Chapter 5

One-dimensional Schrödinger operators with point interactions

Let us demonstrate our findings by considering the simplest possible situation: Fix $\mathcal{L} \in (0, \infty]$ and let

$$(x_k)_{k\geq 0} \subset \mathcal{I} := [0, \mathcal{L})$$

be a strictly increasing sequence such that $x_0 = 0$ and $x_k \uparrow \mathcal{L}$. Considering (x_k) as a vertex set and the intervals $e_k = [x_k, x_{k+1}]$ as edges, we end up with the simplest infinite metric graph – an infinite *path graph*. Then the edge weights $\mu, \nu \colon \mathcal{I} \to \mathbb{R}_{>0}$ are given by

$$\begin{aligned} \mu(x) &= \sum_{k\geq 0} \mu_k \mathbb{1}_{[x_k, x_{k+1})}(x), \\ \nu(x) &= \sum_{k\geq 0} \nu_k \mathbb{1}_{[x_k, x_{k+1})}(x), \end{aligned} \tag{5.1}$$

where $(\mu_k)_{k\geq 0}$ and $(\nu_k)_{k\geq 0}$ are positive real sequences. For a sequence $\alpha = (\alpha_k)_{k\geq 0}$ of reals, conditions (2.13) take the form

$$\begin{cases} f(x_k-) = f(x_k+) =: f(x_k), \\ \nu_k f'(x_k+) - \nu_{k-1} f'(x_k-) = \alpha_k f(x_k) \end{cases} \tag{5.2}$$

for all $k \geq 0$, where we set $f'(0-) = 0$ for notational simplicity and hence for $k = 0$ the corresponding condition is $\nu_0 f'(0) = \alpha_0 f(0)$. The corresponding (maximal) operator $\mathrm{H}_\alpha := \mathrm{H}_{\mu,\nu,\alpha}$ acting in $L^2(\mathcal{I}; \mu)$ is known as the *one-dimensional Schrödinger operator with δ-interactions* on $X = (x_k)_{k\geq 0}$ (see, e.g., [3]), and the corresponding differential expression is given by

$$\tau = \frac{1}{\mu(x)}\left(-\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\geq 0} \alpha_k \delta(x - x_k)\right). \tag{5.3}$$

Remark 5.1. There are manifold reasons to investigate the operator H_α. First of all, it serves as a toy model in quantum mechanics. Indeed, if $\mu_k = \nu_k = 1$ for all $k \geq 0$, then (5.3) turns into the usual δ-coupling on X and H_α in this case is nothing but the Hamiltonian (see [3, 144])

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{k\geq 0} \alpha_n \delta_{x_n}.$$

Moreover, (5.3) naturally appears in the study of Kirchhoff Laplacians and Laplacians with δ-couplings on family preserving graphs (see Section 8.1 for further details).

5.1 The case $\alpha \equiv 0$ and Krein strings

We begin with the study of the "unperturbed" case, that is, when $\alpha \equiv 0$ and hence (5.3) is the classical weighted Sturm–Liouville operator

$$\tau = -\frac{1}{\mu(x)}\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x}. \tag{5.4}$$

Note that in this situation the well-developed spectral theory of Sturm–Liouville operators [208] and Krein strings [120, 127] leads to rather transparent and complete, although far from being trivial, answers to some spectral questions.

Let $\mathrm{H} := \mathrm{H}_{\mu,\nu}$ be the maximal operator associated with (5.4) in $L^2(\mathcal{I};\mu)$ and subject to the Neumann boundary condition at $x = 0$:

$$\mathrm{dom}(\mathrm{H}) = \{f \in L^2(\mathcal{I};\mu) : f, \nu f' \in AC_{\mathrm{loc}}[0,\mathcal{L}),\ f'(0) = 0,\ \tau f \in L^2(\mathcal{I};\mu)\}. \tag{5.5}$$

The corresponding minimal operator H^0 is defined as the closure in $L^2(\mathcal{I};\mu)$ of the pre-minimal operator H':

$$\mathrm{H}' = \mathrm{H} \restriction \mathrm{dom}(\mathrm{H}'), \quad \mathrm{dom}(\mathrm{H}') = \mathrm{dom}(\mathrm{H}) \cap C_c(\mathcal{I}).$$

It is immediate to see that H and H^0 coincide with the maximal and, respectively, minimal Kirchhoff Laplacians defined in Section 2.4.1. The next result provides a rather transparent criterion for the equality $\mathrm{H} = \mathrm{H}^0$ to hold.

Lemma 5.2. *The operator* H *is self-adjoint if and only if the series*

$$\sum_{k\ge 0}\mu_k|e_k|\Big(\sum_{j\le k}\frac{|e_j|}{\nu_j}\Big)^2 \tag{5.6}$$

diverges.

Proof. The self-adjointness criterion follows from the standard limit point/limit circle classification for (5.4) (see, e.g., [208]). Namely, $\tau y = 0$ has two linearly independent solutions

$$y_1(x) \equiv 1, \quad y_2(x) = \int_0^x \frac{\mathrm{d}s}{\nu(s)}, \quad x \in [0,\mathcal{L}),$$

and one simply needs to verify whether or not both y_1 and y_2 belong to $L^2(\mathcal{I};\mu)$. Clearly, $y_1 \in L^2(\mathcal{I};\mu)$ exactly when the series

$$\sum_{k\ge 0}\mu_k|e_k| \tag{5.7}$$

converges. Moreover, it is straightforward to check that $y_2 \in L^2(\mathcal{I};\mu)$ if and only if the series (5.6) converges. The Weyl alternative finishes the proof. ∎

The above considerations suggest to introduce the following quantity:

$$\mathcal{L}_\nu := \int_{\mathcal{I}} \frac{\mathrm{d}x}{\nu(x)} = \sum_{k\geq 0} \frac{|e_k|}{\nu_k}.$$

Observe that $\mathcal{L}_\nu < \infty$ exactly when all solutions to $\tau y = 0$ are bounded.

