Gamma\left(2\sqrt{\frac{1}{4}+q_0}\right)} \cdot (-4\lambda)^{\sqrt{\frac{1}{4}+q_0}},$$

where the branch cut of the function $z^{\sqrt{\frac{1}{4}+q_0}}$ *lies on the negative half line.*

4.2 Standard and Generalized Spectral Representations

Finally we are going to use the spectral resolution of the identity for the model operator $\mathbb{L}_\theta$ in order to show a new expansion result involving functions which are not square integrable locally at 0.

In what follows we fix $\theta \in (0, \pi)$, note that $\theta = 0$ corresponds to the standard case, and we consider the model operator $\mathbb{L}_\theta$. Denote by $N(\theta) \in \mathbb{N} \cup \{\infty\}$ the number of the negative eigenvalues of $\mathbb{L}_\theta$. In the case that 0 is an eigenvalue let the function $e_0(x)$ denote $\varrho\Phi_0$, the embedding of the eigenelement Φ_0 for the eigenvalue 0, which actually can also be written in terms of Bessel functions. In the case 0 is not an eigenvalue let $e_0(x) \equiv 0$. Moreover, on the positive half line we define the function

$$\Psi(x,\lambda) := g_+(x,\lambda) - \frac{1}{d(\lambda + i0)} g(x, \lambda + i0) \qquad \lambda \in \mathbb{R}^+,$$

where the functions on the right hand side are to be understood as the analytic continuation from the upper half plane, as in Corollary 3. We can now formulate our main expansion theorem.

Theorem 4 *With the above notations for every function $U \in C_0^\infty\big((0,\infty)\big)$ it holds*

$$U(x) = \frac{\left\langle \Phi_{\mathbf{0}}, \begin{pmatrix} 0 \\ U \end{pmatrix} \right\rangle_{\mathbb{H}}}{\langle \Phi_{\mathbf{0}}, \Phi_{\mathbf{0}} \rangle_{\mathbb{H}}} e_0(x) + \sum_{j=1}^{N(\theta)} \frac{g(x,\lambda_j)}{d'(\lambda_j)} \int_0^\infty g(s,\lambda_j) U(s)\, ds$$
$$+ \frac{1}{2\pi i} \int_0^\infty \int_0^\infty \Psi(x,\lambda)\overline{\Psi(s,\lambda)}\, U(s)\, ds\, (m(\lambda+i0) - m(\lambda-i0))\, d\lambda. \quad (59)$$

Remark 12 The functions $\Psi(x,\lambda)$ in this expansion are not locally square integrable on $[0,\infty)$, except if $\theta = 0$, where $\Psi = g_+$. In this special case the expansions are well known in the literature (see eg. [19] or more recently [15, 17])

Remark 13 Expansion (59) is obviously dependent on the parameter θ, in particular, the eigenvalues λ_j and the 'generalized eigenfunctions' Ψ (via the function $d(\lambda + i0)$).

As first step we are going to show the following auxiliary lemma, which is a weak version of the spectral decomposition corresponding to the operator $\mathbb{L}_\theta$ in the model space $\mathbb{H}$.

In what follows the notation

$$\langle \mathbf{F}, \mathbf{G} \rangle_{\mathbb{H}} = (\mathbf{f}, \Gamma \mathbf{g})_{\mathbb{C}^{n-2}} + \int\limits_0^\infty \overline{b_{n-2}(L_0) F(x)} G(x)\, dx$$

is used in a natural way also for $\mathbf{F} = \begin{pmatrix} \mathbf{f} \\ F \end{pmatrix}$ and $\mathbf{G} = \begin{pmatrix} \mathbf{g} \\ G \end{pmatrix}$ for which the above integral exists even if the functions F, G do not belong to $\mathcal{H}_{n-2}(L_0)$. However, then it can be interpreted as a pairing with respect to the operator $\mathbb{L}_0$.

