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A growth condition for Hamiltonian systems related with Kreĭn strings

Henrik Winkler and Harald Woracek

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Abstract. We study two-dimensional Hamiltonian systems of the form

$$(*)\qquad y'(x) = zJH(x)y(x), \quad x \in [s_-, s_+),$$

where the Hamiltonian H is locally integrable on $[s_-, s_+)$ and nonnegative, and $J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. The spectral theory of the equation changes depending on the growth of H towards the endpoint s_+; the classical distinction into the Weyl alternatives 'limit point' or 'limit circle' case. A refined measure for the growth of a limit point Hamiltonian H can be obtained by comparing with H-polynomials. This growth measure is concretised by a number $\Delta(H) \in \mathbb{N}_0 \cup \{\infty\}$ and appeared first in connection with a Pontryagin space analogue of the equation $(*)$. It is known that the growth restriction '$\Delta(H) < \infty$' has some striking consequences on the spectral theory of the equation; in many respects, the case 'limit point but still $\Delta(H) < \infty$' is similar to the limit circle case.
In general, the number $\Delta(H)$ is given in a rather implicit way, difficult to handle and not suitable for concrete calculations. In the present paper we provide a more accessible way to compute $\Delta(H)$ for some particular classes of Hamiltonians which occur in connection with Sturm–Liouville equations and Kreĭn strings.

1. Introduction

We consider two-dimensional Hamiltonian systems of differential equations of the form

$$y'(x) = zJH(x)y(x), \quad x \in [s_-, s_+)\,, \tag{1.1}$$

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where y is a 2-vector valued function, the Hamiltonian H takes real and nonnegative 2×2-matrices as values and is locally integrable on $[s_-, s_+)$, J denotes the signature matrix $J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and z is a complex number (the eigenvalue parameter). Equations of this form appear in natural sciences, for example as natural generalizations of Sturm–Liouville equations, see, e.g., [Re], [GKM], [At]. A vast literature is devoted to the study of operator models for the equation (1.1) and their spectral properties from different perspectives, see, e.g., [GK], [O], [dB2], [SN1], [SN2], [HS], [S]. Special emphasis, when studying problems of the kind, is put on inverse spectral problems, e.g., [K], [M2], [Ra].

The spectral properties of the equation (1.1) highly depend on the growth of the Hamiltonian H towards the endpoint s_+. The decisive distinction is between Weyl's limit circle and limit point cases, i.e., whether the integral $\int_{s_-}^{s_+} \operatorname{tr} H(x)\, dx$ is finite or infinite. For example, if the limit circle case prevails, solutions possess boundary values at s_+, the spectrum of the problem is discrete, and the sequences of positive and negative eigenvalues, (λ_n^+) and (λ_n^-), respectively, have regular asymptotics. In fact, the limits $\lim \frac{n}{\lambda_n^+}$ and $\lim \frac{n}{\lambda_n^-}$ exist in $[0, \infty)$ and coincide. On the other hand, if the limit point case takes place, continuous spectrum may occur.

In connection with the study of equations with singular potential, a generalization of the equation (1.1) and its operator model to an indefinite (Pontryagin space) setting was proposed in [KW/IV]. A corresponding version of Weyl's theory, including direct and inverse spectral theorems, was established in [KW/V, KW/VI]. In this generalization the Hamiltonian H is allowed to have a finite number of inner singularities. In addition, a finite number of scalar parameters may be specified which tell how passing a singularity influences the solution. At a singularity, the Hamiltonian function H is not anymore locally integrable (justifying the terminology 'singularity'), however, its growth is restricted. First, locally at a singularity, a certain compactness condition is required; resolvents should be of Hilbert–Schmidt class. Second, the rate of growth of H towards a singularity, measured by means of a number $\Delta(H) \in \mathbb{N} \cup \{\infty\}$ which is obtained by comparing with 'H-polynomials', should be finite.

Viewing the theory from a slightly different perspective, one may say the following:

> *Let H be a Hamiltonian as in* (1.1) *which is in the limit point case at s_+. Assume that selfadjoint realizations of the equation have resolvents of Hilbert–Schmidt class, and that the number $\Delta(H)$ is finite. Then H can be prolongued to an indefinite Hamiltonian $\mathfrak{h}$ in the sense of* [KW/IV]. *Moreover, this indefinite Hamiltonian $\mathfrak{h}$ may be chosen to be in the limit circle case at its right endpoint.*

Though $\mathfrak{h}$ is indefinite, the presence of the limit circle case has similar consequences on the spectral theory of the operator model associated with $\mathfrak{h}$ as known from the classical case. This, in turn, has consequences for the Hamiltonian H we started with in the above quoted statement. Among them the following facts:

- Solutions of equation (1.1) have 'H-polynomially'-regularized boundary values at s_+ (this is shown in the forthcoming manuscript [LaWo3]).
- Eigenvalues are distributed asymptotically according to $\lim \frac{n}{\lambda_n^+} = \lim \frac{n}{\lambda_n^-} \in [0,\infty)$ (this —and more— is shown in [W1, Theorem 4.8]).

Note here that, since H is in the limit point case, actual boundary values at s_+ do not always exist, and that the information on the distribution of eigenvalues which is immediately obtained from the compactness assumption is only $\sum \frac{1}{|\lambda_n^\pm|^{2+\varepsilon}} < \infty$, $\varepsilon > 0$.

An illustrative example (though, in some sense, being a toy example) occurs in connection with the Bessel equation.

Example 1.1. The Bessel equation is the Sturm–Liouville equation

$$-u''(x) + \frac{\nu^2 - 1/4}{x^2} u(x) = \lambda u(x),\ x > 0.$$

Here ν is a parameter $\nu > 1/2$ and λ is the eigenvalue parameter. Obviously, both endpoints 0 and ∞ are singular endpoints.

Rewriting this equation as a first-order-system, making a substitution in the independent variable, and setting $\alpha := 2\nu - 1$, $\lambda = z^2$, yields a Hamiltonian system (1.1) with

$$H_\alpha(x) := \begin{pmatrix} x^{-\alpha} & 0 \\ 0 & x^\alpha \end{pmatrix}, \quad x > 0\,.$$

At the endpoint ∞ always the limit point case prevails. Contrasting this, at the endpoint 0 the limit point case appears if and only if $\alpha \geq 1$. We are interested in a finer analysis of the behaviour at 0, hence, let us isolate this part of the equation: Set

$$\tilde{H}_\alpha(x) := \begin{pmatrix} (1-x)^{-\alpha} & 0 \\ 0 & (1-x)^\alpha \end{pmatrix}, \quad x \in [0,1)\,.$$

It turns out that the Hamiltonian $\tilde{H}_\alpha$ always satisfies the Hilbert–Schmidt condition, and that always $\Delta(\tilde{H}_\alpha) < \infty$, in fact

$$\Delta(\tilde{H}_\alpha) = \left\lfloor \frac{\alpha+1}{2} \right\rfloor . \tag{1.2}$$

Hence, via Pontryagin space theory, we obtain information on the behaviour of solutions and spectrum of the systems with Hamiltonian $\tilde{H}_\alpha$, and thereby gain knowledge about the behaviour of the Bessel equation at its singular endpoint 0.

This example of course only illustrates a *method*. A systematic treatment is given in the forthcoming paper [LaWo3]. The connection of the Bessel equation itself with the theory of indefinite Hamiltonian systems is worked out in detail in the forthcoming manuscript [LaWo4].

The questions appear how to recognize from a given Hamiltonian H whether or not the Hilbert–Schmidt property holds, and whether or not the number $\Delta(H)$ is finite. The first question was answered in [KW1]: Resolvents are of Hilbert–Schmidt type, if and only if a certain double integral involving the entries of H converges. The number $\Delta(H)$, however, can at present only be computed in a quite implicit way, namely from its actual definition, cf. Theorem 2.19. Our aim in the present paper is to provide a more explicit method to compute $\Delta(H)$ (and, in particular, to decide whether $\Delta(H)$ is finite) for some special classes of Hamiltonians. To be precise, we study Hamiltonians of diagonal form and Hamiltonians of (inverse) Stieltjes type[1]. For these classes we describe an inductive process to compute $\Delta(H)$, see Theorem 3.7 and Theorem 5.2.

From a practical viewpoint, the established inductive way to compute $\Delta(H)$ may on first sight seem only a slight improvement compared with the original definition. But, actually, it turns out to be very useful: For example, using Theorem 3.7 only a couple of lines are needed to obtain (1.2)[2], whereas proving this relation by going back to the original definition requires several pages of tedious computations.

From the viewpoint of applications, the classes of Hamiltonians under consideration are often sufficient. As for diagonal Hamiltonians: Each Sturm–Liouville equation can be rewritten as a system (1.1) with H being diagonal. For equations without a potential term, in particular for equations in impedance form, this is immediate; for equations in Schrödinger form, a suitable Liouville transform has to be applied (again we refer to the forthcoming manuscript [LaWo3]). As for (inverse) Stieltjes type Hamiltonians: Each Kreĭn string can immediately be rewritten as a system (1.1) with H being of inverse Stieltjes type; using the mass function of its dual string it can be rewritten as a system (1.1) with a Stieltjes type Hamiltonian (these transformations can be found in [KWW2]).

Let us point out an interesting connection with the recent work [FL]. In this paper a generalised Nevanlinna function is associated with a Sturm–Liouville equation having a singular potential of a certain form. It turns out that the negative index of this generalised Nevanlinna function is nothing but the number $\Delta(\tilde{H})$ for the Hamiltonian constructed from the potential in the same manner as in Theorem 1.1.

[1]For the definition of these classes see Definition 2.6.

[2]Compare with Step 2 of Theorem 3.15, where we elaborate a similar toy example.

The proof of this fact, however, is nontrivial and requires to combine results from [LaWo3] and [KW/IV].

We close this introduction with a brief description of the organisation of the paper. Section 2 has a mainly preliminary character. One, we set up our notation, and recall the classical theory as well as some more specific constructions and theorems up to the extent needed for the present exposition. Two, we provide several supplements and technical lemmas for later reference. After this preparation, in Section 3, we set off for the first main result of the paper: Theorem 3.7, where we show how to compute $\Delta(H)$ for a diagonal Hamiltonian H.

The class of diagonal Hamiltonians is closely related with the classes of (inverse) Stieltjes type Hamiltonians. In fact, (the operator model of) a diagonal Hamiltonian H can be decomposed in two parts, the 'even' and 'odd' parts of H. It is known that the even part corresponds to a Hamiltonian of Stieltjes type, the odd part to one of inverse Stieltjes type, and also converse constructions are available. This interaction between the classes of Hamiltonians often gives the possibility to transfer results, so also in the case of the 'growth measure Δ'. Our aim in Section 4 is to work out quantitatively the relation between the respective numbers Δ, cf. Theorem 4.1. Besides its intrinsic interest, this theorem is a major tool later on. The proposed proof is mainly elementary, by establishing and exploiting an instance of symmetry on the level of polynomials. The origin of the growth measure Δ, however, lies in Pontryagin space theory. Hence, we find it interesting that a (slightly weaker) version of Theorem 4.1 can also be deduced in a more structural but less elementary way from some theorems about indefinite Hamiltonians, cf. Theorem A.1. Since it is not within the scope of the present manuscript to dive into the indefinite world, we present this alternative approach as a supplement in an appendix.

In Section 5, we turn to (inverse) Stieltjes type Hamiltonians, and establish the second main result of the paper: The recursive computation method Theorem 5.2. Its proof relies on Theorem 4.1, which is used to reduce to Theorem 3.7.

2. Preliminaries and supplements about Hamiltonian systems

This section has a mainly preliminary character. We set up our notation, recall the known theory up to the required extent, and provide some supplements needed in the later sections. It is divided into several subsections according to the following schedule:

a. Hamiltonian systems and their operator models. We recall definitions and basic facts.
b. Weyl theory. We recall the definition of the Weyl coefficient associated with

a Hamiltonian system.

c. The operators $\mathcal{I}_H$ and $\mathring{A}_H$. Sometimes it is practical to work with a particular selfadjoint realization of the equation (1.1).
d. Compactness properties. We define and study Neumann–von Schatten class properties.
e. H-polynomials; the number $\Delta(H)$. We define the main object of our present interest: The number $\Delta(H)$ which provides a measure for the growth of the Hamiltonian H.
f. Decomposition of diagonal Hamiltonians into even and odd parts. Hamiltonians of diagonal form and their operator model can be decomposed into two parts. These parts correspond to Stieltjes- and inverse Stieltjes type Hamiltonians, respectively.
g. A lemma on general inverses. We provide a general statement which is frequently used. For example it is needed to justify the application of the substitution rule in some integrals when measures are not absolutely continuous.

a. Hamiltonian systems and their operator models

Let us explicitly state the definition of a Hamiltonian as we use it in the present text. Denote by ξ_ϕ the vector

$$\xi_\phi := \begin{pmatrix} \cos\phi \\ \sin\phi \end{pmatrix}.$$

Definition 2.1. A *Hamiltonian* H is a function defined on some interval $[s_-, s_+)$, $-\infty < s_- < s_+ \leq +\infty$, which takes real 2×2-matrices as values, and has the following properties:

(Ham1) Each entry of H is (Lebesgue-to-Borel) measurable and locally integrable on $[s_-, s_+)$.
(Ham2) We have $H(x) \geq 0$ almost everywhere on $[s_-, s_+)$.
(Ham3) The function H does not vanish on any set of positive measure.
(Ham4) The Hamiltonian H is not of the form

$$H(x) = \operatorname{tr} H(x)\cdot \xi_\phi \xi_\phi^T, \quad x\in[s_-, s_+) \text{ a.e.}, \tag{2.1}$$

with some constant $\phi\in\mathbb{R}$.

The requirements (Ham3) and (Ham4) are put to simplify the treatment technically. As it is shown, e.g., in [WW2, Proposition 4.2], (Ham3) is no loss in generality. The requirement (Ham4) is of course a restriction, but it is only a trivial case which is ruled out.

Intervals where the Hamiltonian is of the particularly simple form (2.1) play a special role: Let $(\alpha,\beta)\subseteq[s_-,s_+)$. Then we call (α,β) an *H-indivisible interval of type $\phi\in\mathbb{R}$*, if

$$H(x)=\operatorname{tr}H(x)\cdot\xi_\phi\xi_\phi^T,\ x\in(\alpha,\beta)\text{ a.e.}$$

In this case the number $\int_\alpha^\beta\operatorname{tr}H(x)\,dx\in[0,\infty]$ is called the *length* of this indivisible interval. Clearly, if two indivisible intervals have nonempty intersection, their types must coincide (up to integer multiples of π) and their union is again indivisible. Hence, each indivisible interval is contained in a maximal indivisible interval.

The equation (1.1) gives rise to an operator model which consists of a Hilbert space, a maximal differential relation in this space, and boundary value maps. First, the space and operator:

Definition 2.2. Let H be a Hamiltonian defined on the interval $[s_-,s_+)$. If $f,g\colon[s_-,s_+)\to\mathbb{C}^2$ are measurable functions, then we write $f=_H g$, if $Hf=Hg$ a.e. Clearly, the relation $=_H$ is an equivalence relation.

We denote by $L^2(H)$ the linear space of all $=_H$-equivalence classes $\hat f$ of measurable functions $f\colon[s_-,s_+)\to\mathbb{C}^2$, which satisfy:

$$\int_{s_-}^{s_+}f(t)^*H(t)f(t)\,dt<\infty\,. \tag{L2}$$

If (α,β) is H-indivisible of type ϕ, then $\xi_\phi^T f$ is constant a.e. on (α,β). (C)

An inner product is defined on $L^2(H)$ as

$$(\hat f,\hat g)_H:=\int_{s_-}^{s_+}g(t)^*H(t)f(t)\,dt,\quad \hat f=[f]_{=_H},\hat g=[g]_{=_H}\,.$$

A linear relation $T_{\max}(H)$ acting in $L^2(H)$ is defined as

$$\begin{aligned}T_{\max}(H):=\{(\hat f;\hat g)\in L^2(H)\times L^2(H)\\ :\hat f=[f]_{=_H},\hat g=[g]_{=_H}\text{ with } f \text{ absolutely continuous},\\ f'=JHg\text{ a.e. on }[s_-,s_+)\}\,.\end{aligned}$$

Moreover, we set $T_{\min}(H):=T_{\max}(H)^*$.

Unless necessary, we suppress the explicit distinction between $=_H$-equivalence classes and their representatives. Let us recall that, due to our requirement (**??**), for each $(\hat f;\hat g)\in T_{\max}(H)$ there exists a unique absolutely continuous representative with $f'=JHg$, cf. [HSW, Lemma 3.5].

The operator theoretic properties of $T_{\max}(H)$, in particular also the definition of boundary value maps, depend on the growth of H towards its endpoints. One says that Weyl's limit circle case prevails, if the entries of H are even integrable on $[s_-, s_+]$. Equivalently, this means that

$$\int_{s_-}^{s_+} \operatorname{tr} H(x)\, dx < \infty .$$

Otherwise, one speaks of Weyl's limit point case. In order to shorten language, we use the (also common) terminology 'regular' and 'singular', instead of 'Weyl's limit circle case' and 'Weyl's limit point case'.

To each element of $T_{\max}(H)$ boundary values can be assigned at the endpoint s_-. In fact, if $(\hat{f};\hat{g}) \in T_{\max}(H)$, then there exists a unique absolutely continuous representative f of $\hat{f}$, and this representative has an absolutely continuous extension to $[s_-, s_+)$. If H is regular, also at the endpoint s_+ boundary values can be assigned. In this case, the absolutely continuous representative has an absolutely continuous extension to all of $[s_-, s_+]$, cf. [HSW, Lemma 3.5].

Definition 2.3. Let H be a Hamiltonian defined on the interval $[s_-, s_+)$.

Case H regular: We define $\Gamma_{H,1}, \Gamma_{H,2} \colon T_{\max}(H) \to \mathbb{C}^2$ as

$$\Gamma_{H,1}(f;g) := \begin{pmatrix} f_1(s_-) \\ f_1(s_+) \end{pmatrix},\ \Gamma_{H,2}(f;g) := \begin{pmatrix} -f_2(s_-) \\ f_2(s_+) \end{pmatrix}, \quad (f;g) \in T_{\max}(H),$$

where we understand by $f = (f_1, f_2)^T$ the unique representative which is absolutely continuous on $[s_-, s_+]$.

Case H singular: We define $\Gamma_{H,1}, \Gamma_{H,2} \colon T_{\max}(H) \to \mathbb{C}$ as

$$\Gamma_{H,1}(f;g) := f_1(s_-),\ \Gamma_{H,2}(f;g) := -f_2(s_-), \quad (f;g) \in T_{\max}(H),$$

where we understand by $f = (f_1, f_2)^T$ the unique representative which is absolutely continuous on $[s_-, s_+)$.

In the next statement we summarize some essential properties of this operator model. Proofs of these facts can be found, e.g., in [HSW].

Theorem 2.4. *Let H be a Hamiltonian defined on the interval $[s_-, s_+)$.*

(i) *The space $L^2(H)$ endowed with the inner product $(.,.)_H$ is a Hilbert space.*

(ii) *The linear relation $T_{\min}(H)$ is a closed symmetric operator. The linear relation $T_{\max}(H)$ is closed.*

Case H regular: The operator $T_{\min}(H)$ *is completely nonselfadjoint, entire*[3], *and has defect index* $(2,2)$. *The triple* $\langle \mathbb{C}^2; \Gamma_{H,1}, \Gamma_{H,2}\rangle$ *is an (ordinary) boundary triplet*[4] *for* $T_{\max}(H)$.

Case H singular: The operator $T_{\min}(H)$ *is completely nonselfadjoint and has defect index* $(1,1)$. *Canonical selfadjoint extensions of* $T_{\min}(H)$ *have simple spectrum. The triple* $\langle \mathbb{C}; \Gamma_{H,1}, \Gamma_{H,2}\rangle$ *is an (ordinary) boundary triplet for* $T_{\max}(H)$.

Of course, 'changes of scale' in the equation (1.1) will not affect the spectral theory of the associated differential relation. The notion of 'changes of scale', however, needs to be defined rigorously.

Definition 2.5. Let H_1 and H_2 be two Hamiltonians defined on respective intervals $[s_-^1, s_+^1)$ and $[s_-^2, s_+^2)$. Then H_1 and H_2 are called *reparametrizations* of each other, if there exists an absolutely continuous and increasing bijection $\varphi\colon [s_-^2, s_+^2) \to [s_-^1, s_+^1)$ with φ^{-1} also being absolutely continuous, such that

$$H_2(x) = H_1(\varphi(x)) \cdot \varphi'(x), \quad x \in [s_-^2, s_+^2)\,.$$

In this case, we write $H_1 \sim H_2$.

Clearly, the relation '$\sim$' is an equivalence relation. Moreover, it is not difficult to show that $H_1 \sim H_2$ implies that the corresponding boundary triplets are isomorphic, see, e.g., [WW2, Theorem 3.8] for a general account on reparametrizations.

Notational convention. Unless specified differently, the symbol 'H' denotes a Hamiltonian defined on an interval $[s_-, s_+)$.

Let us now define the classes of Hamiltonians which we deal with in the present paper. It is clear what is meant by a diagonal Hamiltonian, namely, H is said to be diagonal, if its off-diagonal entries vanish a.e..

Notational convention. Unless explicitly specified differently, we write a diagonal Hamiltonian H as

$$H(x) = \begin{pmatrix} h_1(x) & 0 \\ 0 & h_2(x) \end{pmatrix}.$$

Definition 2.6. We call H of *Stieltjes type*, if there exists a nonincreasing function $\phi\colon [s_-, s_+) \to [0, \frac{\pi}{2}]$, such that

$$H(x) = \operatorname{tr} H(x) \cdot \xi_{\phi(x)} \xi_{\phi(x)}^T, \quad x \in [s_-, s_+) \text{ a.e.} \tag{2.2}$$

[3]In the sense of M. G. Kreĭn, see, e.g., [GG, §2.5].

[4]For the definition of boundary triplets and some theory see, e.g., [DHMS, Definition 3.13] and the references therein.

We call H of *inverse Stieltjes type*, if there exists a nonincreasing function $\phi\colon [s_-, s_+) \to [-\frac{\pi}{2}, 0]$, such that (2.2) holds.

Recall that a function q is said to belong to the Stieltjes class, if
(S1) q is analytic in $\mathbb{C} \setminus [0, \infty)$;
(S2) $q(x) > 0$ for $x \in (-\infty, 0)$;
(S3) $\operatorname{Im} q(z) \geq 0$ for $z \in \mathbb{C}^+$.
Some properties of this class of functions, including integral representations, were established in [KK1].

b. Weyl theory

Denote by $W_H(x; z)$, $x \in [s_-, s_+)$, the unique solution of the initial value problem

$$\begin{cases} \frac{\partial}{\partial x} W_H(x; z)J = zW_H(x; z)H(x), & x \in [s_-, s_+), \\ W_H(s_-; z) = I. \end{cases}$$

We refer to $W_H(x, z)$ as the fundamental solution for H, though, strictly speaking, it is the transposed of the fundamental solution of (1.1). For each fixed $x \in [s_-, s_+)$, the function $W_H(x, .)$ is an entire matrix function of finite exponential type. Each entry $w_{ij}(x, .)$ of $W_H(x, .)$ is of bounded type in the upper and lower half-planes, and its exponential type can be computed as

$$\int_{s_-}^{x} \sqrt{\det H(t)}\, dt\,, \tag{2.3}$$

cf. [dB1, Theorem X].

If H is regular, the limit $W_H(s_+, z) := \lim_{x \nearrow s_+} W_H(x, z)$ exists locally uniformly on $\mathbb{C}$. We refer to $W_H(s_+, z)$ as the monodromy matrix of H. It is again an entire function of finite exponential type, and the formula (2.3) holds also for '$x = s_+$'. The monodromy matrix governs the spectral theory of the differential relation associated with H, in fact, all spectral functions can be constructed explicitly from $W_H(s_+, z)$.