Corollary 5.3. *If*

$$\sum_{k\geq 0} \mu_k |e_k| = \infty, \tag{5.8}$$

then H *is self-adjoint. Moreover, in the case* $\mathcal{L}_\nu < \infty$, (5.8) *is also necessary for the self-adjointness.*

Remark 5.4. A few remarks are in order.

(i) Condition (5.8) admits two transparent geometric reformulations. Namely, equipping the set $X = \{x_k\}_{k\geq 0}$ with weights $m\colon x_k \mapsto \mu_{k-1}|e_{k-1}| + \mu_k|e_k|$, and considering the path graph ($x_k \sim x_n$ exactly when $|k-n| = 1$) as a metric space (X, ϱ_m) equipped with the path metric ϱ_m (see Section 6.4.2 for a detailed definition), condition (5.8) is equivalent to each of the following conditions:

   (a) infinite total volume:

$$m(X) = \sum_{k\geq 0} m(x_k) = 2\sum_{k\geq 0} \mu_k |e_k| = \infty,$$

   (b) completeness of (X, ϱ_m).

   In particular, Lemma 5.2 implies that completeness of (X, ϱ_m) is only sufficient for H to be self-adjoint (cf. Theorem 7.7). Moreover, observe that in the case of a path graph both conditions (a) and (b) become also necessary for the self-adjointness exactly when the constant $\mathcal{L}_\nu$ is finite, that is, when all solutions to $\tau y = 0$ are bounded.

(ii) It is an interesting and, in fact, very difficult question to decide about the self-adjointness by looking at the geometry of a given metric graph. Lemma 5.2 demonstrates that even in the simplest case of a weighted path graph its solution involves non-trivial tools.

Despite the well-developed spectral theory of Sturm–Liouville operators, it turns out that the detailed spectral analysis of the operator (5.5) is already a difficult task even with this very special class of weights (5.1). However, in one particular situation the analysis is rather straightforward.

Lemma 5.5. *If the series* (5.6) *is convergent, then the deficiency indices of* H^0 *are equal to* 1 *and the self-adjoint extensions of* H^0 *form a one-parameter family* H_θ, *where* $\theta \in [0,\pi)$ *and*

$$\mathrm{dom}(\mathrm{H}_\theta) := \{f \in \mathrm{dom}(\mathrm{H}) : \cos(\theta) f_\nu(\mathcal{L}) + \sin(\theta) f'_\nu(\mathcal{L}) = 0\}. \tag{5.9}$$

Here

$$f_\nu(\mathcal{L}) = \lim_{x\to\mathcal{L}} (f(x) - \nu(x) f'(x) y_2(x)) \quad \textit{and} \quad f'_\nu(\mathcal{L}) = \lim_{x\to\mathcal{L}} \nu(x) f'(x).$$

Moreover, the spectrum of H_θ *is purely discrete, bounded from below, and eigenvalues (if ordered in the non-decreasing order) obey the Weyl law:*

$$\lim_{n\to\infty} \frac{n}{\sqrt{\lambda_n(\mathrm{H}_\theta)}} = \frac{1}{\pi}\int_0^{\mathcal{L}} \sqrt{\frac{\mu(x)}{\nu(x)}}\mathrm{d}x = \frac{1}{\pi}\sum_{k\geq 0} |e_k| \sqrt{\frac{\mu_k}{\nu_k}}. \tag{5.10}$$

Proof. The first claim is standard (see, e.g., [208]). The second one follows from, e.g., [85, Chapter 6.7]. ∎

Remark 5.6. A few remarks are in order.

(i) Using the definition (3.1) of the intrinsic edge length, we set

$$\eta_k := \eta(e_k) = |e_k| \sqrt{\frac{\mu_k}{\nu_k}} \tag{5.11}$$

for all $k \in \mathbb{Z}_{\geq 0}$, and then the right-hand side of (5.10) is nothing but

$$\frac{1}{\pi}\sum_{k\geq 0} \eta(e_k) = \frac{1}{\pi} \times \text{intrinsic length of } \mathcal{I}.$$

(ii) If y_2 is bounded, then $f_\nu(\mathcal{L})$ can be replaced by $\lim_{x\to\mathcal{L}} f(x)$.

The next result mostly follows from the work of I. S. Kac and M. G. Krein [119, 120] on spectral theory of Krein strings. Recall that $\lambda_0(A)$ and $\lambda_0^{\mathrm{ess}}(A)$ denote the bottoms of the spectrum, respectively, of the essential spectrum of a self-adjoint operator A.