Lemma 5 *Let elements* $\mathbf{U} := \begin{pmatrix} \mathbf{u} \\ U \end{pmatrix}$ *and* $\mathbf{V} := \begin{pmatrix} \mathbf{v} \\ V \end{pmatrix}$ *be given with* $U, V \in C_0^\infty\big((0,\infty)\big)$. *Then it holds*

$$\langle \mathbf{U}, \mathbf{V} \rangle_{\mathbb{H}} = \langle E_{\mathbb{L}_\theta}(\{0\}) \mathbf{U}, \mathbf{V} \rangle_{\mathbb{H}} + \sum_{j=1}^{N(\theta)} \frac{\langle \mathbf{U}, \Phi_j \rangle_{\mathbb{H}} \langle \Phi_j, \mathbf{V} \rangle_{\mathbb{H}}}{\langle \Phi_j, \Phi_j \rangle_{\mathbb{H}}}$$
$$+ \frac{1}{2\pi i} \int_0^\infty \langle \mathbf{U}, \Psi(\lambda) \rangle_{\mathbb{H}} \langle \Psi(\lambda), \mathbf{V} \rangle_{\mathbb{H}} \frac{m(\lambda + i0) - m(\lambda - i0)}{b_{n-2}(\lambda)}\, d\lambda, \quad (60)$$

where

1. *the operator* $E_{\mathbb{L}_\theta}(\{0\})$ *denotes the spectral projection corresponding to the (possible) eigenvalue* 0,
2. *the elements* $(\Phi_j)_{j=1}^{N(\theta)}$ *are the eigenfunctions for the negative eigenvalues of* $\mathbb{L}_\theta$,
3. *the element* Ψ *is defined as* $\Psi = \begin{pmatrix} 0 \\ g_+ \end{pmatrix} + \frac{1}{Q + \cot\theta} \Phi$,
4. b_{n-2} *is the polynomial introduced in* (34).

Note that the integral in (60) should be understood as an improper integral.

Proof Recall that for the self-adjoint operator $\mathbb{L}_\theta$ in the Hilbert space $\mathbb{H}$ Stones formula (see [13, page 1203]) holds,

$$\langle \mathbf{U}, E_{\mathbb{L}_\theta}((\lambda_1, \lambda_2]) \mathbf{V} \rangle_{\mathbb{H}} = \lim_{\delta \downarrow 0} \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int\limits_{\lambda_1 + \delta}^{\lambda_2 + \delta} \Big(\langle \mathbf{U}, (\mathbb{L}_\theta - (\lambda + i\varepsilon))^{-1} \mathbf{V} \rangle_{\mathbb{H}}$$
$$- \langle \mathbf{U}, (\mathbb{L}_\theta - (\lambda - i\varepsilon))^{-1} \mathbf{V} \rangle_{\mathbb{H}} \Big)\, d\lambda, \quad (61)$$

where $\mathbf{U}, \mathbf{V}$ are as in the formulation of the Lemma and $E_{\mathbb{L}_\theta}((\lambda_1, \lambda_2])$ denotes the spectral projection for the operator $\mathbb{L}_\theta$ corresponding to the interval $(\lambda_1, \lambda_2]$. In what follows we choose $0 < \lambda_1 < \lambda_2$.

Using Krein's formula (37) for the resolvent of $\mathbb{L}_\theta$ and rearranging the integrand we can write (61) as