Let us further discuss the singular case. In this case, the spectral theory of the operator model associated with H is governed by the Weyl coefficient q_H associated with H. Classically, this function is constructed by means of Weyl's limit point procedure: Write again $W_H(x; .) = (w_{ij}(x; .))_{i,j=1}^2$. Then, for each $\tau \in \mathbb{R} \cup \{\infty\}$, the limit

$$\lim_{x \nearrow s_+} \frac{w_{11}(x; z)\tau + w_{12}(x; z)}{w_{21}(x; z)\tau + w_{22}(x; z)} =: q_H(z)$$

exists locally uniformly on $\mathbb{C} \setminus \mathbb{R}$, and its value does not depend on τ. Thereby, for $\tau = \infty$, we understand the quotient as $w_{11}(t; z)/w_{21}(t; z)$.

Alternatively, q_H can be obtained as the Weyl m-function of the boundary triplet associated with H; sometimes this viewpoint is more practical.

The Weyl coefficient q_H associated with a singular Hamiltonian H is a function belonging to the Nevanlinna class and not equal to a real constant, i.e. it satisfies

(N1) q_H is analytic in $\mathbb{C} \setminus \mathbb{R}$;
(N2) $q_H(\overline{z}) = \overline{q_H(z)}$ for $z \in \mathbb{C} \setminus \mathbb{R}$;
(N3) $\operatorname{Im} q_H(z) > 0$ for $z \in \mathbb{C}^+$.

It is a fundamental result due to de Branges that, conversely, for each function q of Nevanlinna class, there exists (up to reparameterization) one and only one singular Hamiltonian H such that q is the Weyl coefficient of H, cf. [dB2], or [W1] for a more explicit presentation.

The significance of the function q_H for the spectral theory of the operator model associated with H is that it gives rise to a Fourier transform of $L^2(H)$ onto a space $L^2(\sigma)$ (or $L^2(\sigma)\oplus\mathbb{C}$ if H starts with an indivisible interval of type 0). Namely, by choosing for σ the measure in the Herglotz integral representation of q_H, and using the transformation $f \mapsto \hat{f}$ given as

$$\hat{f}(z) := \int_{s_-}^{s_+} (0,1) W_H(x;z) H(x) f(x)\, dx\,,$$

when $f \in L^2(H)$ has compact support in $[s_-, s_+)$.

Items (ii) and (iii) of the next result motivate the choice of terminology in Definition 2.6. These items follow from [W2] together with [WW1]; we skip details. Item (i) is a classical fact, and can be found, e.g., in [dB2, §47].

Proposition 2.7.

(i) *The Weyl coefficient q_H of H is an odd function, if and only if H is diagonal.*
(ii) *The Weyl coefficient q_H of H belongs to the Stieltjes class, if and only if H is of Stieltjes type.*
(iii) *The function $-1/q_H$ belongs to the Stieltjes class, if and only if H is of inverse Stieltjes type.*

c. The operators $\mathcal{I}_H$ and $\mathring{A}_H$

Clearly, the resolvents of selfadjoint extensions of $T_{\min}(H)$ can be expressed as integral operators.

Definition 2.8. We denote by $\mathcal{I}_H$ the operator whose domain $\operatorname{dom} \mathcal{I}_H$ consists of all measurable functions $f\colon [s_-, s_+) \to \mathbb{C}^2$ with

$$Hf \in L^1_{\text{loc}}([s_-, s_+))\,,$$

and which acts as

$$(\mathcal{I}_H f)(x) := \int_{s_-}^{x} JH(t)f(t)\,dt\,.$$

The following properties of $\mathcal{I}_H$ are obvious.

Lemma 2.9.

(i) *We have* $L^\infty_{\mathrm{loc}}([s_-, s_+)) \subseteq \operatorname{dom}\mathcal{I}_H$.

(ii) *For each* $f \in \operatorname{dom}\mathcal{I}_H$, *the function* $\mathcal{I}_H f$ *is absolutely continuous on* $[s_-, s_+)$. *In particular, for each* $f \in \operatorname{dom}\mathcal{I}_H$, *all iterates* $\mathcal{I}_H^k f$, $k \in \mathbb{N}$, *are defined.*

(iii) *For each* $f \in \operatorname{dom}\mathcal{I}_H$, *the function* $\mathcal{I}_H f$ *satisfies* (C).

It is often useful to work with a particular selfadjoint extension of $T_{\min}(H)$.

Lemma 2.10. *Assume that* H *is singular, and that* 0 *is a point of regular type of* $T_{\min}(H)$.

(i) *Let* A *be a selfadjoint extension of* $T_{\min}(H)$ *such that* $0 \in \rho(A)$. *Then*

$$(A^{-1}f)(x) = (\mathcal{I}_H f)(x) + \Gamma(H)(A^{-1}f; f)\,. \tag{2.4}$$

(ii) *There exists a unique angle* $\phi(H) \in [0, \pi)$, *such that* $\xi_{\phi(H)} \in L^2(H)$.

Denote by $\mathring{A}_H$ *the selfadjoint extension defined by the boundary condition*

$$\Gamma(H)\mathring{A}_H = \operatorname{span}\{\xi_{\phi(H)+\frac{\pi}{2}}\}\,.$$

(iii) *We have* $0 \in \rho(\mathring{A}_H)$. *The value of* $\Gamma(H)(\mathring{A}_H^{-1} f; f)$ *can be computed as*

$$\Gamma(H)(\mathring{A}_H^{-1} f; f) = \big(-\lim_{x\nearrow s_+} \xi^T_{\phi(H)+\frac{\pi}{2}}(\mathcal{I}_H f)(x)\big)\xi_{\phi(H)+\frac{\pi}{2}}\,.$$

Proof. Both functions $A^{-1}f$ and $\mathcal{I}_H f$ are absolutely continuous on $[s_-, s_+)$ and have derivative JHf. Hence, they differ only by a constant. Evaluating the limit $x \searrow s_-$ gives (2.4).

Since 0 is a point of regular type for $T_{\min}(H)$, a selfadjoint extension A of $T_{\min}(H)$ satisfies either $0 \in \rho(A)$ or $0 \in \sigma_p(A)$. Moreover, since the defect index of $T_{\min}(H)$ equals $(1, 1)$, the second case takes place for exactly one extension A_0, and $\dim\ker A_0 = 1$. However, $\ker T_{\max}(H) \subseteq \mathbb{C}^2$. The assertion in (ii) follows. Moreover, we see that the extension A_0 is given by the boundary condition

$$\Gamma(H)A_0 = \operatorname{span}\{\xi_{\phi(H)}\}\,.$$

To obtain the formula asserted in (iii), we multiply (2.4) with $\xi^T_{\phi(H)+\frac{\pi}{2}}$ from the left. Since $\xi_{\phi(H)+\frac{\pi}{2}} = -\xi_{\phi(H)}J$ and $\Gamma(H)(\mathring{A}_H^{-1} f; f) = \alpha\xi_{\phi(H)+\frac{\pi}{2}}$ with some $\alpha \in \mathbb{C}$, this gives

$$-\xi^T_{\phi(H)}J(\mathring{A}_H^{-1} f) = \xi^T_{\phi(H)+\frac{\pi}{2}}(\mathcal{I}_H f) + \alpha\,.$$

Applying [HSW, Theorem 3.6] with

$$(\xi_{\phi(H)}; 0), (\mathring{A}_H^{-1} f; f) \in T_{\max}(H)\,,$$

shows that the left side of this relation tends to 0 as x increases to s_+. ■

d. Compactness properties

We denote the ideal of all compact operators by $\mathfrak{S}_\infty$. For each $p \in (0, \infty)$ we denote by $\mathfrak{S}_p$ the Neumann–von Schatten class of all compact operators whose s-numbers belong to ℓ^p.

Definition 2.11. Let $p \in (0, \infty]$. We say that H has the property $\mathfrak{S}_p$, if for some (and hence for each) selfadjoint extension A of $T_{\min}(H)$, and for one (and hence for all) points $z \in \rho(A)$

$$(A - z)^{-1} \in \mathfrak{S}_p\,.$$

In the present context, mainly the cases '$p = \infty$', '$p = 2$', and '$p = 1$' appear. For these we also use the terminology 'compact resolvents', 'Hilbert–Schmidt property', and 'trace class property', respectively. Notice that, by isomorphy of boundary triplets, the fact whether or not a Hamiltonian H has the property $\mathfrak{S}_p$ does not depend on the choice of parameterization.

In general, it is an open problem to characterize validity of the property $\mathfrak{S}_p$ in terms of the Hamiltonian H itself. To the best of our knowledge, this problem has been solved only for the case '$p = 2$'[5]. The result reads as follows:

Theorem 2.12. *Let H be a Hamiltonian defined on the interval $I = (s_-, s_+)$ which is regular at s_- and singular at s_+, and set $G(x) := \int_{s_-}^x H(t)\,dt$. Then H has the Hilbert–Schmidt property if and only if there exists an angle $\phi(H) \in [0, \pi)$ with*

$$\int_{s_-}^{s_+} \xi^T_{\phi(H)} H(t) \xi_{\phi(H)}\,dt < \infty\,, \tag{2.5}$$

$$\int_{s_-}^{s_+} \xi^T_{\phi(H)+\frac{\pi}{2}} G(t) \xi_{\phi(H)+\frac{\pi}{2}} \xi^T_{\phi(H)} H(t) \xi_{\phi(H)}\,dt < \infty\,. \tag{2.6}$$

[5] For the case '$p = \infty$' some necessary and some sufficient conditions which are not too far apart from each other are stated without a proof in [K].

A proof for trace normed Hamiltonians, i.e. Hamiltonians with $\operatorname{tr} H(x) \equiv 1$ defined on $(0,\infty)$, is given [KW1]. Each Hamiltonian can be brought to this form with a reparameterization, see, e.g., [WW2, Proposition 4.2]. It remains to notice that the conditions (2.5) and (2.6) do not depend on the choice of a parameterization: Assume that H_1 and H_2 are Hamiltonians defined on intervals $I_1=(s_-^1,s_+^1)$ and $I_2=(s_-^2,s_+^2)$, respectively, which are related as $H_2(x)=H(\varphi(x))\varphi'(x)$ with some increasing bijection $\varphi\colon I_2\to I_1$ such that φ and φ^{-1} are absolutely continuous. Then, for each $\phi\in[0,\pi)$,

$$\int_{s_-^2}^{s_+^2}\xi_\phi^T H_2(y)\xi_\phi\,dy=\int_{s_-^2}^{s_+^2}\xi_\phi^T H_1(\varphi(y))\xi_\phi\cdot\varphi'(y)\,dy=\int_{s_-^1}^{s_+^1}\xi_\phi^T H_1(x)\xi_\phi\,dx\,.$$

Similarly,

$$\int_{s_-^2}^{s_+^2}\xi_{\phi+\frac{\pi}{2}}^T G_2(y)\xi_{\phi+\frac{\pi}{2}}\xi_\phi^T \hat{H}_2(y)\xi_\phi\,dy=\int_{s_-^1}^{s_+^1}\xi_{\phi+\frac{\pi}{2}}^T G_1(x)\xi_{\phi+\frac{\pi}{2}}\xi_\phi^T H_1(x)\xi_\phi\,dx\,,$$

where G_i, $i=1,2$, is defined correspondingly as $G_i(t):=\int_{s_-^i}^t H_i(s)\,ds$.

For a regular Hamiltonian validity of $\mathfrak{S}_p$ is related to the growth of its fundamental solution as an entire function, whereas for a singular Hamiltonian it is related to the distribution of the poles of the Weyl coefficient q_H. These are well-known facts, however, let us make the connection explicit.

Proposition 2.13. *The following hold:*

(i) *Assume that H is singular, and let q_H be the Weyl coefficient of H. Then H has the property $\mathfrak{S}_\infty$ if and only if q_H is meromorphic in the whole plane. In this case, H has the property $\mathfrak{S}_p$ if and only if $\sum\frac{1}{|\lambda_n|^p}<\infty$, where (λ_n) denotes the sequence of poles of q_H.*

(ii) *Assume that H is regular. Then H has the property $\mathfrak{S}_\infty$. Let $W_H(s_+,z)$ be the monodromy matrix of H. If $\rho\geq 0$, and one entry of $W_H(s_+;.)$ is an entire function of order ρ, then H has the property $\mathfrak{S}_p$ whenever $p>\rho$.*

Proof. *Item* (i): The Weyl coefficient q_H is a Q-function of a certain selfadjoint extension $\mathring{A}$ of $T_{\min}(H)$, see, e.g., [HSW, Theorem 4.3]. Thus the set of its poles equals the spectrum of $\mathring{A}$, remember here that $T_{\min}(H)$ is completely nonselfadjoint. For more details see the argument carried out in the proof of [KW1, Theorem 3.1].

Item (ii): Assume that one entry of $W_H(s_+;.)$ has order ρ. By [BP], see also [BW, Proposition 2.3], the entries of $W_H(s_+;.)$ all have the same order. In particular, $w_{21}(s_+;.)$ is an entire function of order ρ.

The function $\frac{w_{11}(s_+;z)}{w_{21}(s_+;z)}$ is a Q-function of some selfadjoint extension A of $T_{\min}(H)$, and its poles coincide with the zeros of $w_{21}(s_+;z)$. We see that the spectrum of A equals the sequence of zeros of some entire function of order ρ. Hence, the convergence exponent of this sequence does not exceed ρ. ■

The next statement turns out to be useful. To simplify language, we agree on the following convention: If H is a function of the form (2.1), possibly with $s_- = s_+$ (i.e., with empty domain), we say that H has the property $\mathfrak{S}_p$ for each $p \in (0,\infty]$.

Proposition 2.14. *Let $p \in (0,\infty]$, $s_0 \in [s_-, s_+)$, and denote $H_- := H|_{[s_-,s_0)}$ and $H_+ := H|_{[s_0,s_+)}$. Then H has the property $\mathfrak{S}_p$ if and only if both H_+ and H_- have.*

Proof. *Step* 1*; The core argument*: Consider the case that

- ⋆ H does not end indivisibly towards s_- or towards s_+.
- ⋆ s_0 is not an inner point of some indivisible interval.

Then we have $L^2(H) = L^2(H_-) \oplus L^2(H_+)$, and

$$T_{\min}(H_-) \oplus T_{\min}(H_+) \subseteq T_{\min}(H)\,.$$

Let A_- and A_+ be selfadjoint extensions of $T_{\min}(H_-)$ and $T_{\min}(H_+)$, respectively, and set $\mathring{A} := A_- \oplus A_+$. Then the resolvents of A belong to $\mathfrak{S}_p$ if and only if the resolvents of both, A_- and A_+, have this property.

Let A be a selfadjoint extension of $T_{\min}(H)$, and let $z \in \rho(A) \cap \rho(\mathring{A})$. Then $(A-z)^{-1}$ is a finite-dimensional perturbation of $(\mathring{A}-z)^{-1}$, and hence $(A-z)^{-1} \in \mathfrak{S}_p$ if and only if $(\mathring{A} - z)^{-1} \in \mathfrak{S}_p$.

Step 2*; Indivisible ends*: Let us first consider the case that (s_-, s_0) is maximal indivisible. If H is regular at s_-, then $L^2(H) = L^2(H|_{(s_-,s_+)}) \oplus \mathbb{C}$ and $T_{\min}(H)$ is a one-dimensional extension of $T_{\min}(H|_{(s_0,s_+)})$. Hence, H has the property $\mathfrak{S}_p$ if and only if $H|_{(s_0,s_+)}$ has. If H is singular at s_-, then $L^2(H) = L^2(H|_{(s_-,s_+)})$ and $T_{\min}(H)$ is a one-dimensional extension of $T_{\min}(H|_{(s_0,s_+)})$. Again, H has the property $\mathfrak{S}_p$ if and only if $H|_{(s_0,s_+)}$ has.

Next, consider the case that (s_-, s_0) is (not necessarily maximal) indivisible. Denote by s_0' the right endpoint of the maximal indivisible interval with left endpoint s_-. By what we just showed, the following equivalences hold:

$$H \text{ has } \mathfrak{S}_p \iff H|_{(s_0',s_+)} \text{ has } \mathfrak{S}_p \iff H|_{(s_0,s_+)} \text{ has } \mathfrak{S}_p.$$

The case that (s_0, s_+) is indivisible is settled in the same way.

Step 3*; The general case*: Denote by s_-^r the right endpoint of the maximal indivisible interval with left endpoint s_-, by s_+^l the left endpoint of the maximal indivisible interval with right endpoint s_+, and by s_0^l and s_0^r the left and right endpoints of the maximal indivisible interval which contains s_0 in its closure.

By what we showed in Steps 1 and 2, we have the following equivalences:

$$H \text{ has } \mathfrak{S}_p \iff H|_{(s_-^r,s_+^l)} \text{ has } \mathfrak{S}_p \iff H|_{(s_-^r,s_0^l)}, H|_{(s_0^l,s_+^l)} \text{ have } \mathfrak{S}_p$$
$$\iff H|_{(s_-,s_0)}, H|_{(s_0^r,s_+^l)} \text{ have } \mathfrak{S}_p \iff H|_{(s_-,s_0)}, H|_{(s_0,s_+)} \text{ have } \mathfrak{S}_p. \blacksquare$$

We can now deduce that some kinds of Hamiltonians always enjoy certain Neumann-von Schatten class properties.

Proposition 2.15. *Assume that H is regular or ends with an indivisible interval towards s_+. Then*

(i) *H has the property $\mathfrak{S}_p$ whenever $p > 1$.*

(ii) *If H has the trace-class property, then* $\det H$ *vanishes a.e.*

Assume in addition that H is of (inverse) Stieltjes type. Then

(iii) *H has the property $\mathfrak{S}_p$ whenever $p > \frac{1}{2}$.*

Proof. *Item* (i): If H is regular, its monodromy matrix if of finite exponential type, in particular, of order 1. If H is singular but ends indivisibly towards s_+, its Weyl coefficient can be written as the quotient of two entire functions with finite exponential type. This shows (i).

Item (ii): Assume that H has the trace-class property, and let $s_0 \in [s_-, s_+)$. Then $H|_{[s_-,s_0)}$ also has the trace-class property. Let $w_{ij}(x,z)$ be the entries of the monodromy matrix of $H|_{[s_-,s_0)}$. Then, using (2.3) and [Bo, Chapter 8], we obtain that the sequence of positive zeros (λ_n) of $w_{ij}(s_0,.)$ satisfies

$$\lim_{n\to\infty} \frac{n}{\lambda_n} = \frac{1}{\pi} \int_{s_-}^{s_0} \sqrt{\det H(t)}\, dt\,.$$

Convergence of the series $\sum_n \frac{1}{\lambda_n}$ thus implies that $\det H(x) = 0$, $x \in [s_-, s_0)$ a.e. Since s_0 was arbitrary, the assertion (ii) follows.

Item (iii): Consider the case that H is regular, and let W be its monodromy matrix. Appending an indivisible interval of type $\phi(s_+)$ and infinite length gives a singular Hamiltonian $\tilde{H}$ which is again of (inverse) Stieltjes type. The Weyl coefficient $q_{\tilde{H}}$ belongs to the (inverse) Stieltjes class, in particular is analytic on $\mathbb{C} \setminus [0,\infty)$. However, $q_{\tilde{H}} = W \star \cot\phi(s_+)$. Since the poles of $W \star \cot\phi(s_+)$ interlace with the poles of $W \star \infty$, the right lower entry of W has at most one pole on $(-\infty, 0)$. An application of [KWW1, Proposition 3.12] yields that the order of W cannot exceed $1/2$. It follows that H has the property $\mathfrak{S}_p$ whenever $p > 1/2$.

Assume that H is singular and ends indivisible towards s_+. Let $s_0 \in [s_-, s_+)$ be such that (s_0, s_+) is maximal indivisible, and consider the regular Hamiltonian

$\tilde{H} := H|_{[s_-,s_0)}$. Then $\tilde{H}$ is of Stieltjes type, and the above proved shows that $\tilde{H}$ has the property $\mathfrak{S}_p$ for all $p > 1/2$. By Theorem 2.14, H inherits this. ∎

Combining Theorem 2.14 with Theorem 2.15, it follows that certain Neumann–von Schatten class properties are local properties at the singular endpoint.

Corollary 2.16. *Let $s_0 \in [s_-, s_+)$ and $p \in (0, \infty]$.*

(i) *If $p > 1$, the Hamiltonian H has the property $\mathfrak{S}_p$ if and only if $H|_{[s_0,s_+)}$ has.*

(ii) *Assume that H is of (inverse) Stieltjes type. If $p > 1/2$, the Hamiltonian H has the property $\mathfrak{S}_p$ if and only if $H|_{[s_0,s_+)}$ has.*

Remark 2.17. Let us notice that the fact that the Hilbert–Schmidt property is a local property, reflects in the conditions (2.5) and (2.6): Let $s_0, s_0' \in [s_-, s_+)$ and let $\tilde{G}$ be any original function of H. Then H satisfies (2.5) and (2.6), if and only if it satisfies

$$\int_{s_0}^{s_+} \xi_{\phi(H)}^T H(t) \xi_{\phi(H)} \, dt < \infty ,$$

$$\int_{s_0'}^{s_+} \xi_{\phi(H)+\frac{\pi}{2}}^T \tilde{G}(t) \xi_{\phi(H)+\frac{\pi}{2}} \xi_{\phi(H)}^T H(t) \xi_{\phi(H)} \, dt < \infty .$$

To see this, first note that we may substitute the interval (s_-, s_+) of integration by (s_0, s_+) and (s_0', s_+), respectively, since the respective integrands are locally integrable functions on $[s_-, s_+)$. Second, the functions $\tilde{G}$ and G, and hence also $\xi_{\phi(H)+\frac{\pi}{2}}^T \tilde{G}(t) \xi_{\phi(H)+\frac{\pi}{2}}$ and $\xi_{\phi(H)+\frac{\pi}{2}}^T G(t) \xi_{\phi(H)+\frac{\pi}{2}}$, differ only by an additive constant. In conjunction with (2.5), we therefore may substitute G by $\tilde{G}$ in (2.6), and obtain an equivalent set of conditions.

e. H-polynomials; the number $\Delta(H)$

We consider functions which are related to the differential relation $T_{\max}(H)$ in the same way as polynomials are related to $\frac{d}{dx}$. Denote by $\mathbb{C}^2[z]$ the polynomial ring in one indeterminate over the ring $\mathbb{C}^2$, and by $\mathrm{Ac}([s_-, s_+))$ the space of absolutely continuous functions on $[s_-, s_+)$.

Definition 2.18. Let $\gamma_H \colon \mathbb{C}^2[z] \to \mathrm{Ac}([s_-, s_+))$ be the map which acts as

$$\gamma_H\Big(\sum_{k=0}^{n} \binom{\alpha_k}{\beta_k} z^k\Big) := \sum_{k=0}^{n} \mathcal{I}_H^k \binom{\alpha_k}{\beta_k} .$$

We refer to each function of this form as an H-polynomial, and denote the set of all H-polynomials as $\mathrm{Pol}(H)$.

Definition 2.19. For $N \in \mathbb{N}_0$ set

$$\mathcal{P}_N := \left\{ \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{C}^2 : \text{There exist } \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix}, k = 0, \dots, N-1, \right.$$
$$\left. \text{such that } \mathcal{I}_H^N \begin{pmatrix} \alpha \\ \beta \end{pmatrix} + \sum_{k=0}^{N-1} \mathcal{I}_H^k \begin{pmatrix} \alpha_k \\ \beta_k \end{pmatrix} \in L^2(H) \right\}.$$

Then we define a number $\Delta(H) \in \mathbb{N}_0 \cup \{\infty\}$ as

$$\Delta(H) := \inf\{N \in \mathbb{N}_0 : \dim \mathcal{P}_N = 2\},$$

where we understand the infimum of the empty set as ∞.