Lemma 5.7. *Suppose that the series* (5.6) *diverges, i.e., the operator* H *is self-adjoint. Then:*

(i) Positive spectral gap: $\lambda_0(\mathrm{H}) > 0$ *if and only if*

$$\mathcal{L}_\nu = \sum_{k\geq 0} \frac{|e_k|}{\nu_k} < \infty \quad \textit{and} \quad \sup_{n\geq 0} \sum_{k\leq n} \mu_k |e_k| \sum_{k\geq n} \frac{|e_k|}{\nu_k} < \infty. \tag{5.12}$$

(ii) Positive essential spectral gap: $\lambda_0^{\mathrm{ess}}(\mathrm{H}) > 0$ *if and only if either* (5.12) *holds true or*

$$\sum_{k\geq 0} \frac{|e_k|}{\nu_k} = \infty \quad \textit{and} \quad \sup_{n\geq 0} \sum_{k\leq n} \frac{|e_k|}{\nu_k} \sum_{k\geq n} \mu_k |e_k| < \infty. \tag{5.13}$$

(iii) Discreteness: *The spectrum of* H *is purely discrete if and only if*

- *either* $\sum_{k\geq 0} \frac{|e_k|}{\nu_k} < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\leq n} \mu_k |e_k| \sum_{k\geq n} \frac{|e_k|}{\nu_k} = 0,$$

- *or* $\sum_{k\geq 0} \mu_k |e_k| < \infty$ *and*

$$\lim_{n\to\infty} \sum_{k\leq n} \frac{|e_k|}{\nu_k} \sum_{k\geq n} \mu_k |e_k| = 0.$$

Proof. Let us only give a sketch of the proof (details can be found in, e.g., [149]). First observe that 0 is an eigenvalue of H exactly when $y_1 = \mathbb{1} \in L^2(\mathcal{I};\mu)$, that is, exactly when the series (5.7) converges. Taking this fact into account together with the divergence of (5.6), to prove (i), (ii) and (iii) it suffices to observe that by using a simple change of variables, the operator H is unitarily equivalent to the minimal operator $\widetilde{H}$ defined in the Hilbert space $L^2([0,\mathcal{L}_\nu);\mu_g)$ by the differential expression

$$\tilde{\tau} = -\frac{1}{\mu_g(x)}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

and subject to the Neumann boundary condition at $x = 0$. Here

$$\mu_g := (\mu\cdot\nu)\circ g^{-1},$$

where the function $g\colon [0,\mathcal{L}) \to [0,\infty)$ is given by

$$g(x) = \int_0^x \frac{\mathrm{d}s}{\nu(s)}, \quad \mathcal{L}_\nu := g(\mathcal{L}) = \int_0^{\mathcal{L}} \frac{\mathrm{d}s}{\nu(s)}.$$

Notice that g is strictly increasing, locally absolutely continuous on $[0,\mathcal{L})$ and maps $[0,\mathcal{L})$ onto $[0,\mathcal{L}_\nu)$. Hence its inverse $g^{-1}\colon [0,\mathcal{L}_\nu) \to [0,\mathcal{L})$ is also strictly increasing and locally absolutely continuous on $[0,\mathcal{L})$. Now the remaining claims follow from the results of M. G. Krein and I. S. Kac (see [119, Theorems 1 and 3] or [120, Section 11] and [127]). ∎

Remark 5.8. A few remarks are in order.

(i) Using the quantities in (5.12) and (5.13), one can obtain sharp estimates on $\lambda_0(\mathrm{H})$ and $\lambda_0^{\mathrm{ess}}(\mathrm{H})$ (cf., e.g., [149, 196]).

(ii) If the spectrum of H is discrete, then it consists of simple eigenvalues such that

$$0 \leq \lambda_0(\mathrm{H}) < \lambda_1(\mathrm{H}) < \lambda_2(\mathrm{H}) < \cdots$$

and the Weyl-type asymptotics (5.10) holds true. If the right-hand side in (5.10) is infinite (i.e., $\mathcal{I} = [0,\mathcal{L})$ has infinite intrinsic length), then there are criteria (see [127]) to decide whether the series

$$\sum_{n\geq 1} \frac{1}{\lambda_n(\mathrm{H})^\gamma}$$

converges with some $\gamma > \frac{1}{2}$ (the series diverges for all $\gamma \in (0, \frac{1}{2}]$).

If the spectrum of H is not discrete, the study of spectral types of H is a highly non-trivial problem. However, we would like to mention only one result on the absolutely continuous spectrum established recently in [26].

Lemma 5.9 ([26]). *Assume that $\mathcal{I} = [0, \mathcal{L})$ has infinite intrinsic length,*

$$\int_0^{\mathcal{L}} \sqrt{\frac{\mu(x)}{\nu(x)}}\,\mathrm{d}x = \sum_{k\geq 0} |e_k| \sqrt{\frac{\mu_k}{\nu_k}} = \sum_{k\geq 0} \eta_k = \infty, \tag{5.14}$$

and define the increasing sequence $(t_n)_{n\geq 0} \subset [0, \mathcal{L})$ by setting

$$\int_0^{t_n} \sqrt{\frac{\mu(x)}{\nu(x)}}\,\mathrm{d}x = n, \quad n \in \mathbb{Z}_{\geq 0}.$$

If

$$\sum_{n\geq 0} \Big(\int_{t_n}^{t_n+2} \mu(x)\,\mathrm{d}x \int_{t_n}^{t_n+2} \frac{\mathrm{d}x}{\nu(x)} - 4 \Big) < \infty,$$

then $\sigma_{\mathrm{ac}}(\mathrm{H}) = [0, \infty)$.

Remark 5.10. The operator H also plays an important role in the analysis of Kirchhoff Laplacians on family preserving graphs $(\mathcal{G}, \mu, \nu)$, which are known to reduce to Sturm-Liouville operators (see [30, 31]). In this situation, the weights admit the following description in terms of graph parameters of $\mathcal{G}$ (for simplicity we restrict to the case when the weights in Section 2.1 are constant on $\mathcal{G}$ and hence $\mu = \nu \equiv \mathrm{const}$ in (5.1)):

- $|e_k|$ is the length of edges between the consecutive combinatorial spheres S_k and S_{k+1},
- $\mu_k = \nu_k$ is the number of edges between the consecutive combinatorial spheres S_k and S_{k+1},
- the series (5.7) equals the total volume of the metric graph $\mathcal{G}$.