$$\begin{aligned}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int\limits_{\lambda_1+\delta}^{\lambda_2+\delta}&\Big[\Big(\mathbf{u}, \Gamma\big((\mathbf{M}-(\lambda+\mathbf{i}\varepsilon))^{-\mathbf{1}}-(\mathbf{M}-(\lambda-\mathbf{i}\varepsilon))^{-\mathbf{1}}\big)\mathbf{v}\Big)_{\mathbb{C}^{\mathbf{n-2}}}\\
&+\Big(U, b_{n-2}(L_0)\big((L-(\lambda+i\varepsilon))^{-1}-(L-(\lambda-i\varepsilon))^{-1}\big)V\Big)_{L^2(0,\infty)}\\
&-\frac{1}{Q(\lambda+i\varepsilon)+\cot\theta}\langle\Phi(\lambda-i\varepsilon)-\Phi(\lambda+i\varepsilon),\mathbf{V}\rangle_{\mathbb{H}}\langle\mathbf{U}, \Phi(\lambda+i\varepsilon)\rangle_{\mathbb{H}}\\
&+\frac{1}{Q(\lambda-i\varepsilon)+\cot\theta}\langle\Phi(\lambda+i\varepsilon),\mathbf{V}\rangle_{\mathbb{H}}\langle\mathbf{U}, \Phi(\lambda-i\varepsilon)-\Phi(\lambda+i\varepsilon)\rangle_{\mathbb{H}}\\
&+\frac{Q(\lambda+i\varepsilon)-Q(\lambda-i\varepsilon)}{|Q(\lambda-i\varepsilon)+\cot\theta|^2}\langle\Phi(\lambda+i\varepsilon),\mathbf{V}\rangle_{\mathbb{H}}\langle\mathbf{U}, \Phi(\lambda+i\varepsilon)\rangle_{\mathbb{H}}\Big]d\lambda.\end{aligned}$$

Since the first summand is holomorphic in the relevant interval the limit for $\varepsilon \downarrow 0$ of its contribution vanishes. In order to investigate the other terms note first that for any solution of the equation

$$-y'' + \frac{q_0 + q_1 x}{x^2} y = \lambda y,$$

which is holomorphic in λ, it holds

$$y(x, \lambda \pm i\varepsilon) = y(x, \lambda) + \mathcal{O}(\varepsilon), \tag{62}$$

where the term $\mathcal{O}(\varepsilon)$ is uniform with respect to (x, λ) on each compact subset of $(0, \infty) \times \mathbb{R}$. Then the second summand

$$\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int\limits_{\lambda_1+\delta}^{\lambda_2+\delta}\Big(U, b_{n-2}(L_0)\big((L-(\lambda+i\varepsilon))^{-1}-(L-(\lambda-i\varepsilon))^{-1}\big)V\Big)_{L^2(0,\infty)}d\lambda$$

can be simplified by inserting the explicit form of the resolvents as integral operators as given in Lemma 3, observing that the function $m(\lambda)$ in the relation $g(x, \lambda) = g_-(x, \lambda) - m(\lambda)g_+(x, \lambda)$ has a holomorphic continuation to the positive real line and, finally, using the uniform estimate (62). This yields

$$\frac{1}{2\pi i}\int\limits_{\lambda_1+\delta}^{\lambda_2+\delta}\int\limits_0^\infty (b_{n-2}(L_0)\overline{U(x)})g_+(x,\lambda)\,dx$$

$$\cdot\int\limits_0^\infty g_+(s,\lambda)V(s)\,ds\big(m(\lambda+i0)-m(\lambda-i0)\big)d\lambda$$

$$=\frac{1}{2\pi i}\int\limits_{\lambda_1+\delta}^{\lambda_2+\delta}\int\limits_0^\infty g_+(x,\lambda)b_{n-2}(L_0)\overline{U(x)}\,dx$$

$$\cdot\int\limits_0^\infty g_+(s,\lambda)b_{n-2}(L_0)V(s)\,ds\frac{m(\lambda+i0)-m(\lambda-i0)}{b_{n-2}(\lambda)}\,d\lambda,$$

where the last equality uses that $g_+(x,\lambda)$ is a solution of (6). For the other terms note that from the definition of Φ in (38) it follows for $\lambda\in\mathbb{R}^+$

$$\langle\mathbf{U},\Phi(\lambda+i\varepsilon)\rangle=\langle\mathbf{U},\Phi(\lambda+i0)\rangle+\mathcal{O}(\varepsilon)$$

and

$$\langle\Phi(\lambda-i\varepsilon)-\Phi(\lambda+i\varepsilon),\mathbf{V}\rangle$$

$$=\int\limits_0^\infty g_+(s,\lambda)b_{n-2}(L_0)V(s)\,ds\,\frac{m(\lambda+i0)-m(\lambda-i0)}{b_{n-2}(\lambda)}+\mathcal{O}(\varepsilon)$$