In general not much can be said about the behaviour of the spaces $\mathcal{P}_N$. However, putting some hypothesis on H, they behave regularly. The next lemma is shown in [KW/IV, §3] under the more restrictive hypothesis of the Hilbert–Schmidt property. However, inspecting the proofs given there, shows that what is really needed is only existence of a selfadjoint extension of $T_{\min}(H)$ having 0 in its resolvent set; we will not repeat details of the proof.

Lemma 2.20. *Assume that H is singular, and that 0 is a point of regular type of $T_{\min}(H)$.*

(i) *We have $\mathcal{P}_N \subseteq \mathcal{P}_{N+1}$, $N \in \mathbb{N}_0$. In particular, the set $\{N \in \mathbb{N}_0 : \dim \mathcal{P}_N = 2\}$ is either empty or the interval $[\Delta(H)+1, \infty)$.*

(ii) *Let $N \in \mathbb{N}_0$, then $\xi_{\phi(H)} \in \mathcal{P}_N$. Thus $\dim \mathcal{P}_N = 2$ if and only if $\xi_\phi \in \mathcal{P}_N$ for some $\phi \not\equiv \phi(H) \bmod \pi$.*

(iii) *Assume that $\Delta(H) < \infty$. Then there exist unique real constants ω_k, $k \in \mathbb{N}$, such that*

$$\mathfrak{w}_n := \mathcal{I}_H^n \xi_{\phi(H)+\frac{\pi}{2}} + \sum_{k=0}^{n-1} \omega_{n-k} \mathcal{I}_H^k \xi_{\phi(H)+\frac{\pi}{2}} \in L^2(H), \quad n \geq \Delta(H). \tag{2.7}$$

For each $n \geq \Delta(H)$, we have $\mathfrak{w}_{n+1} = \mathring{A}_H^{-1} \mathfrak{w}_n$.

We use the right side of (2.7) to define functions $\mathfrak{w}_n$ also for $n < \Delta(H)$, so that

$$\mathfrak{w}_n = \mathcal{I}_H^n \xi_{\phi(H)+\frac{\pi}{2}} + \sum_{k=0}^{n-1} \omega_{n-k} \mathcal{I}_H^k \xi_{\phi(H)+\frac{\pi}{2}} \in L^2(H), \quad n \in \mathbb{N}_0. \tag{2.8}$$

Remark 2.21. Let us state explicitly that the number $\Delta(H)$ does not depend on the choice of parameterization: If $H_1 \sim H_2$, then $\Delta(H_1) = \Delta(H_2)$. This is seen easily by making a change of variables in the integral defining $\mathcal{I}_H$; similar as in [KW/IV, Lemma 2.4, Remark 3.19].

One may say:

> *The number $\Delta(H)$ provides a comparatively fine measure for the growth of H towards the endpoint s_+.*

For the purpose of illustration, let us mention the following two facts:
(i) The Hamiltonian H is regular if and only if $\Delta(H) = 0$; this is obvious.
(ii) If H is singular and ends with an indivisible interval towards s_+, then $\Delta(H) = 1$; this is shown in [KW/IV, Lemma 3.2].
Also, remember Theorem 1.1.

The following fact sheds significant light on the meaning of $\Delta(H)$. This result is rather deep and proved in [LaWo2].

Theorem 2.22. *Let H be singular, and assume that selfadjoint extensions of $T_{\min}(H)$ have compact resolvents of Hilbert–Schmidt class, and that $\Delta(H) < \infty$. Denote by $\mathfrak{w}_n$ the functions (2.8).*

Then, whenever $z \in \mathbb{C}$ and $\psi(x; z)$ is a solution of the differential equation

$$y'(x) = zJH(x)y(x), \quad x \in (s_-, s_+),$$

the limits

$$\lim_{x \nearrow s_+} \xi^T_{\phi(H)} \psi(x; z) =: \rho$$
$$\lim_{x \nearrow s_+} \sum_{l=0}^{\Delta(H)} z^l \mathfrak{w}_l(x)^* J \Big(\psi(x; z) - \rho \sum_{k=\Delta(H)+1}^{2\Delta(H)-l} z^k \mathfrak{w}_k(x) \Big)$$

exist.

Clearly, the value ρ is a directional boundary value of the solution $\psi(x; z)$ at the singular endpoint s_+. The second limit is, in some sense, a polynomially regularized boundary value at s_+.

Remark 2.23. It is an interesting fact that finiteness of the number $\Delta(H)$ influences compactness properties. For example it follows from [W1, Theorem 4.8] (or on combining [LaWo1, Theorem 5.1] with [KW/III, Theorem 7.4]), that

$$H \text{ satisfies } \mathfrak{S}_2 \wedge \Delta(H) < \infty \quad \Rightarrow \quad H \text{ satisfies } \mathfrak{S}_p,\ p > 1.$$

In fact, one can see by inspecting the proofs in [KW/IV] that in this implication the hypothesis that H satisfies $\mathfrak{S}_2$ can be weakened to the requirement that it has compact resolvents. Tracing all proofs, however, is elaborate and actually not so simple, and has nowhere been done explicitly. Thus we will not use the mentioned fact in the present paper; we state it just as another illustration of the power of '$\Delta(H) < \infty$'.

It is an open question whether in general, or under the hypothesis that 0 is a point of regular type for $T_{\min}(H)$, the condition '$\Delta(H) < \infty$' already implies that H has compact resolvents.

f. Diagonal Hamiltonians and their decomposition into even and odd parts

Diagonal Hamiltonians behave much simpler than arbitrary ones. One reason is that many computations greatly simplify when off-diagonal entries are absent. Another reason is the presence of symmetry: Denote by $\mathfrak{i}_H$ the map which acts on 2-vector valued functions as

$$\mathfrak{i}_H \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} := J \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} -f_1 \\ f_2 \end{pmatrix}. \tag{2.9}$$

The following fact is seen by a simple computation; we skip explicit proof.

Lemma 2.24. *Let H be diagonal. Then $\mathfrak{i}_H$ induces an isometric isomorphism of $L^2(H)$ onto itself.*

Since $\mathfrak{i}_H$ is an isometric involution of $L^2(H)$ onto itself, for each diagonal Hamiltonian H, we obtain orthogonal projections

$$P_H^{\mathrm{ev}} := \frac{1}{2}(I + \mathfrak{i}_H)|_{L^2(H)}, \quad P_H^{\mathrm{od}} := \frac{1}{2}(I - \mathfrak{i}_H)|_{L^2(H)}.$$

These projections satisfy $\ker P_H^{\mathrm{ev}} = \operatorname{ran} P_H^{\mathrm{od}}$ and $\ker P_H^{\mathrm{od}} = \operatorname{ran} P_H^{\mathrm{ev}}$. We set

$$L^2(H)^{\mathrm{ev}} := \operatorname{ran} P_H^{\mathrm{ev}}, \quad L^2(H)^{\mathrm{od}} := \operatorname{ran} P_H^{\mathrm{od}},$$

explicitly,

$$L^2(H)^{\mathrm{ev}} = \left\{ \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in L^2(H) : \ f_1 = 0 \text{ a.e.} \right\},$$
$$L^2(H)^{\mathrm{od}} = \left\{ \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in L^2(H) : \ f_2 = 0 \text{ a.e.} \right\}.$$

Then we have the orthogonal decomposition $L^2(H) = L^2(H)^{\mathrm{ev}}[\dot{+}]L^2(H)^{\mathrm{od}}$.

The spaces $L^2(H)^{\mathrm{ev}}$ and $L^2(H)^{\mathrm{od}}$ can be identified with model spaces of some Hamiltonians. To explain this, we need to recall some notation. We denote

$$\check{v}(t) := \int_{s_-}^{t} h_1(x)\,dx, \quad \hat{v}(t) := \int_{s_-}^{t} h_2(x)\,dx, \qquad t \in [s_-, s_+], \tag{2.10}$$

and let $\hat\rho$ and $\check\rho$ be the left-continuous right inverses of $\hat v$ and $\check v$, respectively.

$$[s_-,s_+] \underset{\hat\rho}{\overset{\hat v}{\rightleftarrows}} [0,\textstyle\int_{s_-}^{s_+} h_2(x)\,dx] \qquad [s_-,s_+] \underset{\check\rho}{\overset{\check v}{\rightleftarrows}} [0,\textstyle\int_{s_-}^{s_+} h_1(x)\,dx]$$
$$\hat v\circ\hat\rho=\mathrm{id} \qquad\qquad \check v\circ\check\rho=\mathrm{id}$$

Explicitly, this is

$$\begin{aligned}\hat\rho(y) &:= \inf\{x\in[s_-,s_+):\ \hat v(x)=y\}, \quad y\in[0,\hat v(s_+))\,,\\ \check\rho(y) &:= \inf\{x\in[s_-,s_+):\ \check v(x)=y\}, \quad y\in[0,\check v(s_+))\,.\end{aligned}$$

Moreover, we denote by Θ_H^{ev} and Θ_H^{od} the maps acting on 2-vector valued functions as

$$\begin{aligned}\Theta_H^{\mathrm{ev}}\begin{pmatrix}f_1\\ f_2\end{pmatrix} &:= \begin{pmatrix}0\\ (\check v\circ\hat\rho\circ\hat v)(f_1\circ\hat v)+(f_2\circ\hat v)\end{pmatrix},\\ \Theta_H^{\mathrm{od}}\begin{pmatrix}f_1\\ f_2\end{pmatrix} &:= \begin{pmatrix}(f_1\circ\check v)-(\hat v\circ\check\rho\circ\check v)(f_2\circ\check v)\\ 0\end{pmatrix}.\end{aligned}$$

Definition 2.25. Let H be diagonal. Then we set

$$I^{\mathrm{ev}} := \begin{cases}[0,\int_{s_-}^{s_+} h_2(x)\,dx), & H \text{ regular at } s_+,\\ [0,\int_{s_-}^{s_+} h_2(x)\,dx), & H \text{ singular at } s_+,\ \int_{s_-}^{s_+}(1+\check v(x)^2)h_2(x)\,dx=\infty,\\ [0,\infty), & H \text{ singular at } s_+,\ \int_{s_-}^{s_+}(1+\check v(x)^2)h_2(x)\,dx<\infty,\end{cases}$$

$$I^{\mathrm{od}} := \begin{cases}[0,\int_{s_-}^{s_+} h_1(t)\,dt), & H \text{ regular at } s_+,\\ [0,\int_{s_-}^{s_+} h_1(t)\,dt), & H \text{ singular at } s_+,\ \int_{s_-}^{s_+}(1+\hat v(t)^2)h_1(t)\,dt=\infty,\\ [0,\infty), & H \text{ singular at } s_+,\ \int_{s_-}^{s_+}(1+\hat v(t)^2)h_1(t)\,dt<\infty,\end{cases}$$

and let H^{ev} and H^{od} be the Hamiltonians

$$H^{\mathrm{ev}}(x) := \begin{cases}\begin{pmatrix}(\check v\circ\hat\rho)(x)^2 & (\check v\circ\hat\rho)(x)\\ (\check v\circ\hat\rho)(x) & 1\end{pmatrix}, & x\in[0,\int_{s_-}^{s_+} h_2(t)\,dt),\\ \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, & x\in I^{\mathrm{ev}},\ x\geq\int_{s_-}^{s_+} h_2(t)\,dt,\end{cases}$$

$$H^{\mathrm{od}}(x) := \begin{cases}\begin{pmatrix}1 & -(\hat v\circ\check\rho)(x)\\ -(\hat v\circ\check\rho)(x) & (\hat v\circ\check\rho)(x)^2\end{pmatrix}, & x\in[0,\int_{s_-}^{s_+} h_1(t)\,dt),\\ \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}, & x\in I^{\mathrm{od}},\ x\geq\int_{s_-}^{s_+} h_1(t)\,dt\,.\end{cases}$$

Note that the Hamiltonians H^{ev} and H^{od} are regular or singular if and only if H has the respective property. This is forced by appending the indivisible interval with infinite length as in the respective second lines of the definition of H^{ev} and H^{od}, if necessary.

The following facts are shown in [KWW2]. To be precise, the below item (i) is [KWW2, Theorem 4.2], and item (ii) follows by inspecting the construction of the various spaces, isomorphisms, and relations between them, starting from [KWW2, (4.24)].

Theorem 2.26. *Let H be a diagonal Hamiltonian.*

(i) *Assume that H is singular at s_+, and let q_H, $q_{H^{\text{ev}}}$, and $q_{H^{\text{od}}}$ denote the Weyl coefficients of H, H^{ev}, and H^{od}, respectively. Then*

$$q_{H^{\text{od}}}(z) = z q_{H^{\text{ev}}}(z), \quad q_H(z) = z q_{H^{\text{ev}}}(z^2) = \frac{1}{z} q_{H^{\text{od}}}(z^2). \tag{2.11}$$

(ii) *Assume that $\int_{s_-}^{s_+} (1+\check{v}(x)^2)\, h_2(x)dx = \infty$, and let $f\colon I^{\text{ev}} \to \mathbb{C}^2$ be a measurable function. Then $f \in L^2(H^{\text{ev}})$ if and only if $\Theta_H^{\text{ev}} f \in L^2(H)$. The map Θ_H^{ev} induces an isometric isomorphism*

$$\Theta_H^{\text{ev}}\colon L^2(H^{\text{ev}}) \to L^2(H)^{\text{ev}}.$$

(iii) *Assume that $\int_{s_-}^{s_+} (1+\hat{v}(x)^2)\, h_1(x)dx = \infty$, and let $f\colon I^{\text{od}} \to \mathbb{C}^2$ be a measurable function. Then $f \in L^2(H^{\text{od}})$ if and only if $\Theta_H^{\text{od}} f \in L^2(H)$. The map Θ_H^{od} induces an isometric isomorphism*

$$\Theta_H^{\text{od}}\colon L^2(H^{\text{od}}) \to L^2(H)^{\text{od}}.$$

We may thus say that the constellation of Hamiltonians

$$\begin{array}{ccc} & H & \\ \swarrow & & \searrow \\ H^{\text{ev}} & & H^{\text{od}} \end{array}$$

corresponds to the constellation of Nevanlinna functions

$$\begin{array}{ccc} & zq(z^2) & \\ \swarrow & & \searrow \\ q(z) & & zq(z) \end{array}$$

and we have the decomposition

$$\mathrm{i}_H \circlearrowright L^2(H) = \begin{array}{ccc} L^2(H)^{\text{ev}} & \xleftarrow{\ \Theta_H^{\text{ev}}\ } & L^2(H^{\text{ev}}) \\ [\dot{+}] & & \\ L^2(H)^{\text{od}} & \xleftarrow[\ \Theta_H^{\text{od}}\ ]{} & L^2(H^{\text{od}}) \end{array} \tag{2.12}$$

The class of Hamiltonians which arise as H^{ev} or H^{od} for some diagonal Hamiltonian can be identified.

The items (ii) and (iii) are then immediate from the relation (2.11) and [KK1].

Theorem 2.27. *Let H be a singular diagonal Hamiltonian.*

(i) *The Hamiltonian H^{ev} is of Stieltjes type. Conversely, if $\tilde{H}$ is a Hamiltonian of Stieltjes type, then there exists a diagonal Hamiltonian H, such that $\tilde{H} \sim H^{\mathrm{ev}}$.*

(ii) *The Hamiltonian H^{od} is of inverse Stieltjes type. Conversely, if $\tilde{H}$ is a Hamiltonian of inverse Stieltjes type, then there exists a diagonal Hamiltonian H, such that $\tilde{H} \sim H^{\mathrm{od}}$.*

g. A lemma on general inverses

In the course of the exposition, we will frequently make use of the following elementary statement.

Lemma 2.28. *Let $v\colon [a_1, b_1) \to [a_2, b_2)$ be a continuous, nondecreasing, and surjective function, and let $\rho\colon [a_2, b_2) \to [a_1, b_1)$ be the left-continuous right inverse of v, explicitly this is*

$$\rho(y) := \inf\{x \in [a_1, b_1) : v(x) = y\}, \quad y \in [a_2, b_2)\,.$$

(i) *The function ρ is strictly increasing and $\operatorname{conv}(\operatorname{ran}\rho) = [a_1, b_1)$, where 'conv' denotes the convex hull.*

(ii) *Let $x \in [a_1, b_1)$ and $y \in [a_2, b_2)$. Then*

$$y \leq v(x) \iff \rho(y) \leq \rho(\hat{v}(x)) \iff \rho(y) \leq x.$$

(iii) *For each $y \in [a_2, b_2)$ the function v is constant on $[\rho(y), \rho(y+)]$.*

(iv) *For each $x \in (a_1, b_1)$,*

$$\lim_{x' \nearrow x} [\inf \rho^{-1}((x', \infty))] = v(x)\,.$$

(v) *Assume in addition that v is absolutely continuous, and denote by v' a function which coincides a.e. with its derivative. Then the set*

$$\{x \in (a_1, b_1) : (\rho \circ v)(x) \neq x\} \setminus \{x \in (a_1, b_1) : v'(x) = 0\}$$

has Lebesgue measure zero.

Proof. *Item* (i): Let $y_1, y_2 \in [a_2, b_2)$. If $\rho(y_1) \leq \rho(y_2)$, then

$$y_1 = v(\rho(y_1)) \leq v(\rho(y_2)) = y_2\,.$$

It follows that ρ is strictly increasing. Next, clearly, $a_1 = \rho(a_2) \in \operatorname{ran}\rho$. Let $x \in [a_1, b_1)$ be given. Then we can choose $y \in [a_2, b_2)$ with $y > v(x)$. Assuming $\rho(y) \le x$ would imply $y = v(\rho(y)) \le v(x)$. Hence, we must have $\rho(y) > x$, and this shows that $x \in \operatorname{conv}(\operatorname{ran}\rho)$.

Item (ii): If $y \le v(x)$, then $\rho(y) \le \rho(v(x))$. Since always $\rho(v(x)) \le x$, the latter inequality implies that $\rho(y) \le x$. From this inequality, applying v, we obtain $y = v(\rho(y)) \le v(x)$.

Item (iii): Let $x \in [\rho(y), \rho(y+)]$. Then, for each $y' \in [a_2, b_2)$, $y' > y$, thus $x \in [\rho(y), \rho(y')]$. This implies that

$$y = v(\rho(y)) \le v(x) \le v(\rho(y')) = y' .$$

It follows that $v(x) = y$.

Item (iv): Let $z \in \mathbb{R}$ and $w \in \rho^{-1}([z, \infty))$. Then $\rho(w) \ge z$, and hence $w \ge v(z)$. Thus also $\inf \rho^{-1}([z, \infty)) \ge v(z)$. Using continuity of v, it follows that for each $x \in [a_1, b_1)$

$$\lim_{x' \nearrow x} [\inf \rho^{-1}((x', \infty))] \ge \lim_{x' \nearrow x} [\inf \rho^{-1}([x', \infty))] \ge \lim_{x' \nearrow x} v(x') = v(x) .$$

Let $x, x' \in [a_1, b_1)$ with $x' < x$, and assume that $s \in [a_1, b_1)$ with $v(s) > v(x')$. Then $\rho(v(s)) > x'$, and hence $v(s) \in \rho^{-1}((x', \infty))$. Using continuity and surjectivity of v, it follows that

$$\inf \rho^{-1}((x', \infty)) \le \inf\{v(s) :\, s \in [a_1, b_1), v(s) > v(x')\} = v(x') ,$$

and hence

$$\lim_{x' \nearrow x} [\inf \rho^{-1}((x', \infty))] \le \lim_{x' \nearrow x} v(x') = v(x) .$$

Item (v): Consider now the case that in addition v is absolutely continuous. To simplify notation think of v and ρ as extended to b_1 and b_2, respectively, by $v(b_1) := b_2$ and $\rho(b_2) := b_1$. The set $\{x \in (a_1, b_1] :\, (\rho \circ v)(x) \ne x\}$ can be written as the disjoint union

$$\{x \in (a_1, b_1] :\, (\rho \circ v)(x) \ne x\} = \dot{\bigcup_i} (\alpha_i, \beta_i]$$

taken over all intervals such that $[\alpha_i, \beta_i]$ are the maximal intervals with nonempty interior where v is constant. Clearly, the number of these intervals is at most countable. On the interior of each such interval, the derivative of v exists and is equal to zero. Hence, $v'(x) = 0$ on each interval a.e., and the assertion follows. ■

3. Diagonal Hamiltonians

In this section we investigate Hamiltonians of diagonal form. We establish a recursive method to compute $\Delta(H)$ for such Hamiltonians, see Theorem 3.7 below, which is the first main result of the present paper.

a. Consequences of diagonality for $\mathcal{I}_H$ and $\mathfrak{w}_n$

First, a simple observation; we skip explicit proof.

Lemma 3.1. *Let H be a diagonal Hamiltonian.*

(i) *The type of an H-indivisible interval can only be 0 or $\pi/2$.*

(ii) *The space $L^2(H)$ consists of all functions $f=\binom{f_1}{f_2}$ such that*

$$f_1 \in L^2(h_1(x)dx), \quad f_1 \text{ constant a.e. on indivisible intervals of type } 0,$$

$$f_2 \in L^2(h_2(x)dx), \quad f_2 \text{ constant a.e. on indivisible intervals of type } \frac{\pi}{2}.$$

Next, some facts which are the basis for many simplifications.

Lemma 3.2. *Let H be diagonal, singular, and assume that 0 is a point of regular type of $T_{\min}(H)$.*

(i) *We have $\phi(H)\in\{0,\frac{\pi}{2}\}$.*

(ii) *The operator $\mathcal{I}_H$ acts as*

$$\Big(\mathcal{I}_H\begin{pmatrix}f_1\\f_2\end{pmatrix}\Big)(x)=\int_{s_-}^{x}\begin{pmatrix}-f_2(t)h_2(t)\\ f_1(t)h_1(t)\end{pmatrix}dt, \quad \begin{pmatrix}f_1\\f_2\end{pmatrix}\in\operatorname{dom}\mathcal{I}_H\,. \tag{3.1}$$

(iii) *Consider the case that $\phi(H)=0$. Then*

$$\Big(\mathring{A}_H^{-1}\begin{pmatrix}f_1\\f_2\end{pmatrix}\Big)(x)=-\begin{pmatrix}\int_{s_-}^{x} f_2(t)\,h_2(t)dt\\ \int_{x}^{s_+} f_1(t)\,h_1(t)dt\end{pmatrix}, \quad \begin{pmatrix}f_1\\f_2\end{pmatrix}\in L^2(H)\,, \tag{3.2}$$

in particular,

$$\int_{s_-}^{x} f_2(t)\,h_2(t)dt\in L^2(h_1(x)dx), \quad \int_{x}^{s_+} f_1(t)\,h_1(t)dt\in L^2(h_2(x)dx)\,. \tag{3.3}$$

The analogous statement holds in the case that $\phi(H)=\pi/2$.