For instance, for radially symmetric antitrees $\mu_k = s_k s_{k+1}$, where $(s_k)_{k\geq 0} \subseteq \mathbb{Z}_{\geq 1}$ are the antitree sphere numbers [31, 149] (see also Section 8.1 for weighted metric antitrees); for radially symmetric trees $\mu_k = b_0 \dots b_k$, where $(b_k)_{k\geq 0} \subseteq \mathbb{Z}_{\geq 1}$ are the tree branching numbers [196].

In conclusion, let us quickly discuss parabolic properties of Markovian extensions of H^0. We begin with the characterization of Markovian uniqueness. Recall that the

Gaffney Laplacian H_G is defined (see Lemma 2.18) as the restriction of H to H^1 functions, that is,

$$\mathrm{dom}(\mathrm{H}_G) = \{f \in \mathrm{dom}(\mathrm{H}) : f' \in L^2(\mathcal{I};\nu)\}. \tag{5.15}$$

Lemma 5.11. *The operator* H_G *is self-adjoint if and only if* $y_2(x) = \int_0^x \frac{ds}{\nu(s)}$ *does not belong to* $H^1(\mathcal{I})$*, that is, either the series* (5.6) *diverges or* $\mathcal{L}_\nu = \infty$*. If* H_G *is not self-adjoint, then its Markovian restrictions form a one-parameter family*

$$\mathrm{dom}(\mathrm{H}_\theta) := \{f \in \mathrm{dom}(\mathrm{H}_G) : \cos(\theta) f(\mathcal{L}) + \sin(\theta) f_\nu'(\mathcal{L}) = 0\}, \quad \theta \in [0, \tfrac{\pi}{2}]. \tag{5.16}$$

Here $f(\mathcal{L}) = \lim_{x\to\mathcal{L}} f(x)$ *and* $f_\nu'(\mathcal{L}) = \lim_{x\to\mathcal{L}} \nu(x) f'(x)$.

Proof. If H_G is not self-adjoint, then so is H and hence, by Lemma 5.2, the series (5.6) converges. On the other hand, all self-adjoint extensions in this case are parameterized by (5.9). For each $\theta \neq \frac{\pi}{2}$, $\mathrm{dom}(\mathrm{H}_\theta)$ contains functions such that $f_\nu'(\mathcal{L}) = 1$, that is,

$$f'(x) = \frac{1}{\nu(x)}(1 + o(1)) \quad \text{as } x \to \mathcal{L}.$$

However, if $\mathcal{L}_\nu = \infty$, then $f' \notin L^2(\mathcal{I};\nu)$, which implies that H_G admits a unique self-adjoint restriction corresponding to $\theta = \frac{\pi}{2}$. The latter contradicts our assumption that H_G is not self-adjoint since in this case H_G admits at least two different self-adjoint restrictions H_D and H_N. ■

Remark 5.12. Notice that the self-adjointness of H_G is equivalent to the equality $H^1(\mathcal{I}) = H^1_0(\mathcal{I})$, where

$$H^1(\mathcal{I}) = \{f \in AC_{\mathrm{loc}}(\mathcal{I}) : f \in L^2(\mathcal{I};\mu),\ f' \in L^2(\mathcal{I};\nu)\},$$
$$H^1_0(\mathcal{I}) = \overline{H^1(\mathcal{I}) \cap C_c(\mathcal{I})}^{\|\cdot\|_{H^1}}.$$

The next result provides a characterization of transience/recurrence of Markovian restrictions of H_G.

Lemma 5.13. *Let* H_G *be the Gaffney Laplacian* (5.15).

(i) *If* H_G *is self-adjoint, then it is recurrent if and only if* $\mathcal{L}_\nu = \infty$.

(ii) *If* H_G *is not self-adjoint and* H_θ *is its Markovian restriction* (5.16)*, then* H_θ *is recurrent if and only if* $\theta = \frac{\pi}{2}$.

Proof. It is not difficult to show that H_G (or its Markovian restriction when H_G is not self-adjoint) is transient exactly when the Green's function of H_G is well defined at the zero energy, that is, one needs to look at the limit of the resolvent $(\mathrm{H}_G - z)^{-1}$ when $z \uparrow 0$. It remains to use the form of the resolvent of a second order linear differential operator. ■

Finally, let us state the stochastic completeness criterion, which essentially goes back to W. Feller [70].

Lemma 5.14. *Let* H_G *be the Gaffney Laplacian* (5.15).

(i) *If* H_G *is self-adjoint, then it is stochastically incomplete if and only if*

$$\mathcal{L}_\nu < \infty \quad \textit{and} \quad \frac{1}{\nu(x)} \int_0^x \mu(s)\,\mathrm{d}s \in L^1(\mathcal{I}). \tag{5.17}$$

(ii) *If* H_G *is not self-adjoint and* H_θ *is its Markovian restriction* (5.16)*, then* H_θ *is stochastically complete if and only if* $\theta = \frac{\pi}{2}$.