and for the other expressions correspondingly. Collecting all terms gives

$$\langle\mathbf{U},E_{\mathbb{L}_\theta}((\lambda_1,\lambda_2])\mathbf{V}\rangle_{\mathbb{H}}$$

$$=\lim_{\delta\downarrow 0}\frac{1}{2\pi i}\int\limits_{\lambda_1+\delta}^{\lambda_2+\delta}\langle\mathbf{U},\Psi(\lambda+i0)\rangle\langle\Psi(\lambda+i0),\mathbf{V}\rangle\frac{m(\lambda+i0)-m(\lambda-i0)}{b_{n-2}(\lambda)}\,d\lambda$$

$$=\frac{1}{2\pi i}\int\limits_{\lambda_1}^{\lambda_2}\langle\mathbf{U},\Psi(\lambda+i0)\rangle\langle\Psi(\lambda+i0),\mathbf{V}\rangle\frac{m(\lambda+i0)-m(\lambda-i0)}{b_{n-2}(\lambda)}\,d\lambda,$$

since $\sigma_p(\mathbb{L}_\theta)\cap\mathbb{R}^+=\emptyset$. This implies further

$$\langle\mathbf{U},E_{\mathbb{L}_\theta}((0,\infty))\mathbf{V}\rangle_{\mathbb{H}}$$

$$=\frac{1}{2\pi i}\int\limits_0^\infty\langle\mathbf{U},\Psi(\lambda+i0)\rangle\langle\Psi(\lambda+i0),\mathbf{V}\rangle\frac{m(\lambda+i0)-m(\lambda-i0)}{b_{n-2}(\lambda)}\,d\lambda$$

Finally the decomposition of the identity operator I as

$$I = E_{\mathbb{L}_\theta}(\{0\}) + \sum_{j=1}^{N(\theta)} E_{\mathbb{L}_\theta}(\{\lambda_j\}) + E_{\mathbb{L}_\theta}((0,\infty)),$$

where $\mathbb{E}_{\mathbb{L}_\theta}(\{\lambda_j\}) = \frac{\langle \Phi_j, \cdot \rangle}{\langle \Phi_j, \Phi_j \rangle} \Phi_j$ is the orthogonal projection onto the eigenspace spanned by the eigenelement $\Phi_j := \Phi(\lambda_j)$ corresponding to the eigenvalue λ_j, yields the desired weak expansion. □

Using this result we are now going to prove Theorem 4.

Proof First we show that for every $\mathbf{U} = \begin{pmatrix} \mathbf{0} \\ U \end{pmatrix}$ with $U \in C_0^\infty\big((0,\infty)\big)$ the transformation

$$\mathcal{I}\mathbf{U} := E_{\mathbb{L}_\theta}(\{0\})\mathbf{U} + \sum_{j=1}^{N(\theta)} \frac{\langle \Phi_j, \mathbf{U} \rangle_{\mathbb{H}}}{\langle \Phi_j, \Phi_j \rangle_{\mathbb{H}}} \Phi_j + \frac{1}{2\pi i} \int_0^\infty \langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}} \Psi(\lambda) \frac{m(\lambda + i0) - m(\lambda - i0)}{b_{n-2}(\lambda)}\, d\lambda \tag{63}$$

is well defined, which means that we have to verify the existence of the integral. Let us start with the right endpoint $+\infty$. Since $\mathbf{U}$ belongs to the domain of any power $N \geqslant 0$ of the operator $\mathbb{L}_\theta$ Lemma 5 can be applied to the inner product $\langle \mathbb{L}_\theta^N \mathbf{U}, \mathbf{U} \rangle_{\mathbb{H}}$. Integration by parts and using the eigenvalue property leads to