Proof. We have

$$\int_{s_-}^{s_+}\xi_\phi^T H(t)\xi_\phi\,dt=\cos^2\phi\int_{s_-}^{s_+}h_1(t)\,dt+\sin^2\phi\int_{s_-}^{s_+}h_2(t)\,dt\,.$$

Since H is singular and $\operatorname{tr} H(t) = h_1(t) + h_2(t)$, we must have $\int_{s_-}^{s_+} h_j(t)\,dt = \infty$ for at least one $j \in \{1,2\}$. Hence, if there exists a number ϕ with $\int_{s_-}^{s_+} \xi_\phi^T H(t)\xi_\phi\,dt < \infty$, then either $\phi = 0$ or $\phi = \pi/2$. This shows (i). To see item (ii), it is enough to note that

$$JH(t) = \begin{pmatrix} -h_2(t) & 0 \\ 0 & h_1(t) \end{pmatrix}.$$

To establish (iii), we use Theorem 2.10 and compute

$$\begin{aligned}
&\Big(\mathring{A}_H^{-1}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\Big)(x) \\
&\quad = \int_{s_-}^{x} \begin{pmatrix} -f_2(t)h_2(t) \\ f_1(t)h_1(t) \end{pmatrix} dt - \lim_{x\nearrow s_+} \Big[\begin{pmatrix} 0 \\ 1 \end{pmatrix}^T \int_{s_-}^{x} \begin{pmatrix} -f_2(t)h_2(t) \\ f_1(t)h_1(t) \end{pmatrix} dt\Big] \\
&\quad = -\begin{pmatrix} \int_{s_-}^{x} f_2(t)\,h_2(t)dt \\ \int_{x}^{s_+} f_1(t)\,h_1(t)dt \end{pmatrix}.
\end{aligned}$$

■

If H is of diagonal form, validity of the Hilbert–Schmidt property can be checked in a much simpler way. Using Theorem 3.2, (i), one can easily deduce the following statement from Theorem 2.12; we skip explicit proof.

Lemma 3.3. *Let H be a diagonal Hamiltonian. Then H has the Hilbert–Schmidt property, if and only if*

$$\int_{s_-}^{s_+} h_1(x)\,dx < \infty \quad \text{and} \quad \int_{s_-}^{s_+} \Big(\int_{s_-}^{x} h_2(t)\,dt\Big) h_1(x)\,dx < \infty$$

or

$$\int_{s_-}^{s_+} h_2(x)\,dx < \infty \quad \text{and} \quad \int_{s_-}^{s_+} \Big(\int_{s_-}^{x} h_1(t)\,dt\Big) h_2(x)\,dx < \infty.$$

Remark 3.4. For diagonal Hamiltonians, also the compactness property can be characterized in an explicit way. The following fact is stated (without a proof) in [K]: *Let H be a diagonal Hamiltonian. Then H has the property $\mathfrak{S}_\infty$ if and only if one of the following two conditions holds:*

(i) $\int_{s_-}^{s_+} h_1(x)\,dx < \infty$ *and* $\lim_{x\to s_+} \Big(\int_{x}^{s_+} h_1(t)\,dt \cdot \int_{s_-}^{x} h_2(t)\,dt\Big) = 0.$

(ii) $\int_{s_-}^{s_+} h_2(x)\,dx < \infty$ *and* $\lim_{x\to s_+} \Big(\int_{x}^{s_+} h_2(t)\,dt \cdot \int_{s_-}^{x} h_1(t)\,dt\Big) = 0.$

The presence of symmetry concretised by the map $\mathfrak{i}_H$ defined in (2.9) also has consequences on the functions $\mathfrak{w}_n$.

Lemma 3.5. *Let H be diagonal and singular. Assume that* 0 *is a point of regular type of* $T_{\min}(H)$ *and that* $\Delta(H) < \infty$*. Moreover, let* ω_k *and* $\mathfrak{w}_n$ *be as in Theorem 2.20,* (iii)*. Then*

$$\omega_k = 0,\ k \in 2\mathbb{N} - 1 \quad \textit{and} \quad \mathfrak{i}_H \mathfrak{w}_n = (-1)^n \mathfrak{w}_n,\ n \in \mathbb{N}_0 .$$

Proof. We restrict explicit proof to the case that $\phi(H) = 0$. The case that $\phi(H) = \pi/2$ is treated in the same way.

Since

$$\mathfrak{i}_H \circ \mathcal{I}_H = -\mathcal{I}_H \circ \mathfrak{i}_H , \tag{3.4}$$

it follows that the functions

$$g := \mathfrak{w}_\Delta + \mathfrak{i}_H \mathfrak{w}_\Delta = \sum_{k=0}^{\Delta} (1 + (-1)^k) \omega_{\Delta-k} \mathcal{I}_H^k \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2 \sum_{\substack{k=0 \\ k \text{ even}}}^{\Delta} \omega_{\Delta-k} \mathcal{I}_H^k \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

$$h := \mathfrak{w}_\Delta - \mathfrak{i}_H \mathfrak{w}_\Delta = \sum_{k=0}^{\Delta} (1 - (-1)^k) \omega_{\Delta-k} \mathcal{I}_H^k \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 2 \sum_{\substack{k=0 \\ k \text{ odd}}}^{\Delta} \omega_{\Delta-k} \mathcal{I}_H^k \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

both belong to $L^2(H)$. If $\Delta(H)$ is odd, the minimality property of $\Delta(H)$ implies that the coefficients ω_l which appear in g must vanish. Similarly, if $\Delta(H)$ is even, the coefficients ω_l which appear in h vanish. Let Δ' denote the largest odd integer less than or equal to $\Delta(H)$, then

$$\omega_1 = \omega_3 = \cdots = \omega_{\Delta'} = 0 .$$

It follows from (3.1) that the upper component of $\mathfrak{w}_n$, $n \in \{0, \ldots, \Delta(H)\} \cap (2\mathbb{N})$, vanishes identically, whereas for $n \in \{0, \ldots, \Delta(H)\} \cap (2\mathbb{N} - 1)$ the lower component of $\mathfrak{w}_n$ vanishes identically. An inductive argument using (3.2) yields the assertion.

The second formula is immediate from (3.4). ∎

b. Computation of $\Delta(H)$

The central notion in our recursive procedure is the following operator.

Definition 3.6. Assume that H is diagonal. We denote by Λ_H the operator whose domain $\operatorname{dom} \Lambda_H$ consists of all measurable functions $f\colon [s_-, s_+) \to \mathbb{C}$ with

$$f h_2 \in L^1_{\mathrm{loc}}([s_-, s_+)), \quad \int_{s_-}^{x} f(t)\, h_2(t) dt \in L^1(h_1(x) dx) ,$$

and which acts as

$$(\Lambda_H f)(x) := \int_x^{s_+} \Big(\int_{s_-}^{t} f(s)\, h_2(s)ds\Big)\, h_1(t)dt, \quad x \in [s_-, s_+),\ f \in \operatorname{dom}\Lambda_H\,. \tag{3.5}$$

Theorem 3.7. *Let H be a singular diagonal Hamiltonian defined on the interval $[s_-, s_+)$, and write*

$$H(x) = \begin{pmatrix} h_1(x) & 0 \\ 0 & h_2(x) \end{pmatrix}, \qquad x \in [s_-, s_+)\,.$$

Assume that H has the Hilbert–Schmidt property, and satisfies $\phi(H) = 0$. Then, for each $n \in \mathbb{N}$, the iterate $\Lambda_H^n 1$ is defined. Set

$$N := \sup\big\{n \in \mathbb{N}_0 :\ \Lambda_H^n 1 \notin L^2(h_2(x)dx)\big\} \in \mathbb{N}_0 \cup \{\infty\}\,. \tag{3.6}$$

Then $\Delta(H) < \infty$ if and only if $N < \infty$. In this case

$$\Delta(H) = \begin{cases} 2N+1, & \int_0^x (\Lambda_H^N 1)(t)\, h_2(t)dt \in L^2(h_1(x)dx), \\ 2N+2, & \int_0^x (\Lambda_H^N 1)(t)\, h_2(t)dt \notin L^2(h_1(x)dx), \end{cases} \tag{3.7}$$

and

$$\mathfrak{w}_{2n} = \begin{pmatrix} 0 \\ \Lambda_H^n 1 \end{pmatrix}, \ \mathfrak{w}_{2n+1} = \begin{pmatrix} \int_{s_-}^x (\Lambda_H^n 1)(t)\, h_2(t)dt \\ 0 \end{pmatrix}, \qquad n \in \mathbb{N}_0\,. \tag{3.8}$$

Remark 3.8.

(i) The set $\{n \in \mathbb{N}_0 :\ \Lambda_H^n 1 \notin L^2(h_2(x)dx)\}$ is an interval which contains 0. This will follow from Theorem 3.10 below.

(ii) If $\phi(H)$ equals $\pi/2$ instead of 0 in Theorem 3.7, then an analogous statement holds true. This can be seen by applying the above stated result with the Hamiltonian $-JHJ$. The resulting theorem reads the same as Theorem 3.7 above, only with h_1 and h_2 exchanged.

The proof of Theorem 3.7 is split into several lemmata. First, some general (and obvious) properties of the operator Λ_H; we skip details.

Lemma 3.9.

(i) *Whenever $f \in \operatorname{dom}\Lambda_H$, the function $\Lambda_H f$ is absolutely continuous on (s_-, s_+) and*

$$\lim_{x \nearrow s_+} (\Lambda_H f)(x) = 0\,.$$

(ii) *If $f \in \operatorname{dom}\Lambda_H$ is nonnegative, then $\Lambda_H f$ is nonnegative and nonincreasing.*

(iii) *If $f, g \in \operatorname{dom}\Lambda_H$ are real-valued and $f \leq g$, then $\Lambda_H f \leq \Lambda_H g$.*
(iv) *The domain of Λ_H is closed with respect to complex conjugation, and*

$$\Lambda_H(\overline{f}) = \overline{\Lambda_H f}, \quad f \in \operatorname{dom}\Lambda_H .$$

(v) *$\Lambda_H f$ is constant on indivisible intervals of type $\pi/2$.*

From now on, for the rest of this subsection, fix a Hamiltonian H with the properties assumed in the theorem.

Lemma 3.10.
(i) *We have $L^\infty([s_-, s_+)) \subseteq \operatorname{dom}\Lambda_H$. The restriction of Λ_H to $L^\infty([s_-, s_+))$ maps $L^\infty([s_-, s_+))$ into $L^\infty([s_-, s_+)) \cap \operatorname{Ac}([s_-, s_+))$. We have*

$$\|\Lambda_H|_{L^\infty([s_-,s_+))}\| \leq \int_{s_-}^{s_+} \Big(\int_{s_-}^{x} h_2(t)dt \Big) h_1(x)dx .$$

(ii) *Let $f \in L^2(h_2(x)dx)$ and assume that f is constant a.e. on each indivisible interval of type $\pi/2$. Then $f \in \operatorname{dom}\Lambda_H$ and*

$$\begin{pmatrix} 0 \\ \Lambda_H f \end{pmatrix} = \mathring{A}_H^{-2} \begin{pmatrix} 0 \\ f \end{pmatrix} .$$

In particular, $\Lambda_H f \in L^2(h_2(x)dx)$.

Proof. For the proof of (i), let a measurable and bounded function $f \colon [s_-, s_+) \to \mathbb{C}$ be given. Then, clearly, $f h_2 \in L^1_{\mathrm{loc}}([s_-, s_+))$. Moreover, we can estimate

$$\begin{aligned} \int_{s_-}^{s_+} \Big| \int_{s_-}^{t} f(s)\, h_2(s)ds \Big| h_1(t)dt &\leq \int_{s_-}^{s_+} \int_{s_-}^{t} |f(s)|\, h_2(s)ds\, h_1(t)dt \\ &\leq \|f\|_\infty \int_{s_-}^{s_+} \Big(\int_{s_-}^{x} h_2(t)dt \Big) h_1(x)dx < \infty . \end{aligned} \tag{3.9}$$

This shows that $f \in \operatorname{dom}\Lambda_H$. For each $x \in [s_-, s_+)$

$$|\Lambda_H f(x)| = \Big| \int_{x}^{s_+} \Big(\int_{s_-}^{t} f(s)\, h_2(s)ds \Big) h_1(t)dt \Big| \leq \int_{s_-}^{s_+} \Big| \int_{s_-}^{t} f(s)\, h_2(s)ds \Big| h_1(t)dt ,$$

and, together with (3.9), this shows the required bound for the operator norm of $\Lambda_H|_{L^\infty([s_-,s_+))}$. The fact that $\Lambda_H f$ is absolutely continuous has already been noticed in Theorem 3.9.

We come to the proof of (ii). If $f \in L^2(h_2(x)dx)$, then for each $T \in [s_-, s_+)$

$$\int_{s_-}^{T} |f(t)| h_2(t)\, dt \leq \Big(\int_{s_-}^{T} |f(t)|^2 h_2(t)\, dt \Big)^{\frac{1}{2}} \Big(\int_{s_-}^{T} h_2(t)\, dt \Big)^{\frac{1}{2}} < \infty ,$$

i.e. $fh_2 \in L^1_{\text{loc}}([s_-, s_+))$.

Under the present hypothesis on f, the function $\binom{0}{f}$ belongs to $L^2(H)$. We conclude from (3.3) that $f \in \operatorname{dom}\Lambda_H$. Remember here that $h_1(x)dx$ is a finite measure. Applying (3.2) twice, gives

$$\Big(\mathring{A}_H^{-2}\binom{0}{f}\Big)(x) = -\Big(\mathring{A}_H^{-1}\begin{pmatrix}\int_{s_-}^t f(s)\,h_2(s)ds\\ 0\end{pmatrix}\Big)(x)$$
$$=\begin{pmatrix}0\\ \int_x^{s_+}\int_{s_-}^t f(s)\,h_2(s)ds\; h_1(t)dt\end{pmatrix} = \begin{pmatrix}0\\ \Lambda_H f\end{pmatrix}. \qquad \blacksquare$$

Lemma 3.10, (i), already implies that each iterate $\Lambda_H^n 1$, $n \in \mathbb{N}$, is defined. Lemma 3.10, (ii), implies that $\{n \in \mathbb{N}_0 : \Lambda_H^n 1 \in L^2(h_2(x)dx)\}$ is either empty or the interval $[N+1, \infty)$.

Lemma 3.11. *For each $n \in \mathbb{N}$ the limit*

$$\lambda_n := \lim_{x \searrow s_-} (\Lambda_H^n 1)(x) \tag{3.10}$$

exists and is finite. We have

$$\begin{pmatrix}0\\ \Lambda_H^n 1\end{pmatrix} = \mathcal{I}_H^{2n}\begin{pmatrix}0\\1\end{pmatrix} + \sum_{k=0}^{n-1}\lambda_{n-k}\mathcal{I}_H^{2k}\begin{pmatrix}0\\1\end{pmatrix},\ n \in \mathbb{N}_0\,. \tag{3.11}$$

Proof. An inductive application of Theorem 3.9, (ii), shows that $\Lambda_H^n 1$ is nonnegative and nonincreasing. Hence, the limit (3.10) exists. Referring to Theorem 3.10, (i), it is finite.

We use induction on n to show (3.11). For $n = 0$ this relation is obvious. Assume (3.11) holds for some $n \in \mathbb{N}_0$. Applying (3.1) twice gives

$$\begin{aligned}
&\Big(\mathcal{I}_H^2\begin{pmatrix}0\\ \Lambda_H^n 1\end{pmatrix}\Big)(x)\\
&= -\int_{s_-}^x\int_{s_-}^t \begin{pmatrix}0\\ \Lambda_H^n 1(s)\end{pmatrix} h_2(s)ds\, h_1(t)dt\\
&= \int_x^{s_+}\int_{s_-}^t \begin{pmatrix}0\\ \Lambda_H^n 1(s)\end{pmatrix} h_2(s)ds\, h_1(t)dt - \int_{s_-}^{s_+}\int_{s_-}^t \begin{pmatrix}0\\ \Lambda_H^n 1(s)\end{pmatrix} h_2(s)ds\, h_1(t)dt\\
&= \begin{pmatrix}0\\ (\Lambda_H^{n+1}1)(x)\end{pmatrix} - \lambda_{n+1}\begin{pmatrix}0\\1\end{pmatrix}.
\end{aligned}$$

Thus (3.11) holds also for $n+1$. $\blacksquare$

We denote by $\mathbb{1}_J$ the characteristic function of the set J.

Lemma 3.12. *Let a number $n \in \mathbb{N}_0$ and a measurable function $f\colon [s_-, s_+) \to \mathbb{C}$ which is constant a.e. on each indivisible interval of type $\pi/2$ be given. Assume that $f \cdot \mathbb{1}_{[s_-,T)} \in L^2(h_2(t)dt)$, $T \in [s_-, s_+)$, that $f \in \operatorname{dom}\Lambda_H^n$, and $\Lambda_H^n f \in L^2(h_2(x)dx)$. Moreover, assume that the limit $\lim_{x\nearrow s_+} f(x)$ exists and is nonzero. Then $\Delta(H) \leq 2n$.*

Proof. We start with a preliminary observation: Let $T \in [s_-, s_+)$, assume that $g \cdot \mathbb{1}_{[s_-,T)} \in L^2(h_2(x)dx)$, that g is constant a.e. on each indivisible interval of type $\pi/2$, and that $g \in \operatorname{dom}\Lambda_H^n$. Then $\Lambda_H^n g \in L^2(h_2(x)dx)$ if and only if $\Lambda_H^n(g\cdot\mathbb{1}_{(T,s_+)}) \in L^2(h_2(x)dx)$. This follows from Theorem 3.10, (ii), since

$$\Lambda_H^n(g \cdot \mathbb{1}_{(T,s_+)}) = \Lambda_H^n g - \Lambda_H^n(g \cdot \mathbb{1}_{[s_-,T)})\,.$$

Now let a function f as in the statement of the lemma be given. Remembering Theorem 3.9, (iv), we may without loss of generality assume that f is real-valued. Moreover, since multiplying f with a nonzero constant does not influence the hypothesis, we may assume that $\lim_{x\nearrow s_+} f(x) > 1$.

Choose $T \in [s_-, s_+)$ such that $f(x) \geq 1$, $x \in (T, s_+)$. As we have observed above, $\Lambda_H^n(f \cdot \mathbb{1}_{(T,s_+)}) \in L^2(h_2(x)dx)$. Monotonicity of Λ_H, cf. Theorem 3.9, (iii), gives

$$0 \leq \Lambda_H^n(\mathbb{1}_{(T,s_+)})) \leq \Lambda_H^n(f \cdot \mathbb{1}_{(T,s_+)})\,.$$

Note here that $\mathbb{1}_{(T,s_+)} \in L^\infty([s_-, s_+))$, and hence certainly belongs to $\operatorname{dom}\Lambda_H^n$. We conclude that $\Lambda_H^n 1 \in L^2(h_2(x)dx)$, and (3.11) together with Theorem 2.20, (ii), implies that $2n \geq \Delta(H)$. ∎

Proof of Theorem 3.7. If $N < \infty$, Theorem 3.11 together with Theorem 2.20, (ii), implies that $\Delta(H) \leq 2N + 2$. We will show in the following that $\Delta(H) < \infty$ implies (3.7) and (3.8).

First, a general observation: Let $n \in \mathbb{N}_0$. By Theorem 3.5 the function $\mathfrak{w}_{2n}$ is given as

$$\mathfrak{w}_{2n} = \mathcal{I}_H^{2n}\begin{pmatrix}0\\1\end{pmatrix} + \sum_{l=0}^{n-1} \omega_{2(n-l)}\mathcal{I}_H^{2l}\begin{pmatrix}0\\1\end{pmatrix}. \tag{3.12}$$

Hence, using (3.11), we find

$$\mathfrak{w}_{2n} = \begin{pmatrix}0\\ \Lambda_H^n 1 + \sum_{k=0}^{n-1}\alpha_k\Lambda_H^k 1\end{pmatrix}, \tag{3.13}$$

with some constants $\alpha_0, \dots, \alpha_{n-1}$.

Now we establish the first formula in (3.8) for the index $n_0 := \left[\frac{\Delta(H)+1}{2}\right]$. Assume on the contrary that one of the constants $\alpha_0, \dots, \alpha_{n_0-1}$ in (3.13) is nonzero, and let $k_0 \in \{0, \dots, n_0-1\}$ be the smallest index with this property. Then we have

$$\begin{pmatrix} 0 \\ \Lambda_H^{k_0}\left[\Lambda_H^{n-k_0}1 + \sum_{k=k_0}^{n-1} \alpha_k \Lambda_H^{k-k_0}1\right] \end{pmatrix} = \mathfrak{w}_{2n} \in L^2(H).$$

Since $\lim_{x \nearrow s_+}[\Lambda_H^{n_0-k_0}1 + \sum_{k=k_0}^{n_0-1} \alpha_k \Lambda_H^{k-k_0}1] = \alpha_{k_0} \neq 0$, Theorem 3.12 implies that $\Delta(H) \le 2k_0$. However, $2k_0 \le 2n_0 - 2 \le \Delta(H) - 1$, and we have reached a contradiction. It follows that $\alpha_0 = \dots = \alpha_{n_0-1} = 0$.

We come to the case $n < n_0$ in the first formula in (3.8). Since $2n_0 - 2 < \Delta(H)$, it follows from (3.11) and (3.12) that $\omega_{2k} = \lambda_k$, $k \le n_0$. Using once more (3.11), this shows that $\mathfrak{w}_{2n} = \Lambda_H^n 1$.

Assume now that $n > n_0$. Then it follows from Theorem 2.20, (iii), and Theorem 3.10 that

$$\mathfrak{w}_{2n} = \mathring{A}_H^{-2(n-n_0)} \mathfrak{w}_{2n_0} = \mathring{A}_H^{-2(n-n_0)} \begin{pmatrix} 0 \\ \Lambda_H^{n_0}1 \end{pmatrix} = \begin{pmatrix} 0 \\ \Lambda_H^{n}1 \end{pmatrix}.$$

We see that (3.8) holds for all $n \in \mathbb{N}_0$. The second part of (3.8) follows since, by Theorem 3.5, we have $\mathfrak{w}_{2n+1} = \mathcal{I}_H \mathfrak{w}_{2n}$, $n \in \mathbb{N}_0$.

It remains to show (3.7). By (3.8), we have $\Lambda_H^n 1 \in L^2(h_2(x)dx)$ if and only if $2n \ge \Delta(H)$. Thus $2N < \Delta(H) \le 2N + 2$. The formula (3.7) now follows with the help of (3.1). ∎

c. An example

The formula (3.7) for $\Delta(H)$ might at first sight seem equally useless as its original definition. But actually it turns out to be quite practical, especially when it comes to practical computations or perturbation arguments. The basis for this is the following observation, whose proof is immediate; we skip details.

Lemma 3.13. *Let h_1, h_2 and $\hat{h}_1, \hat{h}_2$ be measurable functions, defined and locally integrable on an interval $[s_-, s_+)$, and let operators Λ and $\hat{\Lambda}$ be defined correspondingly by the formula (3.5). Assume that*

$$0 \le h_1 \le \hat{h}_1, \qquad 0 \le h_2 \le \hat{h}_2.$$

Then, whenever $f \in \operatorname{dom}\Lambda$, $\hat{f} \in \operatorname{dom}\hat{\Lambda}$, and $0 \le f \le \hat{f}$, we have

$$\Lambda f \le \hat{\Lambda}\hat{f}.$$

The same holds of course with h_1 and h_2 exchanged, i.e. suited to the case '$\phi(H) = \pi/2$'.

Corollary 3.14. *Let H and $\hat{H}$ be two singular diagonal Hamiltonians defined on the interval $[s_-, s_+)$, and assume that $H(t) \le \hat{H}(t)$. If $\hat{H}$ has the Hilbert–Schmidt property, so does H. In this case, we have $\phi(H) = \phi(\hat{H})$ and $\Delta(H) \le \Delta(\hat{H})$.*

Proof. It is obvious that the integrals in Theorem 3.3 depend monotonically on the nonnegative functions h_1, h_2. Hence $\hat{H}$ having the Hilbert–Schmidt property implies that H also has. Clearly, in this case, $\phi(H) = \phi(\hat{H})$.

Assume now that $\hat{H}$ has the Hilbert–Schmidt property, and for definiteness that $\phi(\hat{H}) = 0$ (the case that $\phi(\hat{H}) = \pi/2$ is treated in the same way). The functions $\Lambda^n 1$ and $\hat{\Lambda}^n 1$ are always nonnegative. It follows by induction that $\Lambda^n 1 \le \hat{\Lambda}^n 1$ for all $n \in \mathbb{N}_0$. From this we obtain that also always $\int_{s_-}^{x} (\Lambda^n 1)(t)\, h_2(t)dt \le \int_{s_-}^{x} (\hat{\Lambda}^n 1)(t)\, \hat{h}_2(t)dt$.

