

Chapter 3

Connections via boundary triplets

To simplify the exposition, we begin by looking at a weighted metric graph (\mathcal{G}, μ, ν) as a metric realization of one of its models, that is, we start with a given combinatorial graph $\mathcal{G}_d = (\mathcal{V}, \mathcal{E})$ equipped with edge lengths $|\cdot|: \mathcal{E} \rightarrow (0, \infty)$ and weights $\mu, \nu: \mathcal{E} \rightarrow (0, \infty)$. Let also $\alpha: \mathcal{V} \rightarrow \mathbb{R}$, that is, we are going to consider Laplacians with δ -couplings (2.13) at vertices. The main results of this chapter (see Theorem 3.1 and Theorem 3.22 below) relate basic spectral properties of the Laplacian with δ -couplings \mathbf{H}_α with those of a certain Schrödinger-type operator on the corresponding combinatorial graph \mathcal{G}_d . At the very end of this chapter, in Section 3.3, we shall look at a weighted metric graph from the metric space perspective, which allows to understand the whole family of graph Laplacians associated with the models of a given weighted metric graph.

Let us stress once again that we always assume Hypothesis 2.1.

3.1 Spectral properties: Graph Laplacians vs. Kirchhoff Laplacians

To state the result, we first define the *intrinsic edge length*

$$\eta(e) := |e| \sqrt{\frac{\mu(e)}{\nu(e)}}, \quad e \in \mathcal{E}, \quad (3.1)$$

together with the quantity¹

$$\eta^*(\mathcal{E}) := \sup_{e \in \mathcal{E}} \eta(e). \quad (3.2)$$

Now introduce the edge weight $r: \mathcal{E} \rightarrow (0, \infty)$ by distinguishing two cases:

- if the underlying model of a weighted metric graph satisfies $\eta^*(\mathcal{E}) < \infty$, then we set

$$r(e) = |e| \mu(e), \quad e \in \mathcal{E}, \quad (3.3)$$

- if $\eta^*(\mathcal{E}) = \infty$, we define the weight r by

$$r(e) = \begin{cases} |e| \mu(e), & \eta(e) \leq 1, \\ \sqrt{\mu(e)\nu(e)}, & \eta(e) > 1. \end{cases} \quad (3.4)$$

¹In Section 3.3, we shall call it *the intrinsic size of a model* and its meaning will be clarified in Chapter 6 (see Remark 6.19).

Next, with a given metric graph \mathcal{G} and weights μ, ν we associate:

- the *vertex weight* $m: \mathcal{V} \rightarrow (0, \infty)$,

$$m(v) = \sum_{\bar{e} \in \bar{\mathcal{E}}_v} r(e), \quad v \in \mathcal{V}, \quad (3.5)$$

- the *edge weight* $b: \mathcal{V} \times \mathcal{V} \rightarrow [0, \infty)$,

$$b(u, v) = \begin{cases} \sum_{\bar{e} \in \bar{\mathcal{E}}_u, e \in \mathcal{E}_v} \frac{\nu(e)}{|e|}, & u \neq v, \\ 0, & u = v, \end{cases} \quad (u, v) \in \mathcal{V} \times \mathcal{V}. \quad (3.6)$$

It is straightforward to verify that b satisfies all properties (i)–(iv) of Section 2.2. Since \mathcal{G}_d is connected, so is the edge weight b . Moreover, the vertex weight m is strictly positive on \mathcal{V} and hence defines a measure of full support on \mathcal{V} . Therefore, following considerations in Section 2.2, with the discrete Schrödinger expression

$$(\tau f)(v) := \frac{1}{m(v)} \left(\sum_{u \in \mathcal{V}} b(v, u)(f(v) - f(u)) + \alpha(v)f(v) \right), \quad v \in \mathcal{V}, \quad (3.7)$$

we can associate in the weighted Hilbert space $\ell^2(\mathcal{V}; m)$ the minimal operator \mathbf{h}_α^0 and the maximal operator \mathbf{h}_α .

The main aim of this section is to prove the following result:

Theorem 3.1. *Let \mathbf{H}_α^0 be the minimal Laplacian on (\mathcal{G}, μ, ν) equipped with the δ -coupling conditions (2.13) at the vertices and let also \mathbf{h}_α^0 be the corresponding minimal discrete Schrödinger operator defined in $\ell^2(\mathcal{V}; m)$ by (3.7). Then:*

- (i) *The deficiency indices of \mathbf{H}_α^0 and \mathbf{h}_α^0 are equal and*

$$n_+(\mathbf{H}_\alpha^0) = n_-(\mathbf{H}_\alpha^0) = n_\pm(\mathbf{h}_\alpha^0) \leq \infty.$$

In particular, \mathbf{H}_α is self-adjoint if and only if \mathbf{h}_α is self-adjoint.