$$\langle \mathbb{L}_\theta^N \mathbf{U}, \mathbf{U} \rangle_{\mathbb{H}} = \sum_{j=1}^{N(\theta)} \lambda_j^N \frac{|\langle \Phi_j, \mathbf{U} \rangle_{\mathbb{H}}|^2}{\langle \Phi_j, \Phi_j \rangle_{\mathbb{H}}} + \frac{1}{2\pi i} \int_0^\infty \lambda^N |\langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}}|^2 (Q(\lambda + i0) - Q(\lambda - i0))\, d\lambda, \tag{64}$$

where we also used formula (42) and Theorem 2. Since Q as a Nevanlinna function grows at most linearly it follows that

$$\int_0^\infty \lambda^N |\langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}}|^2\, d\lambda < \infty \quad \text{for all } N \in \mathbb{N},$$

and hence $\langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}}$ tends to zero faster than any power of λ.

Let us now consider the second factor in the integral in (63)

$$\Psi(\lambda) = (0) g_+(\cdot, \lambda) - \frac{1}{Q(\lambda + i0) + \cot\theta} \Phi(\lambda + i0).$$

The identity

$$g_+(x, \lambda) = -\frac{g(x, \lambda + i0) - g(x, \lambda - i0)}{m(\lambda + i0) - m(\lambda - i0)}$$

together with Remark 11 and Corollary 4 imply that $g_+(x, \lambda)$ is (locally uniformly in x) bounded in λ as $\lambda \to +\infty$. Similarly also $\varrho\Phi(x, \lambda) = \frac{1}{b_{n-2}(\lambda)} g(x, \lambda)$

is (locally uniformly in x) bounded for large real λ. Since the functions g_k, which are used for the embedding, are independent of λ and bounded at ∞ it follows that both components of $\Phi(\lambda)$ are (locally uniformly in x) bounded and hence the integral in (64) converges (locally uniformly in x) at $+\infty$.

Let us next consider the left endpoint $\lambda = 0$. For $\mathbf{U} = \mathbf{V} = \begin{pmatrix} \mathbf{0} \\ U \end{pmatrix}$ Lemma 5 implies that the integral

$$\int_0^\infty |\langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}}|^2 (Q(\lambda + i0) - Q(\lambda - i0))\, d\lambda$$

exists. Hence

$$\langle \Psi(\lambda), \mathbf{U} \rangle_{\mathbb{H}} \sqrt{\operatorname{Im} Q(\lambda + i0)} \in L^2(0, \infty).$$

So it remains to show that

$$\Psi(\lambda) \sqrt{\operatorname{Im} Q(\lambda + i0)} \in L^2(0, \lambda_0) \quad \text{for some } \lambda_0 > 0, \tag{65}$$

or, equivalently, that both the functions

$$\sqrt{\operatorname{Im} Q(\lambda + i0)} \quad \text{and} \quad \left(g_+(x, \lambda) - \frac{1}{d(\lambda + i0)} g(x, \lambda) \right) \sqrt{\operatorname{Im} Q(\lambda + i0)}$$

are integrable on the interval $(0, \lambda_0)$. Here the second function is just $\varrho \Phi$ and the other corresponds to the first component of Φ. Since g_+ and g_- are both entire functions in λ it is sufficient for (65) that both the functions

$$\sqrt{\operatorname{Im} Q(\lambda + i0)} \quad \text{and} \quad \frac{\sqrt{\operatorname{Im} Q(\lambda + i0)}}{|Q(\lambda + i0) + \cot \theta|} = \sqrt{\operatorname{Im} \frac{-1}{Q(\lambda + i0) + \cot \theta}}$$

belong to $L^2(0, \lambda_0)$. However, this follows directly from the fact that these functions are actually the densities of the spectral measures of the Nevanlinna functions Q and $\frac{-1}{Q}$, respectively. Note that here both functions have no generalized poles in $(0, \infty)$ and hence on this interval the measures are absolutely continuous with respect to the Lebesgue measure. Thus the transformation $\mathcal{I}$ in (63) is well defined. Next we show that actually $\mathcal{I}\mathbf{U} = \mathbf{U}$ for all $\mathbf{U} = \begin{pmatrix} \mathbf{0} \\ U \end{pmatrix}$ with $U \in C_0^\infty\big((0, \infty)\big)$. To this end note that Lemma 5 implies