Hence, if we have $\hat{\Lambda}^n 1 \in L^2(\hat{h}_2(x)dx)$ then also $\Lambda^n 1 \in L^2(h_2(x)dx)$, and if $\int_{s_-}^{x} (\hat{\Lambda}^n 1)(t)\, \hat{h}_2(t)dt \in L^2(\hat{h}_1(x)dx)$ then $\int_{s_-}^{x} (\Lambda^n 1)(t)\, h_2(t)dt \in L^2(h_1(x)dx)$. ■

This observation allows us to exploit (3.7) and obtain examples of Hamiltonians with arbitrary fast growth concerning the scale of measurement concretised by the number $\Delta(H)$. We use a slightly different example than Theorem 1.1, since we also want to show that despite validity of $\mathfrak{S}_2$ the number $\Delta(H)$ may be equal to ∞. The computations needed to establish (2.1), however, are similar.

Example 3.15. Consider the Hamiltonians defined on the interval $[0, 1)$ by

$$H_\alpha(x) := \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{(1-x)^\alpha} \end{pmatrix}, \qquad \alpha \in \mathbb{R},$$

and

$$H_{2-}(x) := \begin{pmatrix} 1 & 0 \\ 0 & \frac{1-\ln(1-x)}{(1-x)^2[3-\ln(1-x)]^3} \end{pmatrix}.$$

Obviously, the constant $\binom{1}{0}$ is square integrable with respect to these Hamiltonians. We will show

value of α		H.-S.	$\Delta(H)$
$\alpha < 1$	regular	yes	0
$\alpha \in \left(2 - \frac{1}{n}, 2 - \frac{1}{n+1}\right),\ n \in \mathbb{N}$	singular	yes	n
$\alpha = 2-$	singular	yes	∞
$\alpha \ge 2$	singular	no	

Step 1: The fact that H_α is regular or singular at s_+ depending whether $\alpha < 1$ or $\alpha > 1$, respectively, is obvious (all inequalities for α include the case '$\alpha = 2-$' in the obvious way). Next, we have

$$\int_0^t (1-s)^{-\alpha}\,ds = \frac{1}{-\alpha+1} - \frac{(1-t)^{-\alpha+1}}{-\alpha+1}, \quad a \neq 1,$$

$$\int_0^t \frac{1-\ln(1-s)}{(1-s)^2[3-\ln(1-s)]^3}\,ds = \frac{1}{9} - \frac{1}{(1-t)[3-\ln(1-t)]^2}.$$

Hence the condition of Theorem 3.3 for the Hilbert–Schmidt property holds if and only if $\alpha < 2$.

Step 2. Computation of $\Delta(H_\alpha)$ for $\alpha < 2, \alpha \neq 2-$:

Put $\alpha' := 2-\alpha$. A computation shows that, whenever $b+\alpha' \neq 0, 1$,

$$\Lambda_{H_\alpha}((1-s)^b)(x) = \frac{(1-x)^{b+\alpha'}}{(b+\alpha')(b+\alpha'-1)} + \frac{1-x}{b+\alpha'-1}.$$

Since we have $(1-s)^c \in L^2(h_2(x)dx)$ if and only if $c > \frac{1-\alpha'}{2}$, the second summand certainly belongs to $L^2(h_2(x)dx)$. Since $\Lambda_{H_\alpha} L^2(h_2(x)dx) \subseteq L^2(h_2(x)dx)$, we obtain inductively that with some nonzero constants γ_m,

$$\Lambda_{H_\alpha}^m((1-s)^b)(x) \in \gamma_m(1-x)^{b+m\alpha'} + L^2(h_2(x)dx),\ m \in \mathbb{N},$$

provided $b + k\alpha' \neq 0, 1,\ k \in \mathbb{N}$. We conclude that

$$\Lambda_{H_\alpha}^{m-1} 1 \notin L^2(h_2(x)dx), \Lambda_{H_\alpha}^m 1 \in L^2(h_2(x)dx),\ \alpha \in \Big(2 - \frac{1}{2m-1}, 2 - \frac{1}{2m+1}\Big).$$

Since $\phi(H_\alpha) = 0$ and, by our computation of $\mathring{A}_H^{-1}$ in (3.2), the operator $f \mapsto \int_0^x f(t)\,h_2(t)dt$ maps $L^2(h_2(x)dx)$ into $L^2(h_1(x)dx)$, we obtain

$$\int_0^x \Lambda_{H_\alpha}^{m-1} 1(t)\,h_2(t)dt \in \gamma_m'(1-x)^{m\alpha'-1} + L^2(h_1(x)dx),$$

and hence

$$\int_0^x \Lambda_{H_\alpha}^{m-1} 1(t)\,h_2(t)dt \in L^2(h_1(x)dx),\ \alpha \in \Big(2 - \frac{1}{2m-1}, 2 - \frac{1}{2m}\Big),$$

$$\int_0^x \Lambda_{H_\alpha}^{m-1} 1(t)\,h_2(t)dt \notin L^2(h_1(x)dx),\ \alpha \in \Big(2 - \frac{1}{2m}, 2 - \frac{1}{2m+1}\Big).$$

Step 3. Computation of $\Delta(H_\alpha)$ for $\alpha = 2-$:

For every $\alpha < 2$ we have

$$\lim_{t\nearrow 1}\Big(\frac{1-\ln(1-t)}{(1-t)^2[3-\ln(1-t)]^3}\Big/\frac{1}{(1-t)^\alpha}\Big) = +\infty\,.$$

Hence for every $\alpha < 2$ there exists $T_\alpha \in [0,1)$ such that $H_\alpha(t) \leq H_{2-}(t)$, $t \in [T_\alpha, 1)$. By [KW/IV, Lemma 3.12] and Theorem 3.14, we thus have

$$\Delta(H_{2-}) = \Delta(H_{2-}|_{[T,1)}) \geq \Delta(H_\alpha|_{[T,1)}) = \Delta(H_\alpha)\,,$$

and conclude that $\Delta(H_{2-}) = \infty$.

4. Decomposition into even and odd parts

Our aim in this section is to prove the following theorem which relates the number $\Delta(H)$ with $\Delta(H^{\mathrm{ev}})$ and $\Delta(H^{\mathrm{od}})$ for a diagonal Hamiltonian H. Here H^{ev} and H^{od} are the 'even' and 'odd' parts of H, cf. Theorem 2.25.

Theorem 4.1. *Let H be a singular diagonal Hamiltonian defined on the interval $[s_-, s_+)$, and assume that 0 is a point of regular type for $T_{\min}(H)$. Then*

$$\Delta(H) < \infty \iff \Delta(H^{\mathrm{ev}}) < \infty \iff \Delta(H^{\mathrm{od}}) < \infty\,.$$

In this case, we have

$$\Delta(H^{\mathrm{ev}}) = \begin{cases} \left[\frac{\Delta(H)+1}{2}\right], & \phi(H) = 0,\\ \left[\frac{\Delta(H)}{2}\right], & \phi(H) = \frac{\pi}{2},\ \Delta(H) \geq 2,\\ 1, & \phi(H) = \frac{\pi}{2},\ \Delta(H) = 1, \end{cases}$$

$$\Delta(H^{\mathrm{od}}) = \begin{cases} \left[\frac{\Delta(H)}{2}\right], & \phi(H) = 0,\ \Delta(H) \geq 2,\\ 1, & \phi(H) = 0,\ \Delta(H) = 1,\\ \left[\frac{\Delta(H)+1}{2}\right], & \phi(H) = \frac{\pi}{2}. \end{cases}$$

Remark 4.2. The Weyl coefficient associated with a Hamiltonian is a Q-function of the minimal operator induced by a certain canonical selfadjoint extension, cf. [HSW, Theorem 4.3]. Hence, the point 0 is a point of regular type for the minimal operator, if and only if the Weyl coefficient is meromorphic in some neighbourhood of 0.

We conclude from Theorem 2.26, (i), that 0 is a point of regular type for a diagonal Hamiltonian H, if and only if it is for H^{ev}, and if and only if it is for H^{od}. In particular, the hypothesis of the theorem implies that Theorem 2.20 is available.

We first settle the cases that H^{ev} ends with an indivisible interval of type 0 or H^{od} ends indivisibly of type $\pi/2$. This is a consequence of the following fact, remember that Hamiltonians which end indivisibly have '$\Delta = 1$'.

Lemma 4.3. *We have $\Delta(H) = 1$ if and only if one of the following two alternatives occurs ($\hat{v}$ and $\check{v}$ are as in (2.10)):*
(i) $\int_{s_-}^{s_+} (1 + \hat{v}(x)^2)\, h_1(x)dx < \infty$;
(ii) $\int_{s_-}^{s_+} (1 + \check{v}(x)^2)\, h_2(x)dx < \infty$.

Proof. Using Theorem 3.2, we compute

$$\mathcal{I}_H \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} -\int_{s_-}^{x} h_2(t)\, dt \\ 0 \end{pmatrix} = -\begin{pmatrix} \hat{v}(x) \\ 0 \end{pmatrix},$$

and similarly

$$\mathcal{I}_H \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ -\int_{s_-}^{x} h_1(t)\, dt \end{pmatrix} = \begin{pmatrix} 0 \\ \check{v}(x) \end{pmatrix}.$$

Assume that (i) holds. Then $\phi(H) = 0$. By Theorem 3.1, we have $\mathcal{I}_H \binom{0}{1} \in L^2(H)$, and hence $\Delta(H) \leq 1$. However, since H is singular, in any case $\Delta(H) \geq 1$. In the same way, validity of (ii) implies $\Delta(H) = 1$.

Conversely, assume that $\Delta(H) = 1$. Consider the case that $\phi(H) = 0$. Then, due to Theorem 3.5, we must have $\mathcal{I}_H \binom{0}{1} \in L^2(H)$. Thus (i) holds. If $\phi(H) = \pi/2$, in the same way (ii) follows. ∎

From now on, for the rest of this section, assume that

$$\int_{s_-}^{s_+} (1 + \hat{v}(x)^2)\, dx = \int_{s_-}^{s_+} (1 + \check{v}(x)^2)\, dx = \infty,$$

so that Theorem 2.26, (ii) and (iii), are available.

In order to relate the numbers $\Delta(H), \Delta(H^{\mathrm{ev}}), \Delta(H^{\mathrm{od}})$, we need to understand the relationship between H-polynomials on the one hand, and H^{ev}- and H^{od}-polynomials on the other. To this end, we realize a decomposition analogous to (2.12) on the level of polynomials.

Definition 4.4. Define a map $\mathfrak{i}_{\mathrm{Pol}} \colon \mathbb{C}^2[z] \to \mathbb{C}^2[z]$ as

$$\mathfrak{i}_{\mathrm{Pol}}\Big(\sum_{l=0}^{n} \begin{pmatrix} \alpha_l \\ \beta_l \end{pmatrix} z^l \Big) := \sum_{l=0}^{n} \begin{pmatrix} (-1)^{l+1}\alpha_l \\ (-1)^l \beta_l \end{pmatrix} z^l.$$

Clearly, $\mathfrak{i}_{\mathrm{Pol}}$ is an involutory bijection of $\mathbb{C}^2[z]$ onto itself. Hence, we obtain projections $P^{\mathrm{ev}}_{\mathrm{Pol}}$ and $P^{\mathrm{od}}_{\mathrm{Pol}}$ by setting

$$P^{\mathrm{ev}}_{\mathrm{Pol}} := \frac{1}{2}(I + \mathfrak{i}_{\mathrm{Pol}}), \quad P^{\mathrm{od}}_{\mathrm{Pol}} := \frac{1}{2}(I - \mathfrak{i}_{\mathrm{Pol}})\,.$$

These projections satisfy $\operatorname{ran} P^{\mathrm{ev}}_{\mathrm{Pol}} = \ker P^{\mathrm{od}}_{\mathrm{Pol}}$ and $\operatorname{ran} P^{\mathrm{od}}_{\mathrm{Pol}} = \ker P^{\mathrm{ev}}_{\mathrm{Pol}}$. Set

$$\mathbb{C}^2[z]^{\mathrm{ev}} := \operatorname{ran} P^{\mathrm{ev}}_{\mathrm{Pol}}, \quad \mathbb{C}^2[z]^{\mathrm{od}} := \operatorname{ran} P^{\mathrm{od}}_{\mathrm{Pol}}\,,$$

explicitly,

$$\mathbb{C}^2[z]^{\mathrm{ev}} = \Big\{ \sum_{l=0}^{n} \binom{\alpha_l}{\beta_l} z^l \in \mathbb{C}^2[z] : \ \alpha_l = 0,\, l \text{ even},\ \beta_l = 0,\ \text{ odd} \Big\}\,,$$

$$\mathbb{C}^2[z]^{\mathrm{od}} = \Big\{ \sum_{l=0}^{n} \binom{\alpha_l}{\beta_l} z^l \in \mathbb{C}^2[z] : \ \alpha_l = 0,\, l \text{ odd},\ \beta_l = 0,\, l \text{ even} \Big\}\,.$$

One can appropriately identify $\mathbb{C}^2[z]^{\mathrm{ev}}$ and $\mathbb{C}^2[z]^{\mathrm{od}}$ with $\mathbb{C}^2[z]$:

Lemma 4.5. *Define maps*

$$\Theta^{\mathrm{ev}}_{\mathrm{Pol}}\Big(\sum_{l=0}^{n} \binom{\alpha_l}{\beta_l} z^l \Big) := \binom{0}{\beta_0} + \binom{\alpha_0}{0} z + \binom{0}{\beta_1} z^2 + \cdots + \binom{0}{\beta_n} z^{2n} + \binom{\alpha_n}{0} z^{2n+1}\,,$$

$$\Theta^{\mathrm{od}}_{\mathrm{Pol}}\Big(\sum_{l=0}^{n} \binom{\alpha_l}{\beta_l} z^l \Big) := \binom{\alpha_0}{0} + \binom{0}{\beta_0} z + \binom{\alpha_1}{0} z^2 + \cdots + \binom{\alpha_n}{0} z^{2n} + \binom{0}{\beta_n} z^{2n+1}\,.$$

Then $\Theta^{\mathrm{ev}}_{\mathrm{Pol}}$ and $\Theta^{\mathrm{od}}_{\mathrm{Pol}}$ map $\mathbb{C}^2[z]$ linearly and bijectively onto $\mathbb{C}^2[z]^{\mathrm{ev}}$ or $\mathbb{C}^2[z]^{\mathrm{od}}$, respectively.

Using a pictogram analogous to (2.12), we thus are in the situation

$$\mathfrak{i}_{\mathrm{Pol}} \circlearrowright \ \mathbb{C}^2[z] = \begin{array}{ccc} \operatorname{ran} P^{\mathrm{ev}}_{\mathrm{Pol}} & \xleftarrow{\ \Theta^{\mathrm{ev}}_{\mathrm{Pol}}\ } & \mathbb{C}^2[z] \\ \dot{+} & & \\ \operatorname{ran} P^{\mathrm{od}}_{\mathrm{Pol}} & \xleftarrow[\ \Theta^{\mathrm{od}}_{\mathrm{Pol}}\ ]{} & \mathbb{C}^2[z] \end{array}$$

The following lemmata contain the basic computations needed for the proof of Theorem 4.1. They show that the decompositions into even and odd parts on the level of polynomials and of Hamiltonians are compatible.

Lemma 4.6. *Let H be a singular diagonal Hamiltonian.*

(i) *We have the commuting diagrams:*

$$
\begin{array}{ccc}
\operatorname{dom}\mathcal{I}_H & \xrightarrow{\ \mathfrak{i}_H\ } & \operatorname{dom}\mathcal{I}_H \\
{\scriptstyle \mathcal{I}_H}\big\downarrow & & \big\downarrow{\scriptstyle \mathcal{I}_H} \\
\operatorname{dom}\mathcal{I}_H & \xrightarrow[-\mathfrak{i}_H]{} & \operatorname{dom}\mathcal{I}_H
\end{array}
\qquad\qquad
\begin{array}{ccc}
\mathbb{C}^2[z] & \xrightarrow{\ \mathfrak{i}_{\mathrm{Pol}}\ } & \mathbb{C}^2[z] \\
{\scriptstyle \gamma_H}\big\downarrow & & \big\downarrow{\scriptstyle \gamma_H} \\
\operatorname{Pol}(H) & \xrightarrow[\mathfrak{i}_H]{} & \operatorname{Pol}(H)
\end{array}
$$

In particular, $\mathfrak{i}_H$ maps $\operatorname{Pol}(H)$ into itself.

(ii) *Let $p \in \mathbb{C}^2[z]$. If $p \in \operatorname{ran} P_{\mathrm{Pol}}^{\mathrm{ev}}$, then $\gamma_H p \in \operatorname{ran} P_H^{\mathrm{ev}}$. If $p \in \operatorname{ran} P_{\mathrm{Pol}}^{\mathrm{od}}$, then $\gamma_H p \in \operatorname{ran} P_H^{\mathrm{od}}$.*

(iii) *Let $p \in \mathbb{C}^2[z]$. Then $\gamma_H p \in L^2(H)$ if and only if $\gamma_H P_{\mathrm{Pol}}^{\mathrm{ev}} p \in L^2(H)^{\mathrm{ev}}$ and $\gamma_H P_{\mathrm{Pol}}^{\mathrm{ev}} p \in L^2(H)^{\mathrm{od}}$.*

Proof. For the proof of the first diagram in (i), let $\binom{f_1}{f_2} \in \operatorname{dom}\mathcal{I}_H$ be given. Then

$$
\begin{aligned}
\Big(\mathcal{I}_H \mathfrak{i}_H \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\Big)(x) &= \Big(\mathcal{I}_H \begin{pmatrix} -f_1 \\ f_2 \end{pmatrix}\Big)(x) = \int_{s_-}^{x} \begin{pmatrix} -f_2(t)h_2(t) \\ -f_1(t)h_1(t) \end{pmatrix} dt \\
&= -\,\mathfrak{i}_H \int_{s_-}^{x} \begin{pmatrix} -f_2(t)h_2(t) \\ f_1(t)h_1(t) \end{pmatrix} dt = -\Big(\mathfrak{i}_H \mathcal{I}_H \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\Big)(x)\,.
\end{aligned}
$$

For the second diagram let $p = \sum_{l=0}^{n} \binom{\alpha_l}{\beta_l} z^l \in \mathbb{C}^2[z]$ be given, and compute

$$
\begin{aligned}
\gamma_H \mathfrak{i}_{\mathrm{Pol}} p &= \gamma_H \Big(\sum_{l=0}^{n} \begin{pmatrix} (-1)^{l+1}\alpha_l \\ (-1)^l \beta_l \end{pmatrix} z^l \Big) = \sum_{l=0}^{n} \mathcal{I}_H^l \begin{pmatrix} (-1)^{l+1}\alpha_l \\ (-1)^l \beta_l \end{pmatrix} \\
&= \sum_{l=0}^{n} (-1)^l \mathcal{I}_H^l \mathfrak{i}_H \begin{pmatrix} \alpha_l \\ \beta_l \end{pmatrix} = \sum_{l=0}^{n} \mathfrak{i}_H \mathcal{I}_H^l \begin{pmatrix} \alpha_l \\ \beta_l \end{pmatrix} = \mathfrak{i}_H \gamma_H p\,.
\end{aligned}
$$

Items (ii) and (iii) follow immediately: If $p \in \operatorname{ran} P_{\mathrm{Pol}}^{\mathrm{ev}}$ (or $p \in \operatorname{ran} P_{\mathrm{Pol}}^{\mathrm{od}}$), then

$$
P_H^{\mathrm{od}} \gamma_H p = \gamma_H P_{\mathrm{Pol}}^{\mathrm{od}} p = 0 \quad (P_H^{\mathrm{ev}} \gamma_H p = \gamma_H P_{\mathrm{Pol}}^{\mathrm{ev}} p = 0,\ \text{respectively})\,.
$$

If $\gamma_H p \in L^2(H)$, then

$$
\gamma_H P_{\mathrm{Pol}}^{\mathrm{ev}} p = P_H^{\mathrm{ev}} \gamma_H p \in L^2(H)^{\mathrm{ev}} \quad \text{and} \quad \gamma_H P_{\mathrm{Pol}}^{\mathrm{od}} p = P_H^{\mathrm{od}} \gamma_H p \in L^2(H)^{\mathrm{od}}\,.
$$

The converse holds since $\gamma_H p = \gamma_H P_{\mathrm{Pol}}^{\mathrm{ev}} p + \gamma_H P_{\mathrm{Pol}}^{\mathrm{od}} p$. ∎

Lemma 4.7. *Let H be a singular diagonal Hamiltonian, and set $s_+^{\mathrm{ev}} := \sup I^{\mathrm{ev}}$ and $s_+^{\mathrm{od}} := \sup I^{\mathrm{od}}$. Then we have the commuting diagrams:*

$$\begin{array}{ccc} L^1_{\mathrm{loc}}([0,s_+^{\mathrm{ev}})) & \xrightarrow{\mathcal{I}_{H^{\mathrm{ev}}}} & L^1_{\mathrm{loc}}([0,s_+^{\mathrm{ev}})) \\ \Theta_H^{\mathrm{ev}}\big\downarrow & & \big\downarrow\Theta_H^{\mathrm{ev}} \\ L^1_{\mathrm{loc}}([s_-,s_+)) & \xrightarrow[(\mathcal{I}_H)^2]{} & L^1_{\mathrm{loc}}([s_-,s_+)) \end{array} \qquad \begin{array}{ccc} L^1_{\mathrm{loc}}([0,s_+^{\mathrm{od}})) & \xrightarrow{\mathcal{I}_{H^{\mathrm{od}}}} & L^1_{\mathrm{loc}}([0,s_+^{\mathrm{od}})) \\ \Theta_H^{\mathrm{od}}\big\downarrow & & \big\downarrow\Theta_H^{\mathrm{od}} \\ L^1_{\mathrm{loc}}([s_-,s_+)) & \xrightarrow[(\mathcal{I}_H)^2]{} & L^1_{\mathrm{loc}}([s_-,s_+)) \end{array}$$

Proof. We are going to provide evidence for the left diagram; the right diagram is treated in the same way.