Assume in addition that \mathbf{H}_α (and hence also \mathbf{h}_α) is self-adjoint. Then:

- (ii) *The operator \mathbf{H}_α is lower semibounded if and only if the operator \mathbf{h}_α is lower semibounded.*
- (iii) *The operator \mathbf{H}_α is non-negative if and only if \mathbf{h}_α is non-negative.*
- (iv) *The total multiplicities of negative spectra of \mathbf{H}_α and \mathbf{h}_α coincide,*

$$\kappa_-(\mathbf{H}_\alpha) = \kappa_-(\mathbf{h}_\alpha).$$

- (v) *The spectrum of \mathbf{H}_α is purely discrete if and only if $\#\{e \in \mathcal{E} : \eta(e) > \varepsilon\}$ is finite for every $\varepsilon > 0$ and the spectrum of \mathbf{h}_α is purely discrete.*

Assume also that $\eta^*(\mathcal{E}) = \sup_{e \in \mathcal{E}} \eta(e) < \infty$. Then:

- (vi) The operator \mathbf{H}_α is positive definite if and only if \mathbf{h}_α is positive definite.
- (vii) If, in addition, the operator \mathbf{h}_α is lower semibounded, then $\lambda_0^{\text{ess}}(\mathbf{H}_\alpha) > 0$ ($\lambda_0^{\text{ess}}(\mathbf{H}_\alpha) = 0$) exactly when $\lambda_0^{\text{ess}}(\mathbf{h}_\alpha) > 0$ (respectively, $\lambda_0^{\text{ess}}(\mathbf{h}_\alpha) = 0$).
- (viii) Moreover, the equivalence

$$\mathbf{H}_\alpha^- \in \mathfrak{S}_p(L^2) \iff \mathbf{h}_\alpha^- \in \mathfrak{S}_p(\ell^2)$$

holds for all $p \in (0, \infty]$. In particular, the negative spectrum of \mathbf{H}_α is discrete if and only if so is the negative spectrum of \mathbf{h}_α .

Here and below for a self-adjoint operator T in a Hilbert space \mathfrak{H} , $\lambda_0(T)$ and $\lambda_0^{\text{ess}}(T)$ denote the bottoms of its spectrum, respectively, of its essential spectrum,

$$\lambda_0(T) = \inf \sigma(T), \quad \lambda_0^{\text{ess}}(T) = \inf \sigma_{\text{ess}}(T).$$

Moreover,

$$T^- := T \mathbb{1}_{(-\infty, 0)}(T),$$

where $\mathbb{1}_{(-\infty, 0)}(T)$ is the spectral projection on the negative subspace of T .

As an immediate corollary we obtain the following result for the Kirchhoff Laplacian.

Corollary 3.2. *Let \mathbf{H}^0 be the minimal Kirchhoff Laplacian on (\mathcal{G}, μ, ν) and let also \mathbf{h}^0 be the corresponding minimal weighted graph Laplacian defined in $\ell^2(\mathcal{V}; m)$ by (3.7) with $\alpha \equiv 0$. Then:*

- (i) The deficiency indices of \mathbf{H}^0 and \mathbf{h}^0 are equal and

$$n_+(\mathbf{H}^0) = n_-(\mathbf{H}^0) = n_\pm(\mathbf{h}^0) \leq \infty.$$

In particular, \mathbf{H}^0 is self-adjoint if and only if \mathbf{h}^0 is self-adjoint.

Assume in addition that \mathbf{H}^0 is self-adjoint (and hence coincides with the maximal Kirchhoff Laplacian \mathbf{H}). Then:

- (ii) The spectrum of \mathbf{H} is purely discrete if and only if $\#\{e \in \mathcal{E} : \eta(e) > \varepsilon\}$ is finite for every $\varepsilon > 0$ and the spectrum of the operator \mathbf{h} is purely discrete.

Assume also that $\sup_{e \in \mathcal{E}} \eta(e) < \infty$. Then:

- (iii) The operator \mathbf{H} is positive definite, $\lambda_0(\mathbf{H}) > 0$ if and only if the operator \mathbf{h} is positive definite, $\lambda_0(\mathbf{h}) > 0$.
- (iv) $\lambda_0^{\text{ess}}(\mathbf{H}) > 0$ exactly when $\lambda_0^{\text{ess}}(\mathbf{h}) > 0$.

Proof. The proof is a straightforward application of Theorem 3.1 to the case $\alpha \equiv 0$. One only needs to take into account that both the minimal Kirchhoff Laplacian \mathbf{H}^0 and the minimal graph Laplacian \mathbf{h}^0 are non-negative operators. \blacksquare

Remark 3.3. A few remarks are in order.

- (i) In the case $\eta^*(\mathcal{E}) = \infty$ the weight r can be chosen in many different ways by changing the threshold 1 in (3.4) to any positive number.
- (ii) In the following specific case

$$\inf_{e \in \mathcal{E}} \eta(e) > 0,$$

the choice of r can be further simplified to

$$r(e) := \sqrt{\mu(e)\nu(e)}, \quad e \in \mathcal{E}.$$

Notice that if $\mu = \nu \equiv \mathbb{1}$, the assumption $\inf_{e \in \mathcal{E}} \eta(e) > 0$ is equivalent to $\inf_{e \in \mathcal{E}} |e| > 0$, which is the most common restriction in the spectral theory of quantum graphs [25, 182]. In this case $r(e) \equiv 1$ for all $e \in \mathcal{E}$ and hence the vertex weight m given by (3.5) is nothing but the combinatorial degree (2.2).

- (iii) In the papers [68, 143] it is assumed that $\mu = \nu \equiv \mathbb{1}$ and $\sup_{e \in \mathcal{E}} \eta(e) = \sup_{e \in \mathcal{E}} |e| < \infty$. Usually, the latter is not a restriction since this condition can always be achieved by adding inessential vertices, that is by choosing an appropriate model of a metric graph since this choice does not have any impact on spectral properties of the corresponding Kirchhoff Laplacian (see Section 2.4.3). However, this changes the combinatorial structure of the underlying graph \mathcal{G}_d , which is important for our future purposes. This will be discussed in greater details in Section 3.3.
- (iv) Let us also mention that the list of equivalences in Theorem 3.1 is not complete and we refer to, e.g., [68] for further details.