$$\langle \mathcal{I}\mathbf{U}, \mathbf{V} \rangle_{\mathbb{H}} = \langle \mathbf{U}, \mathbf{V} \rangle_{\mathbb{H}} \tag{66}$$

for all $\mathbf{V} = \begin{pmatrix} \mathbf{v} \\ V \end{pmatrix}$ with $V \in C_0^\infty\big((0, \infty)\big)$. Considering, particularly, $\mathbf{V} = \begin{pmatrix} \mathbf{v} \\ 0 \end{pmatrix}$ implies that the first component of $\mathcal{I}\mathbf{U}$ has to be the zero vector in $\mathbb{C}^{n-2}$. Writing out (66) yields

$$\int_0^\infty \overline{\big((\mathcal{I}\mathbf{U})_{H_{n-2}} - U \big)(x)}\, b_{n-2}(L) V(x)\, dx = 0,$$

where the index H_{n-2} denotes the second component in the space $\mathbb{H}$. Since $b_{n-2}(L)V(x)$ can be an arbitrary $C_0^\infty\big((0,\infty)\big)$ function it follows that $(\mathcal{I}\mathbf{U})_{H_{n-2}}$

and U coincide as elements in L^2. But then the local uniform convergence of the integral in (63) implies that $(\mathcal{I}\mathbf{U})_{H_{n-2}}(x)$ is a continuous function and hence

$$(\mathcal{I}\mathbf{U})_{H_{n-2}}(x) = U(x) \qquad \text{for all } x \in (0, \infty).$$

In what follows we apply the embedding ϱ to the identity

$$\mathbf{U} = E_{\mathbb{L}_\theta}(\{0\})\mathbf{U} + \sum_{j=1}^{N(\theta)} \frac{\langle \Phi_j, \mathbf{U}\rangle_{\mathbb{H}}}{\langle \Phi_j, \Phi_j\rangle_{\mathbb{H}}} \Phi_j$$
$$+ \frac{1}{2\pi i} \int_0^\infty \langle \Psi(\lambda), \mathbf{U}\rangle_{\mathbb{H}} \Psi(\lambda) \frac{m(\lambda + i0) - m(\lambda + i0)}{b_{n-2}(\lambda)}\, d\lambda.$$

Then the left hand side obviously becomes $\varrho\mathbf{U} = U$. On the right hand side note that due to (41) for every eigenvalue $\lambda_j < 0$ it holds

$$\varrho\Phi_j = \varrho\Phi(\lambda_j) = \frac{1}{b_{n-2}(\lambda_j)} g(\,\cdot\,, \lambda_j)$$

and with the natural extension of ϱ to the generalized eigenfunctions one obtains

$$\varrho\Psi(\lambda) = \Psi(\lambda).$$

Note, furthermore,

$$\langle \Psi_j, \mathbf{U}\rangle_{\mathbb{H}} = \int_0^\infty (L - \lambda_j)^{-1} g_{n-2}(x)(b_{n-2}(L)U)(x)dx = \int_0^\infty g(x, \lambda_j)U(x)dx$$

and

$$\langle \Psi(\lambda), \mathbf{U}\rangle_{\mathbb{H}} = \int_0^\infty b_{n-2}(\lambda)\Psi(x, \lambda)U(x)dx = \int_0^\infty g(x, \lambda_j)U(x)dx.$$

Using the identity

$$b_{n-2}(\lambda_j)\langle \Psi_j, \Psi_j\rangle_{\mathbb{H}} = b_{n-2}(\lambda_j)Q'(\lambda_j) = d'(\lambda_j)$$

finally implies expansion (59). □

5 Concluding Remarks

Our approach using supersingular perturbations heavily relies on the asymptotic behavior of the special solutions g_+ and g_- close to the origin. However, besides the fact that (6) is in limit point case at ∞, these are the only properties of the differential expression (1) that are really used in the construction of the model (Sections 2 and 3). Hence the results actually hold true also for more general holomorphic potentials.