Let $\binom{f_1}{f_2} \in L^1_{\mathrm{loc}}([0,s_+^{\mathrm{ev}}))$ be given. Applying (3.1) gives, for $x \in (s_-,s_+)$,

$$\Big[\mathcal{I}_H\Theta_H^{\mathrm{ev}}\binom{f_1}{f_2}\Big](x) = \begin{pmatrix} -\int_{s_-}^x \big[(\check{v}\circ\hat{\rho}\circ\hat{v})(t)(f_1\circ\hat{v})(t) + (f_2\circ\hat{v})(t)\big]h_2(t)dt \\ 0 \end{pmatrix},$$

and in turn

$$\Big[(\mathcal{I}_H)^2\Theta_H^{\mathrm{ev}}\binom{f_1}{f_2}\Big](x)$$
$$= \begin{pmatrix} 0 \\ -\int_{s_-}^x \big(\int_{s_-}^t \big[(\check{v}\circ\hat{\rho}\circ\hat{v})(u)(f_1\circ\hat{v})(u) + (f_2\circ\hat{v})(u)\big]h_2(u)du\big)\, h_1(t)dt \end{pmatrix}.$$

Integrating by parts, we obtain

$$\Big[(\mathcal{I}_H)^2\Theta_H^{\mathrm{ev}}\binom{f_1}{f_2}\Big](x)$$
$$= \begin{pmatrix} 0 \\ -\check{v}(x)\Big(\int_{s_-}^x\big[(\check{v}\circ\hat{\rho}\circ\hat{v})(u)(f_1\circ\hat{v})(u) + (f_2\circ\hat{v})(u)\big]h_2(u)du\Big) + \\ +\int_{s_-}^x \big[(\check{v}\circ\hat{\rho}\circ\hat{v})(t)(f_1\circ\hat{v})(t) + (f_2\circ\hat{v})(t)\big]h_2(t)\cdot\check{v}(t)\,dt \end{pmatrix}.$$

By Theorem 2.28, (v),

$$\int_{s_-}^x [(\check{v}\circ\hat{\rho}\circ\hat{v})(t)(f_1\circ\hat{v})(t) + (f_2(t)\circ\hat{v})]h_2(t)\cdot\check{v}(t)\,dt$$
$$= \int_{s_-}^x \big[(\check{v}\circ\hat{\rho}\circ\hat{v})(t)(f_1\circ\hat{v})(t) + (f_2(t)\circ\hat{v})\big]h_2(t)\cdot(\check{v}\circ\hat{\rho}\circ\hat{v})(t)\,dt\,,$$

and hence we can further rewrite the above expression for $(\mathcal{I}_H)^2\Theta_H^{\mathrm{ev}}\binom{f_1}{f_2}$ as

$$\Big[(\mathcal{I}_H)^2\Theta_H^{\mathrm{ev}}\binom{f_1}{f_2}\Big](x) = \begin{pmatrix} 0 \\ -\check{v}(x)\Big(\int_0^{\hat{v}(x)}\big[(\check{v}\circ\hat{\rho})(s)f_1(s) + f_2(s)\big]\,ds\Big) + \\ +\int_0^{\hat{v}(x)} \big[(\check{v}\circ\hat{\rho})(r)f_1(r) + f_2(r)\big](\check{v}\circ\hat{\rho})(r)\,dr \end{pmatrix}.$$

In order to compute $\Theta_H^{\text{ev}}\mathcal{I}_{H^{\text{ev}}}\binom{f_1}{f_2}$, let $y \in I^{\text{ev}}$, $y \le \hat{v}(s_+)$. Then

$$\Big[\mathcal{I}_{H^{\text{ev}}}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\Big](y) = \int_0^y \begin{pmatrix} -(\check{v}\circ\hat{\rho})(t)f_1(t) - f_2(t) \\ (\check{v}\circ\hat{\rho})(t)^2 f_1(t) + (\check{v}\circ\hat{\rho})(t)f_2(t) \end{pmatrix} dt\,,$$

and hence, for $x \in (s_-, s_+)$,

$$\Big[\Theta_H^{\text{ev}}\mathcal{I}_{H^{\text{ev}}}\begin{pmatrix} f_1 \\ f_2 \end{pmatrix}\Big](x) = \begin{pmatrix} 0 \\ \check{v}(x)\cdot\int_0^{\hat{v}(x)}[-(\check{v}\circ\hat{\rho})(t)f_1(t) - f_2(t)]dt + \\ +\int_0^{\hat{v}(x)}[(\check{v}\circ\hat{\rho})(t)^2 f_1(t) + (\check{v}\circ\hat{\rho})(t)f_2(t)]dt \end{pmatrix}.$$

This shows that the left diagram commutes. ■

Lemma 4.8. *Let H be a singular diagonal Hamiltonian. Then we have the commuting diagrams:*

$$\begin{array}{ccc} \mathbb{C}^2[z] & \underset{(\Theta_{\text{Pol}}^{\text{ev}})^{-1}}{\overset{\Theta_{\text{Pol}}^{\text{ev}}}{\rightleftarrows}} & \mathbb{C}^2[z]^{\text{ev}} \\ \downarrow{\scriptstyle \gamma_{H^{\text{ev}}}} & & \downarrow{\scriptstyle \gamma_H} \\ \text{Pol}(H^{\text{ev}}) & \underset{\Theta_H^{\text{ev}}}{\longrightarrow} & \text{Pol}(H) \end{array} \qquad \begin{array}{ccc} \mathbb{C}^2[z] & \underset{(\Theta_{\text{Pol}}^{\text{od}})^{-1}}{\overset{\Theta_{\text{Pol}}^{\text{od}}}{\rightleftarrows}} & \mathbb{C}^2[z]^{\text{od}} \\ \downarrow{\scriptstyle \gamma_{H^{\text{od}}}} & & \downarrow{\scriptstyle \gamma_H} \\ \text{Pol}(H^{\text{od}}) & \underset{\Theta_H^{\text{od}}}{\longrightarrow} & \text{Pol}(H) \end{array}$$

Proof. We consider the left diagram. First, we check the desired relation for a constant polynomial $p(z) = \binom{\alpha}{\beta}$: We have

$$\gamma_H\Theta_{\text{Pol}}^{\text{ev}}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ \beta \end{pmatrix} + \mathcal{I}_H\begin{pmatrix} \alpha \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \beta \end{pmatrix} + \begin{pmatrix} 0 \\ \int_{s_-}^x \alpha h_1(t)\,dt \end{pmatrix} = \begin{pmatrix} 0 \\ \beta + \alpha\check{v} \end{pmatrix},$$

and, on the other hand,

$$\Theta_H^{\text{ev}}\gamma_{H^{\text{ev}}}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \Theta_H^{\text{ev}}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ \check{v}\alpha + \beta \end{pmatrix}.$$

Next, we extend this knowledge to polynomials of higher degree. The following diagrams obviously commute:

$$\begin{array}{ccccc} \mathbb{C}^2[z] & \xrightarrow{\Theta_{\text{Pol}}^{\text{ev}}} & \mathbb{C}^2[z] & \xrightarrow{\gamma_H} & \text{Pol}\,H \\ \downarrow{\scriptstyle \cdot z} & & \downarrow{\scriptstyle \cdot z^2} & & \downarrow{\scriptstyle (\mathcal{I}_H)^2} \\ \mathbb{C}^2[z] & \underset{\Theta_{\text{Pol}}^{\text{ev}}}{\longrightarrow} & \mathbb{C}^2[z] & \underset{\gamma_H}{\longrightarrow} & \text{Pol}\,H \end{array} \qquad \begin{array}{ccc} \mathbb{C}^2[z] & \xrightarrow{\gamma_{H^{\text{ev}}}} & \text{Pol}(H^{\text{ev}}) \\ \downarrow{\scriptstyle \cdot z} & & \downarrow{\scriptstyle \mathcal{I}_{H^{\text{ev}}}} \\ \mathbb{C}^2[z] & \underset{\gamma_{H^{\text{ev}}}}{\longrightarrow} & \text{Pol}(H^{\text{ev}}) \end{array}$$

Assume now that the asserted diagram has already been shown for some polynomial p, i.e. that $\gamma_H \Theta_{\text{Pol}}^{\text{ev}}(p(z)) = \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}}(p(z))$. Then we can combine the above diagrams with Theorem 4.7, and compute

$$\begin{aligned} \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}}(z \cdot p(z)) =& \Theta_H^{\text{ev}} \mathcal{I}_{H^{\text{ev}}} \gamma_{H^{\text{ev}}}(p(z)) = (\mathcal{I}_H)^2 \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}}(p(z)) \\ =& (\mathcal{I}_H)^2 \gamma_H \Theta_{\text{Pol}}^{\text{ev}}(p(z)) = \gamma_H \Theta_{\text{Pol}}^{\text{ev}}(z \cdot p(z)) \end{aligned}$$

i.e. the asserted diagram holds also for the polynomial $z \cdot p(z)$.

Since the asserted diagram has been shown to hold for constants, it now follows that it holds for all monomials. By linearity, thus, it holds for all polynomials.

The fact that the right diagram commutes is shown in the same way. ∎

After these preparations, we can now give the proof of Theorem 4.1.

Proof of Theorem 4.1. Let H be given according to the assumptions of the theorem. We can switch between the cases '$\phi(H) = 0$' and '$\phi(H) = \pi/2$' by passing from H to $-JHJ$ since

$$(-JHJ)^{\text{ev}} = H^{\text{od}}, \quad (-JHJ)^{\text{od}} = H^{\text{ev}}.$$

Hence, we may restrict explicit proof to the case that '$\phi(H) = 0$'.

Step 1; The numbers $\phi(H^{\text{ev}})$ and $\phi(H^{\text{od}})$:

Since we assume that $\phi(H) = 0$, we have $\int_{s_-}^{s_+} h_1(t)\,dt < \infty$ and $\int_{s_-}^{s_+} h_2(t)\,dt = \infty$. Thus $I^{\text{ev}} = (0, \infty)$ and the second case in the definition of H^{ev} does not appear. This shows that

$$\begin{pmatrix} 0 \\ 1 \end{pmatrix} \notin L^2(H^{\text{ev}}),$$

i.e. $\phi(H^{\text{ev}}) \neq \frac{\pi}{2}$. Next, I^{od} either equals $(0, \int_{s_-}^{s_+} h_1(t)\,dt)$ or $(0, \infty)$. However, if the second case takes place, H^{od} ends indivisibly of type $\pi/2$. Hence, in any case,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \in L^2(H^{\text{od}}),$$

i.e. $\phi(H^{\text{od}}) = 0$.

We conclude that, in order to determine any of $\Delta(H)$, $\Delta(H^{\text{ev}})$, or $\Delta(H^{\text{od}})$, it is enough to investigate polynomials whose leading coefficient is equal to $\binom{0}{1}$.

Step 2; A preliminary computation:

Let $p \in \mathbb{C}^2[z]$ with even degree and leading coefficient $\binom{0}{1}$. Then the polynomial $P_{\text{Pol}}^{\text{ev}} p$ has the same degree as p and also leading coefficient $\binom{0}{1}$. Consider the polynomial

$$p_e := (\Theta_{\text{Pol}}^{\text{ev}})^{-1} P_{\text{Pol}}^{\text{ev}} p.$$

Then we have $\deg p_e = \frac{\deg p}{2}$ and the leading coefficient of p_e equals $\binom{0}{1}$. Similarly, if $p \in \mathbb{C}^2[z]$ has odd degree and leading coefficient $\binom{0}{1}$, then the polynomial

$$p_o := (\Theta_{\text{Pol}}^{\text{od}})^{-1} P_{\text{Pol}}^{\text{od}} p$$

has degree $\frac{\deg p - 1}{2}$ and leading coefficient $\binom{0}{1}$.

Step 3; Assume that $\Delta(H) < \infty$:

Let n_1 be the smallest even integer such that $n_1 \geq \Delta(H)$ and n_2 the smallest odd integer such that $n_2 \geq \Delta(H)$, and consider the polynomials

$$p_1(z) := \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^{n_1} + \sum_{l=0}^{n_1-1} \omega_{n_1-l} \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^l, \quad p_2(z) := \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^{n_2} + \sum_{l=0}^{n_2-1} \omega_{n_2-l} \begin{pmatrix} 0 \\ 1 \end{pmatrix} z^l,$$

where ω_l are as in Theorem 2.20, (iii). Then we have

$$\gamma_H p_j = \mathfrak{w}_{n_j} \in L^2(H), \quad j = 1, 2.$$

Let $p_{1,e}$ and $p_{2,o}$ be defined from p_1 and p_2, respectively, as in Step 1. Using the above lemmata, we obtain

$$\begin{aligned} \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}} p_{1,e} &= \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}} (\Theta_{\text{Pol}}^{\text{ev}})^{-1} P_{\text{Pol}}^{\text{ev}} p_1 = \gamma_H P_{\text{Pol}}^{\text{ev}} p_1 \\ &= P_H^{\text{ev}} \gamma_H p_1 = P_H^{\text{ev}} \mathfrak{w}_{n_1} \in L^2(H), \\ \Theta_H^{\text{od}} \gamma_{H^{\text{od}}} p_{2,o} &= \Theta_H^{\text{od}} \gamma_{H^{\text{od}}} (\Theta_{\text{Pol}}^{\text{od}})^{-1} P_{\text{Pol}}^{\text{od}} p_2 = \gamma_H P_{\text{Pol}}^{\text{od}} p_2 \\ &= P_H^{\text{od}} \gamma_H p_2 = P_H^{\text{od}} \mathfrak{w}_{n_2} \in L^2(H). \end{aligned}$$

This implies that

$$\Delta(H^{\text{ev}}) \leq \frac{n_1}{2}, \quad \Delta(H^{\text{od}}) \leq \frac{n_2 - 1}{2}.$$

If $\Delta(H)$ is even, we have $n_1 = \Delta(H)$ and $n_2 = \Delta(H) + 1$, whereas, if $\Delta(H)$ is odd, $n_1 = \Delta(H) + 1$ and $n_2 = \Delta(H)$. Hence,

$$\Delta(H^{\text{ev}}) \leq \left.\begin{cases} \frac{\Delta(H)}{2}, & \Delta(H) \text{ even} \\ \frac{\Delta(H)+1}{2}, & \Delta(H) \text{ odd} \end{cases}\right\} = \left\lceil \frac{\Delta(H)+1}{2} \right\rceil, \tag{4.1}$$

$$\Delta(H^{\text{od}}) \leq \left.\begin{cases} \frac{\Delta(H)}{2}, & \Delta(H) \text{ even} \\ \frac{\Delta(H)-1}{2}, & \Delta(H) \text{ odd} \end{cases}\right\} = \left\lceil \frac{\Delta(H)}{2} \right\rceil. \tag{4.2}$$

Step 4; Assume that $\Delta(H^{\text{ev}}) < \infty$:

Choose a polynomial $p \in \mathbb{C}^2[z]$ with degree $\Delta(H^{\text{ev}})$ and leading coefficient $\binom{0}{1}$, such that $\gamma_{H^{\text{ev}}} p \in L^2(H^{\text{ev}})$. Then

$$\gamma_H \Theta_{\text{Pol}}^{\text{ev}} p = \Theta_H^{\text{ev}} \gamma_{H^{\text{ev}}} p \in L^2(H),$$

and we conclude that

$$\Delta(H) \le \deg \Theta^{\mathrm{ev}}_{\mathrm{Pol}} p = 2\Delta(H^{\mathrm{ev}}) < \infty\,.$$

This implies

$$\Delta(H^{\mathrm{ev}}) \ge \begin{cases} \frac{\Delta(H)}{2}, & \Delta(H) \text{ even},\\ \frac{\Delta(H)+1}{2}, & \Delta(H) \text{ odd}. \end{cases}$$

The reverse inequality has been shown in Step 2, and (4.1) follows.

Step 5; Assume that $\Delta(H^{\mathrm{od}}) < \infty$:

Now choose a polynomial $p \in \mathbb{C}^2[z]$ with $\deg p = \Delta(H^{\mathrm{od}})$ whose leading coefficient equals $\binom{0}{1}$ and which has the property that $\gamma_{H^{\mathrm{od}}} p \in L^2(H^{\mathrm{od}})$. Then

$$\gamma_H \Theta^{\mathrm{od}}_{\mathrm{Pol}} p = \Theta^{\mathrm{od}}_H \gamma_{H^{\mathrm{od}}} p \in L^2(H)\,,$$

and hence

$$\Delta(H) \le \deg \Theta^{\mathrm{od}}_{\mathrm{Pol}} p = 2\Delta(H^{\mathrm{od}}) + 1 < \infty\,.$$

The reverse inequality in (4.2) follows. ∎

5. Stieltjes type Hamiltonians

Theorem 4.1 can be used to transfer the method to compute Δ with the help of an operator 'Λ' as established in Theorem 3.7 to the class of (inverse) Stieltjes Hamiltonians.

Definition 5.1. Let H be a Hamiltomian which is of the form

$$H(x) = \operatorname{tr} H(x) \cdot \xi_{\phi(x)} \xi^T_{\phi(x)}, \quad x \in [s_-, s_+)\,, \tag{5.1}$$

with some function ϕ of bounded variation.

We denote by Λ_H the operator whose domain $\operatorname{dom} \Lambda_H$ consists of all measurable functions $f\colon [s_-, s_+) \to \mathbb{C}$ with

$$f \in L^1_{\mathrm{loc}}([s_-, s_+)), \quad \int_{s_-}^x f(\xi) \operatorname{tr} H(\xi)\, d\xi \in L^1(|d\phi|)\,,$$

and which acts as

$$(\Lambda_H f)(x) = \int_{[x,s_+)} \Big(\int_{s_-}^{\xi} f(s) \operatorname{tr} H(s)\, ds \Big) |d\phi(\xi)|, \quad x \in [s_-, s_+),\ f \in \operatorname{dom} \Lambda_H\,.$$

We should say it explicitly that we consciously introduced a double meaning to the symbol Λ_H: Depending whether H is diagonal, or of the form (5.1), the operator Λ_H is given as in Theorem 3.6 or as in Theorem 5.1 above.

In the present paper, we deal with (inverse) Stieltjes type Hamiltonians. For such, the function ϕ can be chosen to be nonincreasing, and then $|d\phi| = d(-\phi)$. Investigation of the more general case, that the function ϕ in (5.1) is of bounded variation, will be the subject of a forthcoming work.

The present section is devoted to the proof of the following result, which is the analogue of Theorem 3.7 for (inverse) Stieltjes type Hamiltonians.

Theorem 5.2. *Let H be a singular Hamiltonian which is of (inverse) Stieltjes type, and write $H(x) = \operatorname{tr} H(x) \cdot \xi_{\phi(x)}\xi_{\phi(x)}^T$ with a nonincreasing function ϕ taking values in $[0, \frac{\pi}{2}]$ ($[-\frac{\pi}{2}, 0]$, respectively). Assume that H has the trace-class property.*

Then, for each $n \in \mathbb{N}$, the iterate $\Lambda_H^n 1$ is defined. Set

$$N := \sup\big\{n \in \mathbb{N}_0 : \Lambda_H^n 1 \notin L^2(\operatorname{tr} H(x)dx)\big\} \in \mathbb{N}_0 \cup \{\infty\}\,. \tag{5.2}$$

Then $\Delta(H) < \infty$ if and only if $N < \infty$, and in this case

$$\Delta(H) = N + 1\,.$$

Remark 5.3. The set $\{n \in \mathbb{N}_0 : \Lambda_H^n 1 \notin L^2(\operatorname{tr} H(x)dx)\}$ is an interval containing 0. This will follow from Theorem 3.8, since in the course of the proof of Theorem 5.2 it turns out that it is equal to the corresponding set (3.6) for an appropriate diagonal Hamiltonian.

The proof of this theorem is somewhat elaborate, and we present it in several subsections. In the first we establish the result for the case that H is of Stieltjes type and $\phi(s_+) := \lim_{x\to s_+} \phi(x) > 0$. This is the core of the proof. In subsections which follow, we show how the general case can be reduced to this one.

a. The case that $\phi(s_+) > 0$

Throughout this subsection let H be a singular Hamiltonian of the form (5.1) with ϕ being nonincreasing, taking values in $[0, \pi/2]$, and satisfying $\phi(s_+) > 0$. Then, actually, $\phi(x) \in [\phi(s_+), \frac{\pi}{2}]$, $x \in [s_-, s_+)$. The method to prove Theorem 5.2 is to associate a diagonal Hamiltonian H_d with H, relate the corresponding operators Λ_H and Λ_{H_d}, and use Theorem 3.7 and Theorem 4.1.

Step 1: The Hamiltonian H_d; employing Theorem 3.7 and Theorem 4.1.

Let H_d be a singular diagonal Hamiltonian with $H_d^{\text{ev}} \sim H$. Existence of a Hamiltonian with these properties is ensured by Theorem 2.27, (i). Denote the domain of definition of H_d by $[s_-^d, s_+^d)$, and write (as usual)

$$H_d(y) = \begin{pmatrix} h_1(y) & 0 \\ 0 & h_2(y) \end{pmatrix}, \quad y \in [s_-^d, s_+^d)\,.$$

Moreover, let $\hat{v}, \hat{\rho}, \check{v}, \check{\rho}$ be as in the definition of H_d^{ev} and H_d^{od}, cf. the paragraph preceding Theorem 2.25.

Since $\phi(s_+) > 0$, in particular, the Hamiltonian H does not end with an indivisible interval of type 0 towards s_+. Its reparameterization H_d^{ev} shares this property, and we conclude that

$$I^{\mathrm{ev}} = [0, \hat{v}(s_+^d)), \qquad \int_{s_-^d}^{s_+^d} (1 + \check{v}(y)^2) h_2(y)\, dy = \infty\,.$$

In particular, the function h_2 cannot vanish a.e. on any interval of the form $(s_+^d - \varepsilon, s_+^d)$. This means that $\hat{v}$ is not constant on any interval of this form, and hence maps $[s_-^d, s_+^d)$ surjectively onto $[0, \hat{v}(s_+^d))$. Theorem 2.28, (i), gives

$$\sup_{t \in [0, \hat{v}(s_+^d))} \hat{\rho}(t) = s_+^d\,. \tag{5.3}$$

Let ψ be an absolutely continuous increasing bijection of $[s_-, s_+)$ onto $[0, \hat{v}(s_+^d))$ with ψ^{-1} also being absolutely continuous, such that

$$(H_d^{\mathrm{ev}} \circ \psi)(x) \psi'(x) = H(x), \quad x \in [s_-, s_+)\,.$$

Comparing the right lower entries, we obtain

$$\psi'(x) = \operatorname{tr} H(x) \sin^2 \phi(x)\,, \tag{5.4}$$

and hence

$$\psi(x) = \int_{s_-}^{x} \operatorname{tr} H(\xi) \sin^2 \phi(\xi)\, d\xi, \quad x \in [s_-, s_+) \text{ a.e.}$$

Comparing the right upper entries, we now obtain

$$(\check{v} \circ \hat{\rho})(t) = \cot(\phi \circ \psi^{-1})(t), \quad t \in [0, \hat{v}(s_+^d)) \text{ a.e.} \tag{5.5}$$

Remember here that $\operatorname{tr} H(x)$ is a.e. positive.

Since $\phi(s_+) > 0$, we obtain from (5.3) and (5.5) that

$$\check{v}(s_+^d) = \lim_{t \to \hat{v}(s_+^d)} (\check{v} \circ \hat{\rho})(t) = \lim_{t \to \hat{v}(s_+^d)} \cot(\phi \circ \psi^{-1})(t) = \cot \phi(s_+) < \infty\,,$$

i.e. $\int_{s_-^d}^{s_+^d} h_1(y)\,dy < \infty$. This means that $\phi(H_d) = 0$. Moreover, since H_d is singular, it follows that $\hat{v}(s_+^d) = \infty$.

Let Λ_{H_d} be the operator defined in (3.5), and set

$$N_d := \sup\{n \in \mathbb{N}_0 : \Lambda_{H_d}^n \not\in L^1(h_2(y)dy)\}\,.$$

By Theorem 3.7, the number $\Delta(H_d)$ is either equal to $2N_d+1$ or $2N_d+2$ (naturally including the case that $N_d = \infty$). Since H and H_d^{ev} are reparameterizations of each other, we have $\Delta(H) = \Delta(H_d^{\text{ev}})$, cf. Theorem 2.21. Theorem 4.1 implies that

$$\Delta(H) = \Big[\frac{\Delta(H_d)+1}{2}\Big]\,.$$

Regardless whether $\Delta(H_d)$ equals $2N_d + 1$ or $2N_d + 2$, thus $\Delta(H) = N_d + 1$.

Step 2: Rewriting H_d.

If λ is any function, we denote by C_λ the composition operator $f \mapsto f \circ \lambda$.