3.2 Graph Laplacians as boundary operators

This section is devoted to the proof of Theorem 3.1, which is based on the boundary triplets approach (see Appendix A) and essentially follows the lines of [68].

3.2.1 Edge-based boundary triplet

We begin with constructing a suitable boundary triplet for the operator \mathbf{H}_{\max} . First of all, the following simple fact holds true (cf. [68, Lemma 2.1]).

Lemma 3.4. *Let $H_{e,\max}$, $e \in \mathcal{E}$ be the maximal operator (2.16). The triplet*

$$\tilde{\Pi}_e = \{\mathbb{C}^2, \tilde{\Gamma}_{0,e}, \tilde{\Gamma}_{1,e}\},$$

where the mappings $\tilde{\Gamma}_{0,e}, \tilde{\Gamma}_{1,e}: H^2(e) \rightarrow \mathbb{C}^2$ are defined by

$$\tilde{\Gamma}_{0,e}: f \mapsto \begin{pmatrix} f(e_l) \\ f(e_\tau) \end{pmatrix}, \quad \tilde{\Gamma}_{1,e}: f \mapsto \begin{pmatrix} v(e)\partial f(e_l) \\ v(e)\partial f(e_\tau) \end{pmatrix}, \quad (3.8)$$

is a boundary triplet for $\mathbf{H}_{e,\max}$. The corresponding Weyl function is

$$\tilde{M}_e: z \mapsto \sqrt{\mu(e)v(e)z} \begin{pmatrix} -\cot(\eta(e)\sqrt{z}) & \csc(\eta(e)\sqrt{z}) \\ \csc(\eta(e)\sqrt{z}) & -\cot(\eta(e)\sqrt{z}) \end{pmatrix}, \quad z \in \mathbb{C} \setminus \mathbb{R}.$$

Next we proceed as follows (see, e.g., [143, Section 4] and also [68, Section 2]): set

$$\mathbf{R}_e := r(e) \mathbf{I}_2, \quad \mathbf{Q}_e := \lim_{z \rightarrow 0} \tilde{M}_e(z) = \frac{v(e)}{|e|} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (3.9)$$

where $r: \mathcal{E} \rightarrow (0, \infty)$ is given by (3.3), (3.4). Define the mappings

$$\Gamma_{0,e} := \mathbf{R}_e^{1/2} \tilde{\Gamma}_{0,e}, \quad \Gamma_{1,e} := \mathbf{R}_e^{-1/2} (\tilde{\Gamma}_{1,e} - \mathbf{Q}_e \tilde{\Gamma}_{0,e}),$$

that is, $\Gamma_{0,e}, \Gamma_{1,e}: H^2(e) \rightarrow \mathbb{C}^2$ are given by

$$\Gamma_{0,e}: f \mapsto \sqrt{r(e)} \begin{pmatrix} f(e_l) \\ f(e_\tau) \end{pmatrix}, \quad \Gamma_{1,e}: f \mapsto \frac{v(e)}{\sqrt{r(e)}} \begin{pmatrix} \partial f(e_l) - \frac{f(e_\tau) - f(e_l)}{|e|} \\ \partial f(e_\tau) + \frac{f(e_\tau) - f(e_l)}{|e|} \end{pmatrix}. \quad (3.10)$$

Clearly, $\Pi_e = \{\mathbb{C}^2, \Gamma_{0,e}, \Gamma_{1,e}\}$ is also a boundary triplet for $\mathbf{H}_{e,\max}$. In addition, the following claim holds (cf. [143, Theorem 4.1] and [68, Theorem 2.2]).

Proposition 3.5. *The direct sum of boundary triplets*

$$\Pi_{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \Pi_e = \{\mathcal{H}_{\mathcal{E}}, \Gamma_0^{\mathcal{E}}, \Gamma_1^{\mathcal{E}}\},$$

where

$$\mathcal{H}_{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \mathbb{C}^2, \quad \Gamma_0^{\mathcal{E}} := \bigoplus_{e \in \mathcal{E}} \Gamma_{0,e}, \quad \Gamma_1^{\mathcal{E}} := \bigoplus_{e \in \mathcal{E}} \Gamma_{1,e},$$

is a boundary triplet for the operator $\mathbf{H}_{\max} = \bigoplus_{e \in \mathcal{E}} \mathbf{H}_{e,\max}$.

Proof. Since $\mathbf{H}_{e,\max}^*$ is a positive symmetric operator for every $e \in \mathcal{E}$, so is \mathbf{H}_{\max}^* . Therefore, we need to apply Theorem A.11 and to verify conditions (A.7). Notice that for each $e \in \mathcal{E}$, the corresponding Weyl function is given by

$$M_e(z) = \mathbf{R}_e^{-1/2} (\tilde{M}_e(z) - \mathbf{Q}_e) \mathbf{R}_e^{-1/2} = \frac{1}{r(e)} \tilde{M}_e(z) - \frac{1}{r(e)} \mathbf{Q}_e.$$