The natural question, which arises next, is whether the construction can also work for the even wider class of potentials considered in [17]. This, however, is work in progress.

Acknowledgements We thank the referee for careful reading of the manuscript and useful critical comments.

Appendix A: The Scale of Hilbert Spaces

Recall that if A is a semi-bounded, self-adjoint linear operator in a Hilbert space $\mathcal{H}$, $A \geqslant \gamma$ for some $\gamma \in \mathbb{R}$, then the scale of spaces $\mathcal{H}_s(A)$ associated with A is defined as follows. For $s \geqslant 0$ the space $\mathcal{H}_s(A)$ is given by the set $\operatorname{dom}(A-\mu)^{\frac{s}{2}}$ equipped with the norm

$$\|y\|_s := \|(A-\mu)^{\frac{s}{2}} y\|_{\mathcal{H}} \tag{67}$$

for some $\mu < \gamma$. However, it can easily be seen that this definition does not depend on μ and furthermore $\mathcal{H}_s(A)$ is complete with this norm. The space $\mathcal{H}_{-s}(A)$ is then defined as the dual of $\mathcal{H}_s(A)$ (with respect to the original space $\mathcal{H}$), it can also be obtained by completing $\mathcal{H}$ with respect to the norm (67). This gives a scale of spaces $\mathcal{H}_s(A) \subset \mathcal{H}_t(A)$ if $s > t$. However, in this note we are dealing with $s \in \mathbb{Z}$ only:

$$\ldots \subset \mathcal{H}_3(A) \subset \overset{\operatorname{dom}(A)}{\overset{\|}{\mathcal{H}_2(A)}} \subset \mathcal{H}_1(A) \subset \overset{\mathcal{H}}{\overset{\|}{\mathcal{H}_0(A)}} \subset \mathcal{H}_{-1}(A) \subset \overset{(\operatorname{dom}(A))^*}{\overset{\|}{\mathcal{H}_{-2}(A)}} \subset \mathcal{H}_{-3}(A) \subset \ldots$$

The notation $\langle \cdot, \cdot \rangle$ is used not only for the usual inner product on the space $\mathcal{H}$, but $\langle g, f \rangle$ denotes also the action of the functional $f \in \mathcal{H}_{-s}(A)$ on an element $g \in \mathcal{H}_s(A)$, $s > 0$. Note that $(A-\mu)^{-\frac{t}{2}}$ can be seen as an isometry from $\mathcal{H}_s(A)$ to $\mathcal{H}_{s+t}$. In particular, $\langle g, (A-\mu)^{\frac{t}{2}} f \rangle$ for $g \in \mathcal{H}_{s+t}$ and $f \in \mathcal{H}_{-s}$ is given by $\langle (A-\mu)^{\frac{t}{2}} g, f \rangle$.

Appendix B: Limit Circle Case

For completeness reasons and in order to establish a connection to the foregoing considerations in the 'singular' situation, we want to recall briefly also the 'regular' case $-\frac{1}{4} \leqslant q_0 < \frac{3}{4}$, in which Lemma 1 implies that the expression ℓ is in limit circle case also at the endpoint 0, see [15, 17] and e.g. [2, 27] for general results on rank one perturbations.

With the differential expression (1)

$$\ell(y)(x) = -y''(x) + \frac{q_0 + q_1 x}{x^2}\, y(x) \qquad \text{on } x \in (0, \infty)$$

there is associated the maximal operator $L_{\max}$ by

$$\operatorname{dom} L_{\max} := \{y \in L^2(0,\infty) \,|\, y, y' \in AC_{loc}(0,\infty),\ \ell(y) \in L^2(0,\infty)\} \tag{68}$$

and

$$(L_{\max}y)(x) := \ell(y)(x).$$

Since here we assume that ℓ is in limit circle case at one and in limit point case at the other endpoint the maximal operator $L_{\max}$ is the adjoint of a symmetric minimal operator $L_{\min}$ with defect one. Its domain is given by

$$\begin{aligned}\operatorname{dom} L_{\min} = \Big\{ y \in \operatorname{dom} L_{\max} \mid \lim_{x\to 0} W(y(x), g_+(x,\lambda_0))\\ = 0 \lim_{x\to 0} W(y(x), g_-(x,\lambda_0)) = 0 \Big\}.\end{aligned}$$

In this case $g(\,\cdot\,,\lambda) \in L^2(0,\infty)$ is a defect element of $L_{\min}$. Note that, in fact, $L_{\min}$ does not depend on the particular choice of $\bar{\mathrm{I}}\lambda_0$.