Proof. (i) If H_G is self-adjoint, then stochastic completeness is equivalent to the fact that for some (and hence for all) $\lambda > 0$ the boundary value problem

$$(\nu(x)y')' = \lambda\mu(x)y, \quad y'(0) = 0, \tag{5.18}$$

has only a trivial non-negative bounded solution on $\mathcal{I}$ (see Remark 7.52 below). Integrating (5.18) with $\lambda = 1$ yields

$$y'(x) = \frac{1}{\nu(x)} \int_0^x y(s)\mu(s)\,\mathrm{d}s, \quad x \in [0, \mathcal{L}).$$

Since a solution to (5.18) is unique up to a scalar multiple, we can assume $y(0) = 1$. Clearly, $y \in L^\infty(\mathcal{I})$ exactly when $y' \in L^1(\mathcal{I})$. Thus, if y is bounded, then (5.17) necessarily holds true. Conversely, taking into account that y is non-decreasing, we get

$$0 \le y'(x) \le \frac{y(x)}{\nu(x)} \int_0^x \mu(s)\,\mathrm{d}s =: y(x)b(x), \quad x \in [0, \mathcal{L}).$$

Since $w' = wb$ has a bounded solution on $\mathcal{I}$ satisfying $w(0) = 1$ whenever $b \in L^1(\mathcal{I})$, and taking into account that $y \le w$ on $\mathcal{I}$, this completes the proof of sufficiency.

(ii) If H_G is not self-adjoint, then each Markovian restriction H_θ of H_G has purely discrete, non-negative spectrum. Moreover, each eigenvalue of H_θ is simple. Thus the claim is an immediate consequence of the spectral theorem and the definition of stochastic completeness. ∎

5.2 Connection via boundary triplets

If $\alpha \neq 0$ and, in particular, if α takes negative values on X, the analysis of H_α, the maximal operator associated with (5.3) in $L^2(\mathcal{I}; \mu)$,[1] becomes more involved. In particular, we shall see that there is no transparent self-adjointness criterion.

Consider the interval $\mathcal{I} = [0, \mathcal{L})$ together with the sequence $X = (x_k)_{k\ge0}$ as a metric path graph: $\mathcal{V} = \mathbb{Z}_{\ge0}$ is a vertex set, and $k \sim n$ exactly when $|k - n| = 1$; the length of the edge e_k connecting k with $k + 1$ equals $|e_k| := x_{k+1} - x_k$. Following

[1] The precise definitions of H_α and the corresponding minimal operator H^0_α are given in Section 2.4.1, see (2.18), (2.19) and take into account (5.2).

(3.3)–(3.6) and using (5.11), we define the weight $r\colon \mathbb{Z}_{\geq 0} \to \mathbb{R}_{>0}$ as follows:

- if $\eta^*(X) := \sup_{k\geq 0} \eta_k < \infty$, then
$$r(k) = |e_k|\mu_k, \quad k \geq 0,$$
- if $\eta^*(X) = \infty$, we set
$$r(k) = \begin{cases} |e_k|\mu_k, & \eta_k \leq 1, \\ \sqrt{\mu_k \nu_k}, & \eta_k > 1. \end{cases}$$

Next, we define the weights $m\colon \mathbb{Z}_{\geq 0} \to (0,\infty)$ and $b\colon \mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0} \to [0,\infty)$ by

$$m(k) = \begin{cases} r(0), & k = 0, \\ r(k-1) + r(k), & k \geq 1, \end{cases} \tag{5.19}$$

and

$$b(k,n) = \begin{cases} \dfrac{\nu_{\min(n,k)}}{|x_k - x_n|}, & |n-k| = 1, \\ 0, & |n-k| \neq 1. \end{cases} \tag{5.20}$$

First, we can associate the minimal $\mathbf{h}_\alpha^0$ and the maximal $\mathbf{h}_\alpha$ operators in the weighted Hilbert space $\ell^2(\mathbb{Z}_{\geq 0}; m)$ with the discrete Schrödinger-type expression

$$(\tau f)(k) := \frac{1}{m(k)}\bigg(\sum_{n\geq 0} b(k,n)(f(k) - f(n)) + \alpha_k f(k)\bigg), \quad k \in \mathbb{Z}_{\geq 0}. \tag{5.21}$$

Next, using the map (3.29), we can consider in $\ell^2(\mathbb{Z}_{\geq 0})$ the minimal $\widetilde{\mathbf{h}}_\alpha^0$ and the maximal $\widetilde{\mathbf{h}}_\alpha$ operators, which are unitarily equivalent to $\mathbf{h}_\alpha^0$ and, respectively, $\mathbf{h}_\alpha$. The corresponding difference expression (3.28) is the following second order difference expression

$$(\widetilde{\tau}_\alpha f)(k) = \begin{cases} a_0 f(0) - b_0 f(1), & k = 0, \\ -b_{k-1} f(k-1) + a_k f(k) - b_k f(k+1), & k \geq 1, \end{cases}$$

where

$$a_k = \frac{1}{m(k)}\bigg(\alpha_k + \frac{\nu_{k-1}}{|e_{k-1}|} + \frac{\nu_k}{|e_k|}\bigg), \quad b_k = \frac{\nu_k}{|e_k|\sqrt{m(k)m(k+1)}}, \tag{5.22}$$

for all $k \geq 0$ with $\nu_{-1}/|e_{-1}| = 0$ for notational simplicity. Hence the operator $\widetilde{\mathbf{h}}_\alpha$ is nothing but the maximal operator associated in $\ell^2(\mathbb{Z}_{\geq 0})$ with the Jacobi (tri-diagonal) matrix

$$J = \begin{pmatrix} a_0 & -b_0 & 0 & 0 & \dots \\ -b_0 & a_1 & -b_1 & 0 & \dots \\ 0 & -b_1 & a_2 & -b_2 & \dots \\ 0 & 0 & -b_2 & a_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{5.23}$$

Therefore, Theorem 3.1 establishes connections between the operator (5.3) and spectral theory of Jacobi (tri-diagonal) matrices. We would like to present only one claim regarding self-adjointness.