(i) First of all, straightforward calculations yield that for all $e \in \mathcal{E}$,

$$M_e(-1) = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \begin{pmatrix} \frac{1}{\eta(e)} - \coth \eta(e) & \frac{1}{\sinh \eta(e)} - \frac{1}{\eta(e)} \\ \frac{1}{\sinh \eta(e)} - \frac{1}{\eta(e)} & \frac{1}{\eta(e)} - \coth \eta(e) \end{pmatrix},$$

and

$$M'_e(-1) = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \begin{pmatrix} \coth \eta(e) - \frac{\eta(e)}{\sinh^2 \eta(e)} & \frac{\eta(e) \cosh \eta(e)}{\sinh^2 \eta(e)} - \frac{1}{\sinh \eta(e)} \\ \frac{\eta(e) \cosh \eta(e)}{\sinh^2 \eta(e)} - \frac{1}{\sinh \eta(e)} & \coth \eta(e) - \frac{\eta(e)}{\sinh^2 \eta(e)} \end{pmatrix},$$

where $r(e)$ is given by (3.4). Clearly, $\|M_e(-1)\| = \max(|\lambda_+(M_e)|, |\lambda_-(M_e)|)$, where $\lambda_+(M_e)$ and $\lambda_-(M_e)$ are the eigenvalues of $M_e(-1)$ given explicitly by

$$\lambda_{\pm}(M_e) = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \left(\frac{1}{\eta(e)} - \coth \eta(e) \pm \left(\frac{1}{\sinh \eta(e)} - \frac{1}{\eta(e)} \right) \right).$$

Since $|\lambda_+(M_e)| > |\lambda_-(M_e)|$, we get

$$\|M_e(-1)\| = |\lambda_+(M_e)| = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \frac{\cosh \eta(e) - 1}{\sinh \eta(e)} = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \tanh \left(\frac{\eta(e)}{2} \right).$$

Similarly, one obtains that

$$\begin{aligned} \|M'_e(-1)\| &= \lambda_+(M'_e) = \frac{\sqrt{\mu(e)v(e)}}{r(e)} \frac{(\sinh \eta(e) + \eta(e))(\cosh \eta(e) - 1)}{2 \sinh^2 \eta(e)}, \\ \|(M'_e(-1))^{-1}\| &= \frac{1}{\lambda_-(M'_e)} = \frac{r(e)}{\sqrt{\mu(e)v(e)}} \frac{2 \sinh^2 \eta(e)}{(\sinh \eta(e) - \eta(e))(\cosh \eta(e) + 1)}, \end{aligned}$$

where $\lambda_+(M'_e)$ and $\lambda_-(M'_e)$ are the eigenvalues of $M'_e(-1)$.

(ii) Assume first that $\eta^*(\mathcal{E}) < \infty$. Then $r(e) = \mu(e)|e|$, $e \in \mathcal{E}$ and in particular,

$$\|M_e(-1)\| \leq \sup_{0 < s \leq \eta^*(\mathcal{E})} \frac{1}{s} \tanh \left(\frac{s}{2} \right) = \sup_{0 < s \leq \eta^*(\mathcal{E})} f(s).$$

Since the function $f(s)$ defined by the right-hand side admits an analytic continuation at 0, we conclude that $\sup_e M_e(-1) < \infty$. Similar considerations imply that

$$\sup_e (\|M'_e(-1)\| + \|(M'_e(-1))^{-1}\|) < \infty$$

and hence (A.7) holds true in this case.

(iii) Suppose now that $\eta^*(\mathcal{E}) = \infty$. If $e \in \mathcal{E}$ is an edge with $\eta(e) > 1$, then we get $r(e) = \sqrt{\mu(e)v(e)}$ and hence

$$\|M_e(-1)\| \leq \sup_{s>1} \tanh \left(\frac{s}{2} \right) = 1$$

and

$$\begin{aligned} \|M'_e(-1)\| &\leq \sup_{s>1} \frac{(\sinh s + s)(\cosh s - 1)}{2 \sinh^2 s} < \infty, \\ \|(M'_e(-1))^{-1}\| &\leq \sup_{s>1} \frac{2 \sinh^2 s}{(\sinh s - s)(\cosh s + 1)} < \infty. \end{aligned}$$

On the other hand, if $\eta(e) \leq 1$, then $r(e) = \mu(e)|e|$ as in (ii), and the same steps as there give uniform bounds on $\|M_e(-1)\|$, $\|M'_e(-1)\|$ and $\|(M'_e(-1))^{-1}\|$. Altogether, we conclude that the condition (A.7) holds true and this completes the proof. ■

Remark 3.6. It is easy to see that Proposition 3.5 holds true if instead of (3.4) the weight r is defined as in Remark 3.3 (i).

Clearly, the Weyl function corresponding to the boundary triplet constructed in Proposition 3.5 has a very transparent form and enjoys some important properties.

Lemma 3.7. *The Weyl function corresponding to the boundary triplet $\Pi_{\mathcal{E}}$ is given by*

$$M_{\mathcal{E}}(z) = \bigoplus_{e \in \mathcal{E}} M_e(z), \quad M_e(z) = R_e^{-1/2}(\tilde{M}_e(z) - Q_e)R_e^{-1/2}. \quad (3.11)$$

Moreover:

(i) $M_{\mathcal{E}}(0) = \mathbb{O}_{\mathcal{H}_{\mathcal{E}}}$, where

$$M_{\mathcal{E}}(0) := s - R - \lim_{x \uparrow 0} M_{\mathcal{E}}(x).$$

(ii) $M_{\mathcal{E}}(x)$ uniformly tends to $-\infty$ as $x \rightarrow -\infty$, that is, for every $N > 0$ there is $x_N < 0$ such that for all $x < x_N$, $M_{\mathcal{E}}$ satisfies

$$M_{\mathcal{E}}(x) < -N \cdot \mathbf{I}_{\mathcal{H}_{\mathcal{E}}}.$$

Proof. First of all, (3.11) is immediate from Proposition 3.5. To prove (i), it suffices to mention that $M_e(0) = \mathbb{O}_2$ for all $e \in \mathcal{E}$.