Remark 14 In case $x = 0$ is a regular endpoint the two expressions $\lim\limits_{x\to 0} W(y(x), g_+(x,\lambda_0))$ and $\lim\limits_{x\to 0} W(y(x), g_-(x,\lambda_0))$ can be written as $y(0)$ and $y'(0)$, respectively.

The self-adjoint extensions of $L_{\min}$ are given by L_τ for $\tau \in \mathbb{R}$ with

$$\operatorname{dom} L_\tau := \Big\{ y \in \operatorname{dom} L_{\max} | \lim_{x\to 0} W(y(x), g_+(x,\lambda_0) + \tau g_-(x,\lambda_0)) = 0 \Big\}$$

and

$$\operatorname{dom} L_\infty := \Big\{ y \in \operatorname{dom} L_{\max} | \lim_{x\to 0} W(y(x), g_-(x,\lambda_0)) = 0 \Big\}.$$

It is then a standard calculation to show that the following integral formulas for the resolvents hold:

$$\big((L_\tau - \lambda)^{-1} y\big)(x) = -g(x,\lambda) \int_0^x g_\tau(s,\lambda) y(s)\, ds - g_\tau(x,\lambda) \int_x^\infty g(s,\lambda) y(s)\, ds,$$

where $g_\tau(\,\cdot\,,\lambda) := \frac{1}{1-\tau m(\lambda)}(g_+(\,\cdot\,,\lambda) - \tau g_-(\,\cdot\,,\lambda))$ for $\tau \in \mathbb{R}$ and in the limit case $g_\infty(\,\cdot\,,\lambda) := \frac{1}{m(\lambda)} g_-(\,\cdot\,,\lambda)$. Furthermore, from this one obtains directly

$$(L_\tau - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{1}{m(\lambda) - \frac{1}{\tau}} \langle g(x,\overline{\lambda}),\,\cdot\,\rangle g(x,\lambda),$$

where $\langle\,\cdot\,,\,\cdot\,\rangle$ denotes the usual inner product in $L^2(0,\infty)$.

We introduce now the singular element $\varphi := (L_0 - \lambda_0) g(\,\cdot\,,\lambda_0)$ for some $\lambda_0 \in \mathbb{C}$. Note that $\varphi \notin L^2(0,\infty)$ since $g \notin \operatorname{dom} L_0$, however, $\varphi \in \mathcal{H}_{-2}(L_0)$.

With the formal expression

$$L_0 + t\langle\varphi,\,\cdot\,\rangle\varphi \qquad t \in \mathbb{R} \cup \{\infty\}$$

there is associated a family of self-adjoint operators L_γ given by

$$(L_\gamma - \lambda)^{-1} = (L_0 - \lambda)^{-1} - \frac{\langle (L_0 - \overline{\lambda})^{-1}\varphi,\,\cdot\,\rangle}{Q(\lambda) + \gamma}(L_0 - \lambda)^{-1}\varphi, \quad \gamma \in \mathbb{R} \cup \{\infty\},$$

where the Q-function is defined as

$$Q(\lambda) := (\lambda - \mu_1)\langle \varphi, (L_0 - \lambda)^{-1}(L_0 - \mu_1)^{-1}\varphi \rangle$$

with some $\mu_1 \in \rho(L_0) \cap \mathbb{R}$. It can easily be checked that $Q(\lambda) = m(\lambda) + c$ with some constant $c \in \mathbb{R}$, which fits as a well known special case to Theorem 2.

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