Theorem 5.15. *Let* $\widetilde{\mathbf{h}}_\alpha^0$ *be the minimal operator defined in* $\ell^2(\mathbb{Z}_{\geq 0})$ *by the Jacobi matrix* (5.23) *with Jacobi parameters* (5.22)*. Then the deficiency indices of* H_α^0 *and* $\widetilde{\mathbf{h}}_\alpha^0$ *are equal and*

$$\mathrm{n}_+(\mathrm{H}_\alpha^0) = \mathrm{n}_-(\mathrm{H}_\alpha^0) = \mathrm{n}_\pm(\widetilde{\mathbf{h}}_\alpha^0) \leq 1.$$

In particular, H_α *is self-adjoint if and only if* $\widetilde{\mathbf{h}}_\alpha$ *is self-adjoint.*

Applying spectral theory of Jacobi matrices and using Theorem 3.1, we would be able to investigate spectral properties of the operators H_α and this approach was taken in [143, Section 5.2] for the case $\mu = \nu \equiv \mathbb{1}$. Let us only provide some simple self-adjointness criteria.

Lemma 5.16. *Let* H_α *be the maximal operator defined by* (5.3) *in* $L^2(\mathcal{I};\mu)$*.*

(i) *If the series*

$$\sum_{k\geq 0} \eta_k^2 = \sum_{k\geq 0} |e_k|^2 \frac{\mu_k}{\nu_k} \tag{5.24}$$

diverges, then H_α *is self-adjoint for any* α*.*

(ii) *If* $\mathcal{I}$ *has infinite intrinsic length, i.e.,* (5.14) *holds, and* $\alpha\colon X \to \mathbb{R}$ *is such that* $\widetilde{\mathbf{h}}_\alpha^0$ *is bounded from below, then* H_α *is self-adjoint and bounded from below.*

Proof. (i) By the Carleman test [2, Problem I.1], $\widetilde{\mathbf{h}}_\alpha^0$ is self-adjoint if the series

$$\sum_{k\geq 0} \frac{1}{b_k} \tag{5.25}$$

diverges. However,

$$\frac{1}{b_k} = \frac{|e_k|\sqrt{m(k)m(k+1)}}{\nu_k} \geq \frac{|e_k|r(k)}{\nu_k} \geq \begin{cases} \eta_k^2, & \eta_k \leq 1, \\ 1, & \eta_k > 1. \end{cases} \tag{5.26}$$

Therefore, (5.25) diverges if so is (5.24). It remains to apply Theorem 5.15.

(ii) By the Wouk test [2, Problem I.4], $\widetilde{\mathbf{h}}_\alpha^0$ is self-adjoint if it is bounded from below and

$$\sum_{k\geq 0} \frac{1}{\sqrt{b_k}} = \infty.$$

It remains to take into account (5.26) and then apply Theorem 5.15. ■

Remark 5.17. One can apply other self-adjointness tests (see, e.g., [2, Chapter I]) to J with the Jacobi parameters given by (5.22) in order to get various self-adjointness conditions for the operator H_α (cf., e.g., [143, Section 5]). For instance, Berezanskii's test [2, Problem I.5] would lead to examples with non-trivial deficiency indices even if (5.14) is satisfied.

5.3 Jacobi matrices and Krein–Stieltjes strings as boundary operators

The results in the previous section connect spectral properties of Sturm–Liouville operators with a certain family of Jacobi matrices. The natural question arising in this context is:

How large is the class of Jacobi matrices with Jacobi parameters (5.22)?

The next result shows that for each choice of Jacobi parameters $(a_k, b_k)_{k\geq 0}$ one can find weights μ, ν and strengths α such that (5.22) holds.

Proposition 5.18. *For every symmetric Jacobi (tri-diagonal) matrix (5.23) normalized by the condition $b_k > 0$ for all $k \geq 0$ there exist lengths $(|e_k|)_{k\geq 0} \subset \mathbb{R}_{>0}$, weights $(\nu_k)_{k\geq 0} \subset \mathbb{R}_{>0}$ and strengths $(\alpha_k)_{k\geq 0} \subset \mathbb{R}$ such that:*

(i) Normalization: *lengths $(|e_k|)_{k\geq 0}$ and weights $(\nu_k)_{k\geq 0}$ satisfy*

$$\eta_k = \frac{|e_k|}{\sqrt{\nu_k}} \leq 1 \tag{5.27}$$

for all $k \geq 0$.

(ii) Jacobi parameters *have the form*

$$a_k = \frac{1}{|e_{k-1}| + |e_k|}\left(\alpha_k + \frac{\nu_{k-1}}{|e_{k-1}|} + \frac{\nu_k}{|e_k|}\right), \tag{5.28}$$

$$b_k = \frac{\nu_k}{|e_k|\sqrt{(|e_{k-1}| + |e_k|)(|e_k| + |e_{k+1}|)}} \tag{5.29}$$

for all $k \geq 0$.