(ii) Denote by $\lambda_e^+(x)$ and $\lambda_e^-(x)$ the eigenvalues of $M_e(-x^2)$. Straightforward calculations yield

$$\lambda_e^{\pm}(x) = -x \frac{\sqrt{\mu(e)v(e)}}{r(e)} \cdot \frac{\cosh(\eta(e)x) \mp 1}{\sinh(\eta(e)x)} + \frac{v(e)}{|e|r(e)}(1 \mp 1),$$

and noting that $\lambda_e^+(x) < \lambda_e^-(x) < 0$ for all $x > 0$, we get

$$\begin{aligned} M_e(-x^2) &\leq \lambda_e^-(x) \mathbf{I}_2 \\ &= \mathbf{I}_2 \times \begin{cases} \frac{2}{\eta(e)^2} - \frac{x}{\eta(e)} \coth\left(\frac{\eta(e)x}{2}\right) & \text{if } r(e) = |e|\mu(e), \\ \frac{2}{\eta(e)} - x \coth\left(\frac{\eta(e)x}{2}\right) & \text{if } r(e) = \sqrt{\mu(e)v(e)}. \end{cases} \end{aligned}$$

For an $e \in \mathcal{E}$ with $r(e) = \sqrt{\mu(e)v(e)}$, we have $\eta(e) > 1$ and one easily verifies

$$M_e(-x^2) \leq (2-x)\mathbf{I}_2.$$

If $r(e) = |e|\mu(e)$, then $\eta(e) \leq C$ for all such edges e and some uniform constant $C > 0$ (e.g., take $C = \eta^*(\mathcal{E})$ if $\eta^*(\mathcal{E}) < \infty$ and $C = 1$ otherwise). Let us now proceed

as in the proof of [143, Proposition 4.10] and consider the function

$$F(s) = \frac{\coth(s)}{s} - \frac{1}{s^2}, \quad s > 0.$$

Clearly, F is strictly positive and continuous on $(0, \infty)$. Moreover, $F(s) = \frac{1}{3} + \mathcal{O}(s^2)$ as $s \rightarrow 0$ and $F'(s) = -\frac{1}{s^2} + \mathcal{O}(s^{-3})$ as $s \rightarrow +\infty$ and hence

$$\inf_{s \in (0, a)} F(s) = F(a) = \frac{1}{a} \coth(a) - \frac{1}{a^2}$$

for all sufficiently large $a > 1$. It remains to notice that

$$\lambda_e^-(x) = -\frac{x^2}{2} F\left(\frac{\eta(e)x}{2}\right)$$

and hence

$$\lambda_e^-(x) \leq -\frac{x^2}{2} \inf_{s \in (0, Cx/2)} F(s) = -\frac{x^2}{2} F\left(\frac{Cx}{2}\right) = \frac{2}{C^2} - \frac{x}{C} \coth\left(\frac{Cx}{2}\right) \leq -\frac{x}{2C}$$

for all sufficiently large $x > 1$. Taking into account (3.11), we get

$$M_{\mathcal{E}}(-x^2) \leq I_{\mathcal{H}} \inf_{e \in \mathcal{E}} \lambda_e^-(x) \leq -\frac{x}{2 \max\{1, C\}} I_{\mathcal{H}}$$

for all sufficiently large $x > 1$. ■

3.2.2 Vertex-based boundary triplet

It will be convenient for us to work with another boundary triplet for \mathbf{H}_{\max} , which can be obtained from the triplet $\Pi_{\mathcal{E}}$ by regrouping all its components with respect to the vertices. Define

$$\mathcal{H}_{\mathcal{V}} = \bigoplus_{v \in \mathcal{V}} \mathbb{C}^{\deg(v)}, \quad \Gamma_0^{\mathcal{V}} = \bigoplus_{v \in \mathcal{V}} \Gamma_{0,v}, \quad \Gamma_1^{\mathcal{V}} = \bigoplus_{v \in \mathcal{V}} \Gamma_{1,v}, \quad (3.12)$$

where

$$\Gamma_{0,v} f = (\sqrt{r(e)} f_{\vec{e}}(v))_{\vec{e} \in \vec{\mathcal{E}}_v}, \quad (3.13)$$

$$\Gamma_{1,v} f = \left(\frac{v(e)}{\sqrt{r(e)}} \left(\partial_{\vec{e}} f(v) - \pi_v(\vec{e}) \frac{f(e_{\tau}) - f(e_l)}{|e|} \right) \right)_{\vec{e} \in \vec{\mathcal{E}}_v}, \quad (3.14)$$

with $\pi_v: \vec{\mathcal{E}}_v \rightarrow \{-1, 1\}$ denoting the orientation function

$$\pi_v(\vec{e}) := \begin{cases} 1, & \vec{e} \in \vec{\mathcal{E}}_v^+, \\ -1, & \vec{e} \in \vec{\mathcal{E}}_v^-. \end{cases}$$