Lemma 5.4. *We have*

(i) *The operator $C_{\hat{v}}$ induces an isometry of $L^\infty([0,\infty))$ into $L^\infty([s_-^d, s_+^d))$. The operator $C_{\hat{\rho}}$ induces a surjective contraction of $L^\infty([s_-^d, s_+^d))$ onto $L^\infty([0,\infty))$. Moreover, $C_{\hat{\rho}} \circ C_{\hat{v}} = \mathrm{id}$.*

(ii) *The operators C_ψ and $C_{\psi^{-1}}$ are mutually inverse isometric bijections between $L^\infty([0,\infty))$ and $L^\infty([s_-, s_+))$.*

(iii) *Whenever f is a measurable function with values in $[0,\infty]$ (and being defined on the appropriate interval), we have*

$$\int_a^b (C_{\hat{v}} f)(y) h_2(y)\,dy = \int_{\hat{v}(a)}^{\hat{v}(b)} f(t)\,dt, \qquad \int_{\hat{v}(a)}^{\hat{v}(b)} (C_{\hat{\rho}} f)(t)\,dt = \int_a^b f(y) h_2(y)\,dy\,.$$

The same relations hold if f is a measurable complex valued function, such that in the relation under consideration one (and hence also the other) integrand is integrable.

(iv) *Whenever f is a measurable function with values in $[0,\infty]$ (and being defined on the appropriate interval), we have*

$$\int_{\psi(a)}^{\psi(b)} f(t)\,dt = \int_a^b (C_\psi f)(x)\,\mathrm{tr}\,H(x)\sin^2\phi(x)\,dx\,,$$

$$\int_{\psi(a)}^{\psi(b)} (C_{\psi^{-1}} f)(t)\,dt = \int_a^b f(x)\,\mathrm{tr}\,H(x)\sin^2\phi(x)\,dx\,.$$

The same relations hold if f is a measurable complex valued function, such that in the relation under consideration one (and hence also the other) integrand is integrable.

Proof. We show (i): Since $\hat{v}$ maps $[s_-^d, s_+^d)$ surjectively onto $[0,\infty)$, we have

$$\sup_{y\in[s_-^d,s_+^d)} f(\hat{v}(y)) = \sup_{t\in[0,\infty)} f(t)\,,$$

i.e. $C_{\hat{v}}$ is isometric. Clearly, $\sup_{t\in[0,\infty)} f(\hat{\rho}(t)) \leq \sup_{y\in[s_-^d,s_+^d)} f(y)$, i.e. $C_{\hat{\rho}}$ is contractive, and $(f\circ\hat{v})\circ\hat{\rho} = f$.

For (ii), it is enough to remember that ψ and ψ^{-1} are mutually inverse bijections between $[s_-,s_+)$ and $[0,\infty)$.

We come to the proof of (iii). The function $\hat{v}$ is absolutely continuous, and $\hat{v}' = h_2$. Hence, the substitution rule applies and the first relation follows. Applying this with the function $C_{\hat{\rho}}f$ yields

$$\int_{\hat{v}(a)}^{\hat{v}(b)} (C_{\hat{\rho}}f)(t)\,dt = \int_a^b \big[C_{\hat{v}}(C_{\hat{\rho}}f)\big](y)h_2(y)\,dy\,.$$

However, by Theorem 2.28, (v), the set of all points with $[C_{\hat{v}}(C_{\hat{\rho}}f)](y)\neq f(y)$ and $h_2(y)\neq 0$ has Lebesgue measure zero. Hence,

$$\int_a^b \big[C_{\hat{v}}(C_{\hat{\rho}}f)\big](y)h_2(y)\,dy = \int_a^b f(y)h_2(y)\,dy\,.$$

Finally, remembering (5.4), the first relation in (iv) follows by applying the substitution rule with the absolutely continuous function ψ. The second relation follows by applying the first with $C_{\psi^{-1}}f$. ■

Definition 5.5. We denote by Ξ_1 the operator whose domain $\operatorname{dom}\Xi_1$ consists of all measurable functions $f\colon [s_-,s_+)\to\mathbb{C}$ with

$$f\in L^1_{\text{loc}}([0,\infty)),\qquad \int_0^t f(r)\,dr \in L^1(d(\check{v}\circ\hat{\rho})(t))\,,$$

and which acts as

$$(\Xi_1 f)(t) := \int_{[t,\infty)} \Big(\int_0^\tau f(r)\,dr\Big)\,d(\check{v}\circ\hat{\rho})(t),\quad t\in[0,\infty),\ f\in\operatorname{dom}\Xi_1\,.$$

We denote by Ξ_2 the operator whose domain $\operatorname{dom}\Xi_2$ consists of all measurable functions $f\colon [s_-,s_+)\to\mathbb{C}$ with

$$f\operatorname{tr}H\sin^2\phi \in L^1_{\text{loc}}([s_-,s_+)),\qquad \int_{s_-}^x f(s)\operatorname{tr}H(s)\sin^2\phi(s)\,ds \in L^1(\delta(x)|d\phi(x)|)\,,$$

where

$$\delta(x) := \begin{cases} \frac{1}{\sin^2 \phi(x)}, & \phi \text{ continuous at } x, \\ \frac{\cot \phi(x_+) - \cot \phi(x_-)}{\phi(x_-) - \phi(x_+)}, & \text{otherwise} \end{cases}$$

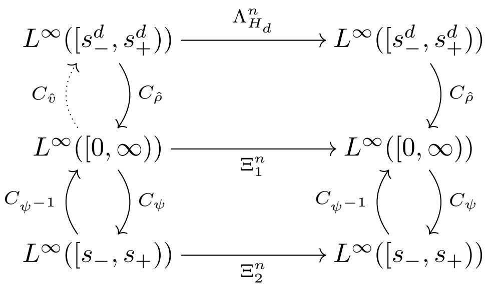
and which acts as

$$(\Xi_2 f)(t) := \int_{[x,s_+)} \Big(\int_{s_-}^{\xi} f(s) \operatorname{tr} H(s) \sin^2 \phi(s)\, ds \Big) \delta(\xi) |d\phi(\xi)|, \qquad t \in [s_-, s_+),\ f \in \operatorname{dom} \Xi_2 .$$

Proposition 5.6. *We have*

$$L^\infty([0,\infty)) \subseteq \operatorname{dom} \Xi_1, \quad \Xi_1(L^\infty([0,\infty))) \subseteq L^\infty([0,\infty)),$$
$$L^\infty([s_-,s_+)) \subseteq \operatorname{dom} \Xi_2, \quad \Xi_2(L^\infty([s_-,s_+))) \subseteq L^\infty([s_-,s_+)).$$

For each $n \in \mathbb{N}$ the following diagram commutes:



that is,

$$\begin{aligned} &C_{\hat{\rho}} \circ \Lambda_{H_d}^n = \Xi_1^n \circ C_{\hat{\rho}}, \quad f \in L^\infty([s_-^d, s_+^d)),\ n \in \mathbb{N}, \\ &C_{\hat{\rho}} \circ \Lambda_{H_d}^n \circ C_{\hat{v}} = \Xi_1, \quad n \in \mathbb{N}, \end{aligned} \tag{5.6}$$

$$C_\psi \circ \Xi_1^n = \Xi_2^n \circ C_\psi, \quad f \in L^\infty([0,\infty)),\ n \in \mathbb{N}. \tag{5.7}$$

Proof of (5.6). Let a measurable function $f\colon [s_-^d, s_+^d) \to [0,\infty]$ be given. We are going to apply the general form of the substitution rule as provided in [T]. Let us match notation: We use [T, Corollary 5.2] with the functions '$\bar{\mu}, \bar{\nu}, \bar{g}$' given as ($t \in [0,\infty)$ fixed)

$$\bar{\mu}(\tau) := \begin{cases} s_-^d, & \tau < 0, \\ \hat{\rho}(\tau), & 0 \le \tau, \end{cases}$$

$$\bar{\nu}(\eta) := \begin{cases} 0, & \eta < s_-^d, \\ \check{v}(\eta), & s_-^d \le \eta < s_+^d, \\ \check{v}(s_+^d), & s_+^d \le \eta, \end{cases} \quad \bar{g}(\eta) := \begin{cases} 0, & \eta < \hat{\rho}(t), \\ \int_0^{\hat{v}(\eta)} (C_{\hat{\rho}} f)(r)\, dr, & \hat{\rho}(t) \le \eta < s_+^d, \\ 0, & s_+^d \le \eta. \end{cases}$$

Thereby, the last cases in the definitions of $\bar{\nu}$ and $\bar{g}$ occur only if $s_+^d < \infty$. By Theorem 2.28, (iv), the function '$\iota_{\bar{\mu}}$' defined in [T, (5.3)] is equal to

$$\iota_{\bar{\mu}}(y) = (\hat{\rho} \circ \hat{v})(y), \quad y \in \mathbb{R}\,.$$

Remembering Theorem 2.28, (ii), (v), Theorem 5.4, and that $\hat{v}$ and $\check{v}$ are absolutely continuous with derivatives h_2 and h_1, respectively, we obtain

$$\begin{aligned}
&\int_{\hat{\rho}(t)}^{s_+^d} \Big(\int_{s_-^d}^{\eta} f(u)\, h_2(u) du \Big)\, h_1(\eta) d\eta \\
&= \int_{\hat{\rho}(t)}^{s_+^d} \Big(\int_{s_-^d}^{\eta} (f \circ \hat{\rho} \circ \hat{v})(u)\, h_2(u) du \Big)\, h_1(\eta) d\eta = \int_{\hat{\rho}(t)}^{s_+^d} \Big(\int_0^{\hat{v}(\eta)} (C_{\hat{\rho}} f)(r)\, dr \Big)\, d\check{v}(\eta) \\
&= \int_{[s_-^d, s_+^d)} \chi_{[\hat{\rho}(t), s_+^d)}(\eta) \Big(\int_0^{\hat{v}(\eta)} (C_{\hat{\rho}} f)(r)\, dr \Big)\, d\check{v}(\eta) \\
&= \int_{[s_-^d, s_+^d)} \chi_{[\hat{\rho}(t), s_+^d)}((\hat{\rho} \circ \hat{v})(\eta)) \Big(\int_0^{\hat{v}((\hat{\rho}\circ\hat{v})(\eta))} (C_{\hat{\rho}} f)(r)\, dr \Big)\, d\check{v}(\eta) \\
&= \int_{\mathrm{conv\,ran}\,\bar{\mu}} (\bar{g} \circ \iota_{\bar{\mu}})(\eta)\, d\bar{\nu}(\eta) = \int_{\mathbb{R}} (\bar{g} \circ \bar{\mu})(\tau)\, d(\bar{\nu} \circ \bar{\mu})(\tau) \\
&= \int_{[0,\infty)} \chi_{[\hat{\rho}(t), s_+^d)}(\hat{\rho}(\tau)) \Big(\int_0^{\hat{v}(\hat{\rho}(\tau))} (C_{\hat{\rho}} f)(r)\, dr \Big)\, d(\check{v} \circ \hat{\rho})(\tau) \\
&= \int_{[0,\infty)} \chi_{[t,\infty)}(\tau) \Big(\int_0^{\tau} (C_{\hat{\rho}} f)(r)\, dr \Big)\, d(\check{v} \circ \hat{\rho})(\tau) \\
&= \int_{[t,\infty)} \Big(\int_0^{\tau} (C_{\hat{\rho}} f)(r)\, dr \Big) d(\check{v} \circ \hat{\rho})(\tau)\,.
\end{aligned} \tag{5.8}$$

The application of the substitution rule [T, Corollary 5.2] is justified since the integrand is nonnegative.

Next, let $f \in L^\infty([0,\infty))$ be given. Then, trivially, also $f \in L^1_{\mathrm{loc}}([0,\infty))$. Moreover, $C_{\hat{v}}|f| = |C_{\hat{v}} f| \in L^\infty([s_-^d, s_+^d))$, and by Theorem 3.10, (i), thus $C_{\hat{v}}|f| \in$

$\operatorname{dom}\Lambda_{H_d}$. In particular,

$$\int_{s_-^d}^{\eta} (C_{\hat{v}}|f|)(u)\, h_2(u)du \in L^1(h_1(\eta)d\eta)\,.$$

Using the computation (5.8) with the nonnegative function $C_{\hat{v}}|f|$ and $t=0$, shows that

$$\int_{[0,\infty)} \Big(\int_0^\tau |f(r)|\, dr \Big)\, d(\check{v}\circ\hat{\rho})(\tau) < \infty\,.$$

Hence, also $\int_0^\tau f(r)\, dr \in L^1(d(\check{v}\circ\hat{\rho})(\tau))$, and we see that $f \in \operatorname{dom}\Xi_1$.

Finally, let $f \in L^\infty([s_-^d, s_+^d))$. Redoing the calculation (5.8), the application of the substitution rule now being justified since integrands are integrable, gives

$$(C_{\hat{\rho}} \circ \Lambda_{H_d})(f) = (\Xi_1 \circ C_{\hat{\rho}})(f)\,. \tag{5.9}$$

Multiplying this equation with $C_{\hat{v}}$ from the right, gives

$$C_{\hat{\rho}} \circ \Lambda_{H_d} \circ C_{\hat{v}} = \Xi_1\,. \tag{5.10}$$

Moreover, by Theorem 2.28, (v), we have

$$\Lambda_{H_d} \circ C_{\hat{v}} \circ C_{\hat{\rho}} = \Lambda_{H_d}\,.$$

Now we use induction on n to show (5.6). The case '$n=1$' is just (5.9) and (5.10). Let $n \geq 2$, then

$$\begin{aligned} C_{\hat{\rho}} \circ \Lambda_{H_d}^n &= (C_{\hat{\rho}} \circ \Lambda_{H_d}^{n-2}) \circ \Lambda_{H_d} \circ \Lambda_{H_d} = (C_{\hat{\rho}} \circ \Lambda_{H_d}^{n-2}) \circ (\Lambda_{H_d} \circ C_{\hat{v}} \circ C_{\hat{\rho}}) \circ \Lambda_{H_d} \\ &= (C_{\hat{\rho}} \circ \Lambda_{H_d}^{n-1} \circ C_{\hat{v}}) \circ (C_{\hat{\rho}} \circ \Lambda_{H_d}) = \Xi_1^{n-1} \circ (\Xi_1 \circ C_{\hat{\rho}}) = \Xi_1^n \circ C_{\hat{\rho}}\,. \end{aligned}$$

This is the first of the required relations. Again multiplying with $C_{\hat{v}}$ from the right, gives the second. ∎

Proof of (5.7). Since C_ψ and $C_{\psi^{-1}}$ are mutually inverse bijections, it is enough to show that

$$C_\psi \circ \Xi_1 = \Xi_2 \circ C_\psi\,. \tag{5.11}$$

Let $x \in [s_-, s_+)$ be fixed. The function $\psi\colon [x, s_+) \to [\psi(x), \infty)$ is a continuous and strictly increasing bijection, and hence maps half-open intervals to half-open intervals. This implies that the image of the measure $d\cot\phi$ under ψ is equal to

$d(\cot\phi\circ\psi^{-1})$. Moreover, ψ is absolutely continuous and $\psi'=\operatorname{tr}H\sin^2\phi$. Remembering that $\check{v}\circ\hat{\rho}=\cot\phi\circ\psi^{-1}$, cf. (5.5), we can thus compute

$$\begin{aligned}\int\limits_{[\psi(x),\infty)}\Big(\int\limits_0^\tau f(r)\,dr\Big)\,d(\check{v}\circ\hat{\rho})(\tau)&\\ =\int\limits_{[\psi(x),\infty)}\Big(\int\limits_{s_-}^{\psi^{-1}(\tau)}(f\circ\psi)(s)\psi'(s)\,ds\Big)\,d(\check{v}\circ\hat{\rho})(\tau)&\qquad(5.12)\\ =\int\limits_{[x,\infty)}\Big(\int\limits_{s_-}^{\xi}(C_\psi f)(x)\operatorname{tr}H(s)\sin^2\phi(s)\,ds\Big)\,d\cot\phi(\xi)\,.&\end{aligned}$$

Now we argue similarly as in the above 'proof of the first half': The relation (5.12) holds for any nonnegative measurable function f defined on $[0,\infty)$. From this, and the fact that $L^\infty([0,\infty))\subseteq\operatorname{dom}\Xi_1$, we obtain that $L^\infty([s_-,s_+))\subseteq\operatorname{dom}\Xi_2$. Now the computation (5.12) can be carried out for each $f\in L^\infty([0,\infty))$ being justified by integrability.

The integral on the left side of (5.12) is nothing but $(C_\psi\circ\Xi_1)(f)$. We have to further consider the right side. The function $\cot x$ is continuously differentiable on $[\phi(s_+),\phi(s_-)]$, in particular, its derivative is bounded on this interval. By the intermediate value theorem, thus

$$\cot\phi(x')-\cot\phi(x)\le C(\phi(x)-\phi(x')),\quad s_-\le x<x'<s_+\,,$$

where $C:=\sup_{x\in[\phi(s_+),\phi(s_-)]}|\frac{d}{dx}\cot x|$. It follows that $d\cot\phi$ is absolutely continuous with respect to $|d\phi|$. The symmetric derivative of $d\cot\phi$ with respect to $|d\phi|$ exists for every $x\in(s_-,s_+)$, in fact it computes as

$$\lim_{r\searrow 0}\frac{d[\cot\phi]([x-r,x+r])}{|d\phi|([x-r,x+r])}=\lim_{r\searrow 0}\frac{\cot\phi(x+r+)-\cot\phi(x-r-)}{\phi(x-r-)-\phi(x+r+)}=\delta(x)\,.$$

However, the symmetric derivative is a Radon–Nikodym derivative, i.e. $d[\cot\phi]=\delta\cdot|d\phi|$, see, e.g., [Be, Proposition 10.2]. Hence, the right side of (5.12) is equal to $(\Xi_2\circ C_\psi)(f)$. The relation (5.11) follows. ■

Step 3: Completing the proof.

In order to translate the definition of the number N_d into the language of Λ_H, we still need to relate Ξ_2 with Λ_H.

For nonnegative functions f,g, we write $f\asymp g$, if there exist constants $c,c'>0$ with $cg\le f\le c'g$.

Lemma 5.7. *Let $f, g \in L^\infty([s_-, s_+))$ and assume that $f \asymp g$. Then*

$$\Xi_2 f \asymp \Lambda_H g\,.$$

Proof. Set $c_0 := \sin\phi(s_+)$. Then $c_0 > 0$ and

$$c_0 \le \sin\phi(x) \le 1,\ 1 \le \delta(x) \le \frac{1}{c_0^2}, \quad x \in [s_-, s_+)\,.$$

To obtain the estimate for δ at points of discontinuity of ϕ, we again used the intermediate value theorem.

Let $c, c' > 0$ be such that $cg \le f \le c'g$. Then

$$(\Xi_2 f)(x) = \int_{[x,s_+)} \Big(\int_{s_-}^{\xi} f(s) \operatorname{tr} H(s) \sin^2\phi(s)\, ds \Big) \delta(\xi) |d\phi(\xi)| \begin{cases} \le \frac{c'}{c_0^2} \int_{[x,s_+)} \big(\int_{s_-}^{\xi} g(s) \operatorname{tr} H(s)\, ds \big) \, |d\phi(\xi)| \\ \ge cc_0 \int_{[x,s_+)} \big(\int_{s_-}^{\xi} g(s) \operatorname{tr} H(s)\, ds \big) \, |d\phi(\xi)| \end{cases}$$

■

Using this lemma, we obtain inductively that

$$\Xi_2^n f \asymp \Lambda_H^n f, \quad f \in L^\infty([s_-, s_+)),\ n \in \mathbb{N}\,.$$

Now it is easy to complete the proof of Theorem 5.2. Let $n \in \mathbb{N}_0$. Then

$$\Lambda_H^n 1 \asymp \Xi_2^n 1 = (\Xi_2^n \circ C_\psi \circ C_{\hat\rho})(1) = (C_\psi \circ C_{\hat\rho})(\Lambda_{H_d}^n 1)\,.$$

By Theorem 5.4, we thus have

$$\Lambda_{H_d}^n 1 \in L^2(h_2(y)dy) \quad \Longleftrightarrow \quad \Lambda_H^n 1 \in L^2(\operatorname{tr} H(x) \sin^2\phi(x) dx).$$

However, since $\sin^2\phi$ is bounded above and away from zero, the latter condition is equivalent to $\Lambda_H^n 1 \in L^2(\operatorname{tr} H(x)dx)$. We arrive at the conclusion that

$$N_d = \sup\{n \in \mathbb{N}_0 :\ \Lambda_H^n 1 \notin L^2(\operatorname{tr} H(x)dx)\} = N\,,$$

and hence that $\Delta(H) = N + 1$. The proof of Theorem 5.2 for the considered case is complete.

■

b. Locality at the singular endpoint

Throughout this subsection let H be a Hamiltonian as in Theorem 5.2.

We know from [KW/IV, Lemma 3.12] that the number $\Delta(H)$ is a local property at the endpoint s_+, meaning that

$$\Delta(H) = \Delta(H|_{[s_0,s_+)})$$

whenever $s_0 \in [s_-, s_+)$ and (s_0, s_+) is not indivisible (just to ensure (Ham4)). Moreover, by Theorem 2.16, (ii), the trace-class property is a local property at the endpoint s_+. Now we show that also the number N defined in (5.2) is a local property at s_+.

Lemma 5.8.

(i) *The function* $V(x) := |d\phi|([x, s_+))$ *belongs to* $L^1(\operatorname{tr} H(x)dx)$.
(ii) *We have* $L^1(\operatorname{tr} H(x)dx) \subseteq \operatorname{dom} \Lambda_H$.
(iii) Λ_H *induces a bounded linear operator of* $L^1(\operatorname{tr} H(x)dx)$ *into itself.*

Proof. We have $\operatorname{dom} \Lambda_H = \operatorname{dom} \Xi_2$, and hence $L^\infty([s_-, s_+)) \subseteq \operatorname{dom} \Lambda_H$. In particular, $1 \in \operatorname{dom} \Lambda_H$, and hence

$$\int_{[s_-,s_+)} \Big(\int_{s_-}^{x} \operatorname{tr} H(\xi)\, d\xi \Big) |d\phi(x)| < \infty\,.$$

Using Fubini's theorem, we obtain

$$\begin{aligned}
\infty > & \int_{[s_-,s_+)} \Big(\int_{s_-}^{x} \operatorname{tr} H(\xi)\, d\xi \Big) |d\phi(x)| \\
= & \int_{[s_-,s_+)} \Big(\int_{[s_-,s_+)} \chi_{[s_-,x]}(\xi)\ \operatorname{tr} H(\xi) d\xi \Big) |d\phi(x)| \\
= & \int_{[s_-,s_+)} \Big(\int_{[s_-,s_+)} \chi_{[\xi,s_+]}(x)\, |d\phi(x)| \Big) \operatorname{tr} H(\xi) d\xi = \int_{[s_-,s_+)} V(\xi)\ \operatorname{tr} H(\xi) d\xi\,.
\end{aligned}$$

This shows (i). Since $|d\phi|$ is a finite measure, item (ii) is obvious. To show (iii), we estimate ($\|.\|_1$ denotes the norm in $L^1(\operatorname{tr} H(x)dx)$)

$$\big|(\Lambda_H f)(x)\big| \le \int_{[x,s_+)} \Big(\int_{s_-}^{\xi} |f(s)|\ \operatorname{tr} H(s) ds \Big) |d\phi(\xi)| \le \|f\|_1 V(x)\,,$$

and hence $\|\Lambda_H f\|_1 \le \|V\|_1 \cdot \|f\|_1$. ■

Proposition 5.9. *Let $s_0 \in [s_-, s_+)$, and set $\tilde{H} := H|_{[s_0,s_+)}$. Then, for each $n \in \mathbb{N}_0$, we have*

$$\Lambda_H^n 1 \in L^1(\operatorname{tr} H(x)dx) \iff \Lambda_{\tilde{H}}^n 1 \in L^1(\operatorname{tr} \tilde{H}(x)dx)\,.$$

Hence, the numbers N and $\tilde{N}$ defined as in (5.2) for H and $\tilde{H}$, respectively, coincide.