(iii) Boundary operator: *the minimal operator $\widetilde{\mathbf{h}}$ associated in $\ell^2(\mathbb{Z}_{\geq 0})$ with the matrix (5.23) having Jacobi parameters (5.28)–(5.29) serves as a boundary operator (in the sense of Proposition 3.11) for the minimal operator $\mathrm{H}^0 = \mathrm{H}^0_{\mathbb{1},\nu,\alpha}$ defined by the differential expression*

$$\tau_{\nu,\alpha} = -\frac{\mathrm{d}}{\mathrm{d}x}\nu(x)\frac{\mathrm{d}}{\mathrm{d}x} + \sum_{k\geq 0}\alpha_k\delta(x - x_k), \tag{5.30}$$

in the Hilbert space $L^2(\mathcal{I})$. Here $\mathcal{I} = [0, \mathcal{L})$ and the weight $\nu\colon \mathcal{I} \to \mathbb{R}_{>0}$ is defined by

$$x_k = \sum_{j=0}^{k-1}|e_j|, \quad \mathcal{L} = \sum_{k\geq 0}|e_k|, \quad \nu(x) = \sum_{k\geq 0}\nu_k \mathbb{1}_{[x_k, x_{k+1})}(x). \tag{5.31}$$

Proof. Since $\alpha_k \in \mathbb{R}$ in (5.22) can be chosen arbitrary, the main difficulty is of course to show that every sequence $(b_k)_{k\geq 0}$ of positive real numbers can be realized as (5.22). Let $(b_k)_{k\geq 0} \subset (0,\infty)$ be given. First set $|e_0| = 1$. Then (5.29) holds for $k = 0$ if

$$|e_1| = \frac{\nu_0^2}{b_0^2} - 1.$$

If $b_0 < 1$, we set $\nu_0 = 1$ and define $|e_1|$ by the above equation, otherwise, we set $\nu_0 = \sqrt{2}b_0 > 1$ and $|e_1| = 1$. Clearly, both (5.27) and (5.29) hold true for $k = 0$.

Next we proceed inductively. Assume we have already defined positive numbers $\nu_0, \dots, \nu_{n-1}$ and $|e_0|, \dots, |e_n|$ such that (5.29) holds for $k = 0, \dots, n-1$. Set

$$s_n := \frac{|e_n|}{\sqrt{|e_{n-1}| + |e_n|}\sqrt{|e_n| + 1}}.$$

If $s_n \leq b_n$, we set

$$|e_{n+1}| = 1, \quad \nu_n = \frac{b_n}{s_n}|e_n|^2 \geq |e_n|^2,$$

and otherwise we choose

$$|e_{n+1}| = \frac{s_n^2}{b_n^2}(1 + |e_n|) - |e_n| > 1, \quad \nu_n = |e_n|^2.$$

Clearly, by construction, both (5.27) and (5.29) hold true for $k = n$. Therefore, proceeding inductively, we obtain sequences of lengths $(|e_k|)_{k\geq 0}$ and weights $(\nu_k)_{k\geq 0}$ such that (5.29) holds together with (5.27). ■

Remark 5.19. A few remarks are in order.

(i) Combining Proposition 5.18 with Theorem 3.1, we conclude that basic spectral theory of Jacobi matrices (e.g., self-adjointness, semiboundedness, etc.) can be included into the spectral theory of Sturm–Liouville operators of the form (5.30)–(5.31).

(ii) The choice of lengths and weights is not unique. Indeed, taking into account that (3.1)–(3.6) are invariant under the scaling $|e| \to |e|c(e)$, $\mu(e) \to \frac{\mu(e)}{c(e)}$, and $\nu(e) \to \nu(e)c(e)$ for any $c\colon \mathcal{E} \to (0,\infty)$, one can rescale parameters and construct lengths and weights with the following properties:
- $|e_k| \leq 1$ and $\mu_k = \nu_k$ for all $k \geq 0$ (hence $\mu = \nu$ in (5.3)),
- $\nu_k = 1$ and $|e_k|^2\mu_k \leq 1$ for all $k \geq 0$ (hence $\nu \equiv 1$ in (5.3)),
- $|e_k| = 1$ and $\mu_k \leq \nu_k$ for all $k \geq 0$ (hence $X = \mathbb{N}$ in (5.3)).

(iii) Let us also stress that for Jacobi (tri-diagonal) matrices (5.23) still there is no self-adjointness criterion formulated in closed form in terms of Jacobi parameters (there are only various necessary and sufficient conditions). This in particular means that even in the simplest case of a weighted path graph one cannot hope for a transparent self-adjointness criterion formulated in terms of weights and interaction strengths.

If $\alpha \geq 0$, then the Hamiltonian H_α generates a Markovian semigroup in $L^2(\mathcal{I};\mu)$ (assume, for a moment, that H_α is self-adjoint). However, the boundary operator $\widetilde{\mathbf{h}}_\alpha$ does not reflect the parabolic properties of H_α (it is not difficult to see that the semigroup generated by $\widetilde{\mathbf{h}}_\alpha$ in $\ell^2(\mathbb{Z}_{\geq 0})$ is positivity preserving, however, in general it is not ℓ^∞ contractive). From this perspective, let us look at the minimal operator $\mathbf{h}^0$ defined in $\ell^2(\mathbb{Z}_{\geq 0}; m)$ by (5.21) with the coefficients (5.19) and (5.20) and $\alpha \equiv 0$. It serves as the boundary operator for the Sturm–Liouville operator H, however, it also captures the parabolic properties of H (see Chapter 4). Following the setting of Section 2.2, every weight function b given by (5.20) defines an infinite path graph. Since the coefficients of b depend only on the weight ν and edge lengths, it is clear that every weighted path graph can be obtained via (5.20). However, the difference expression (5.21) (see (3.7)) also contains the vertex weight m defined by (5.19). Thus, we can reformulate the question posed at the very beginning of Section 5.3 as follows:

Does every path graph b over $(\mathbb{Z}_{\geq 0}, m)$ arise as a boundary operator for H*?*

Taking into account Proposition 5.18, the answer may look a bit surprising.