Corollary 3.8. *The triplet $\Pi_{\mathcal{V}} = \{\mathcal{H}_{\mathcal{V}}, \Gamma_0^{\mathcal{V}}, \Gamma_1^{\mathcal{V}}\}$ given by (3.12)–(3.14) is a boundary triplet for \mathbf{H}_{\max} .*

Proof. For $f_{\mathcal{E}} = ((f_{e_i}, f_{e_\tau}))_{e \in \vec{\mathcal{E}}}$ define the operator $U_{\mathcal{G}}: \mathcal{H}_{\mathcal{E}} \rightarrow \mathcal{H}_{\mathcal{V}}$ by

$$U_{\mathcal{G}}: f_{\mathcal{E}} \mapsto ((f_{v, \vec{e}})_{\vec{e} \in \vec{\mathcal{E}}_v})_{v \in \mathcal{V}}, \quad f_{v, \vec{e}} := \begin{cases} f_{e_i}, & \vec{e} \in \vec{\mathcal{E}}_v^+, \\ f_{e_\tau}, & \vec{e} \in \vec{\mathcal{E}}_v^-, \end{cases} \quad \vec{e} \in \vec{\mathcal{E}}_v, v \in \mathcal{V}. \quad (3.15)$$

Clearly, $U_{\mathcal{G}}$ is an isometric isomorphism. Moreover, it is straightforward to check that

$$\Gamma_0^{\mathcal{V}} = U_{\mathcal{G}} \Gamma_0^{\mathcal{E}}, \quad \Gamma_1^{\mathcal{V}} = U_{\mathcal{G}} \Gamma_1^{\mathcal{E}},$$

which completes the proof. \blacksquare

Let us also mention other important relations.

Corollary 3.9. *The Weyl function $M_{\mathcal{V}}$ corresponding to the boundary triplet (3.12)–(3.14) is given by*

$$M_{\mathcal{V}}(z) = U_{\mathcal{G}} M_{\mathcal{E}}(z) U_{\mathcal{G}}^{-1}, \quad (3.16)$$

where $M_{\mathcal{E}}$ is given by (3.11) and $U_{\mathcal{G}}$ is the operator defined by (3.15). In particular, $s - R - \lim_{x \uparrow 0} M_{\mathcal{V}}(x) = \mathbb{O}_{\mathcal{H}_{\mathcal{V}}}$ and, moreover, $M_{\mathcal{V}}(x)$ uniformly tends to $-\infty$ as $x \rightarrow -\infty$.

Proof. The proof is straightforward and the last claim is an immediate consequence of Lemma 3.7 and equality (3.16). \blacksquare

Remark 3.10. Consider the mappings $\tilde{\Gamma}_0^{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \tilde{\Gamma}_{0,e}$ and $\tilde{\Gamma}_1^{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \tilde{\Gamma}_{1,e}$ given by (3.8). If $f \in \text{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{E})$, then

$$\tilde{\Gamma}_0^{\mathcal{V}} f := U_{\mathcal{G}} \tilde{\Gamma}_0^{\mathcal{E}} f, \quad \tilde{\Gamma}_1^{\mathcal{V}} f := U_{\mathcal{G}} \tilde{\Gamma}_1^{\mathcal{E}} f, \quad (3.17)$$

have the following form:

$$\tilde{\Gamma}_0^{\mathcal{V}} = \bigoplus_{v \in \mathcal{V}} \tilde{\Gamma}_{0,v} \quad \text{and} \quad \tilde{\Gamma}_1^{\mathcal{V}} = \bigoplus_{v \in \mathcal{V}} \tilde{\Gamma}_{1,v},$$

where

$$\tilde{\Gamma}_{0,v} f = (f_{\vec{e}}(v))_{\vec{e} \in \vec{\mathcal{E}}_v}, \quad \tilde{\Gamma}_{1,v} f = (v(e) \partial_{\vec{e}} f(v))_{\vec{e} \in \vec{\mathcal{E}}_v}. \quad (3.18)$$

3.2.3 Boundary operators for Laplacians on metric graphs

Let Θ be a linear relation in $\mathcal{H}_{\mathcal{V}}$ and define the following operator:

$$\begin{aligned} \mathbf{H}_{\Theta} &:= \mathbf{H}_{\max} \upharpoonright \text{dom}(\mathbf{H}_{\Theta}), \\ \text{dom}(\mathbf{H}_{\Theta}) &:= \{f \in \text{dom}(\mathbf{H}_{\max}) : (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \Theta\}, \end{aligned} \quad (3.19)$$

where the mappings $\Gamma_0^{\mathcal{V}}$ and $\Gamma_1^{\mathcal{V}}$ are defined by (3.12)–(3.14). Since $\Pi_{\mathcal{V}}$ is a boundary triplet for \mathbf{H}_{\max} , every proper extension of the operator \mathbf{H}_{\min} has the form (3.19) (see Theorem A.4) and hence so does \mathbf{H}_{α}^0 . The next result provides the explicit form of the linear relation parameterizing \mathbf{H}_{α}^0 .