Proof. Denote by ρ and ι the restriction map and the embedding map defined as

$$\rho : f \mapsto f|_{[s_0,s_+)}, \quad f \in L^\infty([s_-, s_+))\,,$$

$$(\iota f)(x) := \begin{cases} 0, & s_- \leq x < s_0 \\ f(x), & s_0 \leq x < s_+ \end{cases}, \quad f \in L^\infty([s_0, s_+))\,.$$

Then, clearly, $\rho\iota = \mathrm{id}$ and $\iota\rho$ acts as multiplication with the indicator function $\chi_{[s_-,s_+)}$. It follows that

$$(\iota\rho - \mathrm{id})f = -\chi_{[s_-,s_0)}f, \quad f \in L^\infty([s_-, s_+))\,,$$

and hence that

$$(\iota\rho - \mathrm{id})\big(L^\infty([s_-, s_+))\big) \subseteq L^1(\operatorname{tr} H(x)dx)\,. \tag{5.13}$$

Moreover, we have

$$f \in L^1(\operatorname{tr} H(x)dx) \iff \rho f \in L^1(\operatorname{tr} \tilde{H}(x)dx), \quad f \in L^\infty([s_-, s_+))\,,$$
$$f \in L^1(\operatorname{tr} \tilde{H}(x)dx) \iff \iota f \in L^1(\operatorname{tr} H(x)dx), \quad f \in L^\infty([s_0, s_+))\,.$$

In order to relate Λ_H^n and $\Lambda_{\tilde{H}}^n$, we first observe that $\Lambda_{\tilde{H}} = \rho\Lambda_H\iota$: Let $f \in L^\infty([s_0, s_+))$, then for each $x \in [s_0, s_+)$

$$\begin{aligned}[]
[\Lambda_H(\iota f)](x) &= \int_{[x,s_+)} \Big(\int_{s_-}^{\xi} (\iota f)(s) \operatorname{tr} H(s)ds \Big) |d\phi(\xi)| \\
&= \int_{[x,s_+)} \Big(\int_{s_0}^{\xi} f(s) \operatorname{tr} \tilde{H}(s)ds \Big) |d\phi(\xi)| = (\Lambda_{\tilde{H}} f)(x)\,.
\end{aligned}$$

Next, we use induction on n to show that

$$(\Lambda_{\tilde{H}}^n - \rho\Lambda_H^n\iota)(L^\infty([s_0, s_+))) \subseteq L^1(\operatorname{tr} \tilde{H}(x)dx), \quad n \in \mathbb{N}\,. \tag{5.14}$$

The case '$n = 1$' is trivial, since actually $\Lambda_{\tilde{H}} - \rho\Lambda_H\iota = 0$. Let $n \geq 2$, and assume that (5.14) holds for $n - 1$. We can write

$$\begin{aligned}
\Lambda_{\tilde{H}}^n =& \Lambda_{\tilde{H}}\Lambda_{\tilde{H}}^{n-1} \\
=& \rho\Lambda_H\iota\Lambda_{\tilde{H}}^{n-1} - \rho\Lambda_H\iota\rho\Lambda_H^{n-1}\iota + +\rho\Lambda_H\iota\rho\Lambda_H^{n-1}\iota - \rho\Lambda_H\Lambda_H^{n-1}\iota + \rho\Lambda_H^n\iota \\
=& \rho\Lambda_H\iota\big[\Lambda_{\tilde{H}}^{n-1} - \rho\Lambda_H^{n-1}\iota\big] + \rho\Lambda_H\big[\iota\rho - \mathrm{id}\big]\Lambda_H^{n-1}\iota + \rho\Lambda_H^n\iota\,.
\end{aligned}$$

The first summand maps $L^\infty([s_0,s_+))$ into $L^1(\operatorname{tr}\tilde H(x)dx)$ by the inductive hypothesis. The second summand has the same property by (5.13). In total, (5.14) follows for the number n under consideration.

Consider the function $1\in L^\infty([s_-,s_+))$. Then $\rho 1=1\in L^\infty([s_0,s_+))$. We obtain

$$\begin{aligned}\Lambda_{\tilde H}^n(\rho 1)\in&\big(\rho\Lambda_H^n\iota\big)(\rho 1)+L^1(\operatorname{tr}\tilde H(x)dx)\\ =&\rho\Lambda_H^n 1+\rho\Lambda_H^n[\iota\rho-\mathrm{id}](1)+L^1(\operatorname{tr}\tilde H(x)dx)\\ =&\rho\Lambda_H^n 1+L^1(\operatorname{tr}\tilde H(x)dx)\,,\end{aligned}$$

and hence

$$\begin{aligned}\Lambda_{\tilde H}^n(\rho 1)\in L^1(\operatorname{tr}\tilde H(x)dx)\quad&\Longleftrightarrow\quad\rho\Lambda_H^n 1\in L^1(\operatorname{tr}H(x)dx)\\ &\Longleftrightarrow\quad\Lambda_H^n 1\in L^1(\operatorname{tr}H(x)dx)\,.\end{aligned}$$

■

c. Invariance with respect to shift of angle

Let H be a Hamiltonian of the form (5.1) with ϕ being of bounded variation. Moreover, let $\alpha\in\mathbb{R}$, and consider the Hamiltonian

$$\tilde H(x):=\operatorname{tr}H(x)\cdot\xi_{\phi(x)+\alpha}\xi_{\phi(x)+\alpha}^T,\quad x\in[s_-,s_+)\,.$$

It is obvious that $\Lambda_{\tilde H}=\Lambda_H$, and that the numbers N and $\tilde N$ defined as in (5.2) for H and $\tilde H$, respectively, coincide.

Let N_α denote the matrix

$$N_\alpha:=\begin{pmatrix}\cos\alpha & \sin\alpha\\ -\sin\alpha & \cos\alpha\end{pmatrix}.$$

Then $\tilde H=N_{-\alpha}HN_\alpha$. By [KW/IV, Remark 2.28], the boundary triplets associated with $\tilde H$ and H are isomorphic. In fact, the map $\varpi\colon f\mapsto N_{-\alpha}f$ induces a unitary operator of $L^2(H)$ onto $L^2(\tilde H)$ which intertwines $T_{\max}(H)$ and $T_{\max}(\tilde H)$, and transforms boundary values correspondingly by multiplication with $N_{-\alpha}$.

It follows that, for each $p\in(0,\infty]$, the Hamiltonian $\tilde H$ has the property $\mathfrak{S}_p$ if and only if H has. Moreover, 0 is a point of regular type for $T_{\min}(\tilde H)$ if and only if it is for $T_{\min}(H)$, and in this case $\phi(\tilde H)=\phi(H)+\alpha$. Next, we have $\mathcal{I}_{\tilde H}\circ\varpi=\varpi\circ\mathcal{I}_H$, and hence ($n \in \mathbb{N}_0$, $\alpha_k \in \mathbb{C}$)

$$\sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \xi_{\phi(\tilde{H})+\frac{\pi}{2}} = \sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \xi_{\phi(H)+\alpha+\frac{\pi}{2}} \\ = \sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \varpi \xi_{\phi(H)+\frac{\pi}{2}} = \varpi\Big(\sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \xi_{\phi(H)+\frac{\pi}{2}}\Big).$$

Thus, the function $\sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \xi_{\phi(\tilde{H})+\frac{\pi}{2}}$ belongs to $L^2(\tilde{H})$ if and only the function $\sum_{k=1}^{n} \alpha_k \mathcal{I}_{\tilde{H}}^k \xi_{\phi(H)+\frac{\pi}{2}}$ belongs to $L^2(H)$. We conclude that $\Delta(\tilde{H}) = \Delta(H)$.

d. Reduction of the general case

Let a Hamiltonian H as in Theorem 5.2 be given.

We first settle the case that H ends with an indivisible interval, say (s_0, s_+), towards s_+. Then $\Delta(H) = 1$, cf. [KW/IV, Lemma 3.2]. On the other hand, the function ϕ is constant on (s_0, s_+), and hence

$$(\Lambda_H f)(x) = 0, \quad f \in \operatorname{dom} \Lambda_H,\ x \in (s_0, s_+)\,.$$

In particular, $\Lambda_H^n 1 \in L^2(\operatorname{tr} H(x)dx)$, $n \in \mathbb{N}$, and hence $N = 0$. We see that the asserted equality '$\Delta(H) = N + 1$' indeed holds true.

Now assume that H does not end indivisibly towards s_+. Choose $s_0 \in (s_-, s_+)$ such that $\phi(s_0) - \phi(s_+) < \pi/4$, and consider the Hamiltonian ((Ham4) being ensured since (s_0, s_+) cannot be indivisible)

$$\tilde{H}(x) := \operatorname{tr} H(x) \cdot \xi_{\phi(x)-\phi(s_+)+\frac{\pi}{4}} \xi^T_{\phi(x)-\phi(s_+)+\frac{\pi}{4}}, \quad x \in [s_0, s_+)\,.$$

Then $\tilde{H}$ is a singular Hamiltonian of Stieltjes type whose angle function has a nonzero limit. By subsection **a.**, the assertion of Theorem 5.2 is true for $\tilde{H}$, i.e.

$$\Delta(\tilde{H}) = \tilde{N} + 1$$

where $\tilde{N}$ is defined by (5.2) for $\tilde{H}$.

However, by what we showed in subsections **b.** and **c.**, $\Delta(\tilde{H}) = \Delta(H)$ and $\tilde{N} = N$.

A. A Pontryagin space approach to Theorem 4.1

A weaker version of Theorem 4.1 can be proved in a different, less elementary but more structural, way by using Pontryagin space methods. Since the origin of the number $\Delta(H)$ lies in the indefinite theory, we believe this alternative approach provides interesting structural insight, and is thus worth being presented.

Theorem A.1. *Let H be a singular diagonal Hamiltonian defined on the interval $[s_-, s_+)$, and assume that H has the Hilbert–Schmidt property. Then the following are equivalent:*

(i) *H satisfies $\mathfrak{S}_2$ and $\Delta(H) < \infty$.*
(ii) *H^{ev} satisfies $\mathfrak{S}_2$ and $\Delta(H^{\text{ev}}) < \infty$.*
(iii) *H^{od} satisfies $\mathfrak{S}_2$ and $\Delta(H^{\text{od}}) < \infty$.*

In this case, the relations between $\Delta(H)$, $\Delta(H^{\text{ev}})$, and $\Delta(H^{\text{od}})$, given in Theorem 4.1 hold true.

Remark A.2. (i) The difference between Theorem A.1 and Theorem 4.1 is obvious: In Theorem 4.1 it is only assumed that 0 is a point of regular type for $T_{\min}(H)$, i.e. that q_H is meromorphic in some neighbourhood of 0. In the above statement the, much stronger, Hilbert–Schmidt property is required, i.e. it is assumed that q_H is meromorphic throughout the whole plane, and that the sequence of its poles is sufficiently sparse.

(ii) The Pontryagin space theory employed in the proof of the above statement given below is not known to be available in the general situation of Theorem 4.1. Although, according to Theorem 2.23, the assumption could be weakened to H having compact resolvents.

(iii) In the formulation of this result one statement is hidden, which is worth being mentioned explicitly: *Assume that H is of (inverse) Stieltjes type. Then*

$$H \text{ satisfies } \mathfrak{S}_2 \wedge \Delta(H) < \infty \quad \Rightarrow \quad H \text{ satisfies } \mathfrak{S}_p,\ p > \frac{1}{2}.$$

This follows using Theorem 2.23, and the relation (2.11) between Weyl coefficients.

Throughout the following, we use without further notice the theory of indefinite Hamiltonians as developed in [KW/IV]–[KW/VI]. Some, more specific, tools from the 'indefinite world' enter in the form of statements taken from [KWW1] and [W1], and the below Theorem A.4. Making the present exposition self-contained would require to include a detailed introduction to these notions and results. This is, in our opinion, beyond the scope of the present paper. Hence, we content ourself with providing detailed references to definitions and theorems in the mentioned sources. Moreover, in order to mimimize distracting technical labour, we restrict explicit proof to a certain particular situation which features the core ideas.

a. Situation under consideration

We assume in addition to the hypothesis of the theorem that $s_+\infty$, $\phi(H) = \pi/2$, and that $\int_{s_-}^{s_+}(1 + \check{v}(x)^2)h_2(x)\,dx = \infty$. We prove the required relations between $\Delta(H)$ and $\Delta(H^{\text{ev}})$.

Remark A.3. Why is this the core case?

- ⋆ Of course, $s_+ < \infty$ can always be achieved with a reparameterization, so this requirement is no loss of generality.
- ⋆ If $\int_{s_-}^{s_+}(1+\check{v}(x)^2)h_2(x)\,dx < \infty$, we have obtained the required assertions by simple and explicit inspection, cf. Theorem 4.3.
- ⋆ The relation between $\Delta(H)$ and $\Delta(H^{\mathrm{od}})$ can be understood with the same methods; only slight modifications are necessary.
- ⋆ Once the case that $\phi(H) = \pi/2$ is completely settled, the case that $\phi(H) = 0$ can be deduced by passing from H to $-JHJ$; a standard reduction technique.

Before we come to the actual proof, we collect some preliminary facts.

b. Some preliminaries

First, some consequences of our additional hypothesis: Since $\phi(H) = \pi/2$ and H is singular, we have

$$\check{v}(s_+) = \int_{s_-}^{s_+} h_1(x)\,dx = \infty, \quad \hat{v}(s_+) = \int_{s_-}^{s_+} h_2(x)\,dx < \infty\,.$$

Since $\int_{s_-}^{s_+}(1+\check{v}(x)^2)h_2(x)\,dx = \infty$, we have $I^{\mathrm{ev}} = [0, \hat{v}(s_+))$, and hence this interval is bounded. Moreover, divergence of the integral implies that, in particular, h_2 cannot vanish on any interval of the form $(s_+ - \varepsilon, s_+)$. Hence, $\hat{v}$ maps $[s_-, s_+)$ surjectively onto $[0, \hat{v}(s_+))$, and Theorem 2.28, (i), gives

$$\lim_{t \nearrow \hat{v}(s_+)} \hat{\rho}(t) = s_+\,.$$

Since I^{ev} is bounded, we have $\binom{0}{1} \in L^2(H^{\mathrm{ev}})$, i.e. $\phi(H^{\mathrm{ev}}) = \pi/2$. Moreover, we have

$$\lim_{t \nearrow \hat{v}(s_+)} (\check{v} \circ \hat{\rho})(t) = \lim_{x \nearrow s_+} \check{v}(x) = \infty\,.$$

By [WW1, Theorem 3.9], this implies that

$$\lim_{z \nearrow 0} q_{H^{\mathrm{ev}}}(z) = \infty\,,$$

i.e. $q_{H^{\mathrm{ev}}}$ has a pole at 0.

Second, a lemma about indefinite Hamiltonians $\mathfrak{h}$. The fact that this statement holds true can be seen from their structure theory; we skip explicit proof. For the definition of general Hamiltonians and their monodromy matrices see [KW/IV, Definition 8.1] and [KW/V, Proposition 4.29, Definition 4.3]. For the definition of the notion of negative index 'ind$_-$' for the occuring types of functions, see, e.g., [KW/V, Definition 2.17] for scalar functions and [KW/V, Definition 2.1] for matrix functions.

Lemma A.4. *Let $\mathfrak{h}$ be a regular general Hamiltonian with* $\operatorname{ind}_-\mathfrak{h} > 0$*, and let* $W := \omega(\mathfrak{B}(\mathfrak{h}))$ *be its monodromy matrix. Then* $\operatorname{ind}_-(W \star \infty) = 0$ *if and only if* $\mathfrak{h}$ *has only one singularity and is indivisible of type* 0 *on the right of the singularity. In this case, the function* $W \star \infty$ *is the Weyl coefficient of the Hamiltonian function of* $\mathfrak{h}$ *to the left of the singularity.*

Now we are ready for the proof of the theorem.

Proof of equivalence '(i)$\Longleftrightarrow$(ii)'. Assume (i). Then the collection of data

$$\begin{cases} n = 1, \quad s_-, s_+, s_+ + 1, \\ H(x),\ x \in [s_-, s_+), \quad H_1(x) := \frac{1}{(x-s_+)^2}\xi_0\xi_0^T,\ x \in (s_+, s_+ + 1], \\ \ddot{o}_1 := 0,\ b_{1,1} := 0, \quad d_{1,0} = \cdots = d_{1,2\Delta(H)-1} := 0, \\ E := \{s_-, s_+ + 1\}, \end{cases}$$

constitutes a regular general Hamiltonian $\mathfrak{h}$. Let W be the monodromy matrix of $\mathfrak{h}$, then by the above lemma $W \star \infty = q_H$.

Consider the function $\tilde{W} := \mathcal{T}_{\surd}W$ defined as in [KWW1, Definition 3.1], and let $\tilde{\mathfrak{h}}$ be a regular general Hamiltonian whose monodromy matrix equals $\tilde{W}$; existence follows from [KWW1, Theorem 3.2] and the Inverse Spectral Theorem [KW/VI, 1.3]. Then, by [KWW1, Lemma 3.3, (3.4)],

$$z(\tilde{W} \star \infty)(z^2) = (W \star \infty)(z) = q_H(z)\,.$$

This implies that $\tilde{W} \star \infty = q_{H^{\mathrm{ev}}}$. If we had $\operatorname{ind}_- \tilde{W} = 0$, this relation would imply that H^{ev} ends with an indivisible interval of type 0, which it does not. Hence, $\operatorname{ind}_- \tilde{W} > 0$, and the above lemma yields that $\tilde{\mathfrak{h}}$ has only one singularity, and that the Weyl coefficient of the Hamiltonian function of $\tilde{\mathfrak{h}}$ to the left of its singularity equals $q_{H^{\mathrm{ev}}}$. Thus, H^{ev} is a reparameterization of the Hamiltonian function of $\tilde{\mathfrak{h}}$ to the left of the singularity, and hence satisfies $\Delta(H^{\mathrm{ev}}) < \infty$.

Conversely, assume (ii). In essence, we reverse the above procedure. Consider the regular general Hamiltonian $\tilde{\mathfrak{h}}$ given by the data

$$\begin{cases} n = 1, \quad 0, \hat{v}(s_+), \hat{v}(s_+) + 1, \\ H^{\mathrm{ev}}(x),\ x \in [0, \hat{v}(s_+)), \quad H_1(x) := \frac{1}{(x-s_+)^2}\xi_0\xi_0^T,\ x \in (\hat{v}(s_+), \hat{v}(s_+) + 1], \\ \ddot{o}_1 := 0,\ b_{1,1} := 0, \quad d_{1,0} = \cdots = d_{1,2\Delta(H^{\mathrm{ev}})-1} := 0, \\ E := \{0, \hat{v}(s_+) + 1\}, \end{cases}$$

and let $\tilde{W}$ be its monodromy matrix. Then $\tilde{W} \star \infty = q_{H^e v}$.

Consider the function $W := \mathcal{T}_{2,0}\tilde{W}$ defined as in [KWW1, Definition 3.1], then $\mathcal{T}_{\surd}W = \tilde{W}$, cf. [KWW1, Lemma 3.3, (iii)]. Let $\mathfrak{h}$ be a regular general Hamiltonian whose monodromy matrix equals W. We have $\operatorname{ind}_- W \geq \operatorname{ind}_- \tilde{W} > 0$ and

$$(W \star \infty)(z) = z(\tilde{W} \star \infty)(z^2) = zq_{H^{\mathrm{ev}}}(z^2) = q_H(z)\,.$$

By the above lemma, this general Hamiltonian has only one singularity, and the Weyl coefficient of the Hamiltonian function of $\mathfrak{h}$ to the left of the singularity equals q_H. As before it follows that $\Delta(H) < \infty$. ■

In order to establish the relation between the quantities $\Delta(H)$ and $\Delta(H^{\mathrm{ev}})$, assuming they are finite, we employ [W1, Corollary 4.10]; the case we use is in essence [LaWo1, Theorem 5.1].

Proof of the formula relating $\Delta(H)$ with $\Delta(H^{\mathrm{ev}})$. Denote the sequences of poles of $q_{H^{\mathrm{ev}}}$ by (λ_k), and assume that this sequence is arranged increasingly, i.e.

$$0 = \lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \cdots .$$

Then the sequence (γ_k) of poles of q_H is nothing but

$$\gamma_0 = 0, \quad \gamma_{\pm k} = \pm\sqrt{\lambda_k},\ k \geq 1 .$$

Set

$$\begin{aligned} \tilde{A}(z) :=& z\prod_{k\geq 1}\Big(1-\frac{z}{\lambda_k}\Big), \\ A(z) :=& z\prod_{k\neq 0}\Big(1-\frac{z}{\gamma_k}\Big) = z\prod_{k\geq 1}\Big(1-\frac{z^2}{\lambda_k}\Big), \end{aligned}$$

and consider the conditions (on positive integers $\tilde{N}, N$)

$$\tilde{I}_{\tilde{N}} := \sum_{k\in\mathbb{N}} \lambda_k^{-2\tilde{N}} \frac{1}{\tilde{A}'(\lambda_k)^2 |\operatorname{Res}(q_{H^{\mathrm{ev}}},\lambda_k)|} < \infty , \tag{A.1}$$

$$I_N := \sum_{k\in\mathbb{N}} \lambda_k^{-N} \frac{1}{A'(\sqrt{\lambda_k})^2 |\operatorname{Res}(q_H,\sqrt{\lambda_k})|} < \infty . \tag{A.2}$$

Then [W1, Corollary 4.10] says that (remember that q_H is odd)

$$\Delta(H^{\mathrm{ev}}) = \begin{cases} 1, & \text{(A.1) holds for } \tilde{N}=1, \\ \min\{\tilde{N}\in\mathbb{N} : \text{(A.1) holds for } \tilde{N}\} - 1, & \text{otherwise,} \end{cases} \tag{A.3}$$

$$\Delta(H) = \begin{cases} 1, & \text{(A.2) holds for } N=1, \\ \min\{N\in\mathbb{N} : \text{(A.2) holds for } N\} - 1, & \text{otherwise.} \end{cases} \tag{A.4}$$

We compute

$$\begin{aligned} \operatorname{Res}(q_{H^{\mathrm{ev}}},\lambda_k) &= \lim_{z\to\lambda_k} (z-\lambda_k) q_{H^{\mathrm{ev}}}(z) \\ &= \lim_{z\to\lambda_k} (\sqrt{z}-\sqrt{\lambda_k})(\sqrt{z}+\sqrt{\lambda_k}) \frac{q_H(\sqrt{z})}{\sqrt{z}} = 2\operatorname{Res}(q_H,\sqrt{\lambda_k}) . \end{aligned}$$

Next, $\tilde{A}(z^2) = zA(z)$, and hence $2z\tilde{A}'(z^2) = A(z) + zA'(z)$. For $z = \sqrt{\lambda_k}$, thus

$$2\tilde{A}'(\lambda_k) = A'(\sqrt{\lambda_k}) .$$

Hence, the fraction in one summand of the series in (A.1) is just double the fraction in the corresponding summand of the series in (A.2). Hence, (A.1) holds for some $\tilde{N}$ if and only if (A.2) holds for $2\tilde{N}$. Combining this with (A.3) and (A.4), it is easily seen that

$$\Delta(H^{\mathrm{ev}}) = \begin{cases} 1, & \Delta(H) = 1, \\ [\Delta(H)/2], & \text{otherwise.} \end{cases}$$

and this is the required formula. ■

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H. Winkler, Institut für Mathematik, Technische Universität Ilmenau, Curiebau, Weimarer Straße 25, D–98693 Illmenau, Germany; *e-mail*: henrik.winkler@tu-ilmenau.de

H. Woracek, Institut für Analysis und Scientific Computing, Technische Universität Wien, Wiedner Hauptstraße. 8–10/101, 1040 Wien, Austria;
e-mail: harald.woracek@tuwien.ac.at