Proposition 5.20. *Let $m\colon \mathbb{Z}_{\geq 0} \to (0,\infty)$ and $b\colon \mathbb{Z}_{\geq 0} \times \mathbb{Z}_{\geq 0} \to [0,\infty)$ be positive weights such that b defines an infinite path graph (i.e., $b(k,n) = b(n,k) > 0$ exactly when $|k-n| = 1$). Then the minimal operator $\mathbf{h}^0$ associated in $\ell^2(\mathbb{Z}_{\geq 0}; m)$ with the weighted Laplacian*

$$(\tau f)(k) := \frac{1}{m(k)} \sum_{n\geq 0} b(n,k)(f(k) - f(n)), \quad k \in \mathbb{Z}_{\geq 0}, \tag{5.32}$$

arises as a boundary operator for some Sturm–Liouville operator (5.4) with the weights (5.1) if and only if

$$\sum_{k=0}^{n} (-1)^{n-k} m(k) > 0 \tag{5.33}$$

for all $n \geq 0$.

Proof. The necessity of (5.33) follows from (5.19) since $m(0) = r(0) > 0$ and for all $n \geq 1$ we have

$$\begin{aligned}\sum_{k=0}^{n} (-1)^{n-k} m(k) &= (-1)^n m(0) + \sum_{k\geq 1}^{n} (-1)^{n-k} (r(k-1) + r(k)) \\ &= r(n) > 0.\end{aligned}$$

To prove sufficiency, suppose that $m\colon \mathbb{Z}_{\geq 0} \to (0,\infty)$ satisfies (5.33) for all $n \geq 0$ and set $b(k) := b(k,k+1)$, $k \geq 0$. Thus the left-hand side of (5.33) defines a positive sequence $r\colon \mathbb{Z}_{\geq 0} \to (0,\infty)$. Setting

$$|e_k| := \begin{cases} \sqrt{\dfrac{r(k)}{b(k)}}, & r(k) \leq b(k), \\ \dfrac{r(k)}{b(k)}, & r(k) > b(k), \end{cases} \qquad \mu_k := \begin{cases} \sqrt{r(k)b(k)}, & r(k) \leq b(k), \\ r(k), & r(k) > b(k), \end{cases}$$

for all $k \geq 0$, we end up with a suitable and, in fact unique, choice of the weight function

$$\mu(x) = \sum_{k\geq 0} \mu_k \mathbb{1}_{[x_k, x_{k+1})}, \quad x_k = \sum_{j=0}^{k-1} |e_j|,$$

such that the minimal operator $\mathbf{h}^0$ associated in $\ell^2(\mathbb{Z}; m)$ with (5.32) is the boundary operator for H^0 associated with (5.4) (with the weights $\mu = \nu$). ■

Remark 5.21. Surprisingly enough, we are not able to obtain all difference expressions of the form (3.7) even in the simplest case of a path graph. The main restriction is the form of the weight function m. More precisely, the *formal Laplacian* L associated to a path graph b over the measure space $(\mathbb{Z}_{\geq 0}, m)$ can be obtained via (5.19) and (5.20) only if the weight function m belongs to the image of the cone of strictly positive functions $C^+(\mathbb{Z}_{\geq 0})$ under the map $\mathrm{I} + \mathcal{S}$, where $\mathcal{S}$ is the right shift operator defined on $C(\mathbb{Z}_{\geq 0})$ by

$$\mathcal{S}\colon (f(k))_{k\geq 0} \mapsto (f(k-1))_{k\geq 0},$$

where $f(-1) := 0$ for notational simplicity. Indeed, with this notation (5.19) takes the form

$$m = (\mathrm{I} + \mathcal{S})r,$$

and then the validity of (5.33) for all $n \geq 0$ is exactly the inclusion $m \in C^+(\mathbb{Z}_{\geq 0})$.

Remark 5.22 (Krein–Stieltjes strings). Set

$$\ell_k = \frac{1}{b(k,k+1)} = \frac{|e_k|}{\nu_k}, \quad \xi_k = \sum_{j=0}^{k-1} \ell_j, \quad \omega_k = m(k)$$

for all $k \geq 0$. Next define the positive measure ω on $[0,\ell)$, where $\ell := \sum_{k\geq 0} \ell_k$, by

$$\omega([0,\xi)) := \sum_{\xi_k \leq \xi} \omega_k.$$

If $\alpha_k = 0$ for all $k \geq 0$, then the spectral problem $\tau f = zf$ associated with the difference expression (5.21), (5.19), (5.20) admits a mechanical interpretation (see [2, Appendix], [120, Section 13]): it describes small oscillations of a string of length ℓ with mass density ω. The corresponding spectral problem can be written as

$$-y'' = z\omega y, \quad \xi \in [0,\ell),$$

which is similar to the form of (5.4), however, the coefficient ω is a measure bearing point masses only. Strings whose mass density has the above form are usually called *Krein–Stieltjes strings* (the corresponding finite difference expressions appear in the study of the Stieltjes moment problem and their mechanical interpretation was observed by M. G. Krein [120]). Thus, the results of this section establish a connection between two classes of strings: strings whose mass density is piecewise constant and Krein–Stieltjes strings. However, Proposition 5.20 says that we cannot cover the whole class of Krein–Stieltjes strings.