Proposition 3.11. *Assume Hypotheses 2.1 and let $\Pi_{\mathcal{V}}$ be the boundary triplet (3.12)–(3.14). Suppose Θ_{α}^0 is the boundary relation for the operator \mathbf{H}_{α}^0 ,*

$$\text{dom}(\mathbf{H}_{\alpha}^0) = \{f \in \text{dom}(\mathbf{H}_{\max}) : (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \Theta_{\alpha}^0\}. \quad (3.20)$$

Then the operator part $\Theta_{\alpha}^{\text{op}}$ of Θ_{α}^0 is unitarily equivalent to the operator $\mathbf{h}_{\alpha}^0 = \overline{\mathbf{h}_{\alpha}^{\prime}}$ acting in $\ell^2(\mathcal{V}; m)$ and defined by (3.7) with (3.4), (3.5) and (3.6).

Proof. We divide its proof into several steps.

(i) For each vertex $v \in \mathcal{V}$, the boundary conditions (2.13) can be written as

$$\tilde{D}_v \tilde{\Gamma}_{1,v} f = \tilde{C}_v \tilde{\Gamma}_{0,v} f,$$

where we recall that (see (3.18))

$$\tilde{\Gamma}_{0,v} f = (f_{\bar{e}}(v))_{\bar{e} \in \bar{\mathcal{E}}_v}, \quad \tilde{\Gamma}_{1,v} f = (v(e) \partial_{\bar{e}} f(v))_{\bar{e} \in \bar{\mathcal{E}}_v},$$

and the matrices $\tilde{C}_v, \tilde{D}_v \in \mathbb{C}^{\text{deg}(v) \times \text{deg}(v)}$ are given by

$$\tilde{C}_v = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 \\ 0 & 1 & -1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & -1 \\ \alpha(v) & 0 & 0 & \dots & 0 \end{pmatrix}, \quad \tilde{D}_v = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix}.$$

It is straightforward to verify the Rofe–Beketov conditions (A.3), that is,

$$\tilde{C}_v \tilde{D}_v^* = \tilde{D}_v \tilde{C}_v^*, \quad \text{rank}(\tilde{C}_v | \tilde{D}_v) = \text{deg}(v),$$

holds for all $v \in \mathcal{V}$, and hence

$$\tilde{\Theta}_v := \{(f, g) \in \mathbb{C}^{\text{deg}(v)} \times \mathbb{C}^{\text{deg}(v)} : \tilde{C}_v f = \tilde{D}_v g\}$$

is a self-adjoint linear relation in $\mathbb{C}^{\text{deg}(v)}$. Now set

$$\tilde{C} := \bigoplus_{v \in \mathcal{V}} \tilde{C}_v, \quad \tilde{D} := \bigoplus_{v \in \mathcal{V}} \tilde{D}_v.$$

Both \tilde{C} and \tilde{D} are closed operators in $\mathcal{H}_{\mathcal{V}}$. Clearly, $f \in \text{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{E})$ satisfies

$$\tilde{D} \tilde{\Gamma}_1^{\mathcal{V}} f = \tilde{C} \tilde{\Gamma}_0^{\mathcal{V}} f$$

if and only if $f \in \text{dom}(\mathbf{H}'_\alpha) = \text{dom}(\mathbf{H}_\alpha) \cap C_c(\mathcal{E})$. In view of (3.17), we get

$$\Gamma_0^\mathcal{V} f = R_\mathcal{V} \tilde{\Gamma}_0^\mathcal{V} f, \quad \Gamma_1^\mathcal{V} f = R_\mathcal{V}^{-1} (\tilde{\Gamma}_1^\mathcal{V} - Q_\mathcal{V} \tilde{\Gamma}_0^\mathcal{V}) f$$

for all $f \in \text{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{E})$, where

$$R_\mathcal{V} = U_\mathcal{E} R_\mathcal{E} U_\mathcal{E}^{-1}, \quad Q_\mathcal{V} = U_\mathcal{E} Q_\mathcal{E} U_\mathcal{E}^{-1},$$

$R_\mathcal{E} = \bigoplus_{e \in \mathcal{E}} R_e^{1/2}$, $Q_\mathcal{E} = \bigoplus_{e \in \mathcal{E}} Q_e$ are defined by (3.9) and $U_\mathcal{E}$ is given by (3.15). Hence $f \in \text{dom}(\mathbf{H}'_\alpha)$ if and only if $f \in \text{dom}(\mathbf{H}_{\max}) \cap C_c(\mathcal{E})$ satisfies

$$D \Gamma_1^\mathcal{V} f = C \Gamma_0^\mathcal{V} f,$$

where

$$D = \tilde{D} R_\mathcal{V}, \quad C = (\tilde{C} - \tilde{D} Q_\mathcal{V}) R_\mathcal{V}^{-1}.$$

The operators D and C are well defined on $\mathcal{H}_{\mathcal{V},c}$, which consists of vectors of $\mathcal{H}_\mathcal{V}$ having only finitely many non-zero coordinates.

(ii) Define the linear relation

$$\Theta'_\alpha = \{(f, g) \in \mathcal{H}_{\mathcal{V},c} \times \mathcal{H}_{\mathcal{V},c} : Cf = Dg\} \quad (3.21)$$

and let $\mathbf{H}_{\Theta'_\alpha}$ be the corresponding restriction given by (3.19). By construction, Θ'_α is symmetric and hence so is $\mathbf{H}_{\Theta'_\alpha}$ (see Theorem A.4 (i)). Moreover, $\mathbf{H}'_\alpha \subseteq \mathbf{H}_{\Theta'_\alpha}$ and it is straightforward to check that $\mathbf{H}_{\Theta'_\alpha} \subseteq \mathbf{H}_\alpha^0$. Then, by Theorem A.4 (i), $\Theta_\alpha^0 := \overline{\Theta'_\alpha}$ is the boundary relation parameterizing (via (3.19)) the minimal operator \mathbf{H}_α^0 .

(iii) To proceed further, let $f = (f_v)_{v \in \mathcal{V}} \in \mathcal{H}_\mathcal{V}$, where $f_v = (f_{v,\bar{e}})_{\bar{e} \in \bar{\mathcal{E}}_v}$. For each $v \in \mathcal{V}$, let us denote by P_v the orthogonal projection in $\mathcal{H}_\mathcal{V}$ onto \mathcal{H}_v , the subspace consisting of elements $f = (f_u)_{u \in \mathcal{V}} \in \mathcal{H}_\mathcal{V}$ with all entries equal zero except f_v , that is,

$$(P_v f)_u = (\delta_{vu} f_{u,\bar{e}})_{\bar{e} \in \bar{\mathcal{E}}_u}, \quad \delta_{vu} = \begin{cases} 1, & u = v, \\ 0, & u \neq v. \end{cases}$$

By construction, the operators \tilde{C} , \tilde{D} , $R_\mathcal{V}$ (and hence D) commute with P_v . In particular,

$$R_\mathcal{V} = \bigoplus_{v \in \mathcal{V}} R_v, \quad R_v = \text{diag}(\sqrt{r(e)})_{\bar{e} \in \bar{\mathcal{E}}_v},$$

and

$$D = \bigoplus_{v \in \mathcal{V}} D_v, \quad D_v = \tilde{D}_v R_v = \tilde{D}_v \cdot \text{diag}(\sqrt{r(e)})_{\bar{e} \in \bar{\mathcal{E}}_v}.$$

However, the form of $Q_\mathcal{V}$ (and hence of C) is a bit more complicated:

$$Q_\mathcal{V} = \tilde{Q}^0 - \bigoplus_{v \in \mathcal{V}} Q_v, \quad Q_v = \text{diag}\left(\frac{v(e)}{|e|}\right)_{\bar{e} \in \bar{\mathcal{E}}_v},$$

where

$$(\tilde{Q}^0 f)_{v,\vec{e}} = \frac{\nu(e)}{|e|} f_{u,-\vec{e}},$$

and $u \in \mathcal{V}$ and $-\vec{e} \in \vec{\mathcal{E}}_u$ are given by

$$u := \begin{cases} e_\tau, & \vec{e} \in \vec{\mathcal{E}}_v^+, \\ e_l, & \vec{e} \in \vec{\mathcal{E}}_v^-, \end{cases} \quad -\vec{e} := \begin{cases} (-, e), & \vec{e} \in \vec{\mathcal{E}}_v^+, \\ (+, e), & \vec{e} \in \vec{\mathcal{E}}_v^-. \end{cases}$$

The operators $P_v C$ and $P_v D$ are finite rank and hence admit a bounded extension onto $\mathcal{H}_\mathcal{V}$. By abusing the notation, we shall denote these extensions by $P_v C$ and $P_v D$ as well. It is straightforward to verify that $f \in \text{dom}(\mathbf{H}_{\max})$ satisfies (2.13) exactly when

$$P_v D \Gamma_1^\mathcal{V} f = P_v C \Gamma_0^\mathcal{V} f.$$

Therefore, combining the definition of \mathbf{H}_α (see (2.18)) with (A.4), we conclude that the boundary relation Θ_α parameterizing \mathbf{H}_α in the sense of (3.19) is explicitly given by

$$\Theta_\alpha = \{(f, g) \in \mathcal{H}_\mathcal{V} \times \mathcal{H}_\mathcal{V} : P_v C f = P_v D g \text{ for all } v \in \mathcal{V}\}. \quad (3.22)$$

In particular, by Theorem A.4 (i), $\Theta_\alpha = (\Theta'_\alpha)^* = (\Theta_\alpha^0)^*$.

(iv) By (3.21), $\text{mul}(\Theta'_\alpha) = \ker(D)$ (notice that we consider D as the operator defined only on $\mathcal{H}_{\mathcal{V},c}$ and hence $\ker(D)$ is not closed). On the other hand, (3.22) implies that

$$\text{mul}(\Theta_\alpha) = \{f \in \mathcal{H}_\mathcal{V} : P_v D f = 0 \text{ for all } v \in \mathcal{V}\}, \quad (3.23)$$

and hence

$$\text{mul}(\Theta_\alpha) = \overline{\text{mul}(\Theta'_\alpha)} = \text{mul}(\Theta_\alpha^0).$$

Therefore, Θ_α^0 is densely defined on $\mathcal{H}_\mathcal{V}^{\text{op}} := \text{mul}(\Theta_\alpha)^\perp$ and hence admits the decomposition (A.1), that is,

$$\Theta_\alpha^0 = \Theta_{\text{op}}^0 \oplus \Theta_{\text{mul}}, \quad \Theta_{\text{mul}} = \{0\} \times \text{mul}(\Theta_\alpha), \quad (3.24)$$

where Θ_{op}^0 is the graph of a densely defined closed symmetric operator acting in $\mathcal{H}_\mathcal{V}^{\text{op}}$. Next observe that

$$\mathcal{H}_\mathcal{V}^{\text{op}} = \text{mul}(\Theta_\alpha)^\perp = \ker(D)^\perp = \overline{\text{ran}(D^*)} = \text{span}\{\mathbf{f}^v\}_{v \in \mathcal{V}},$$

where $\mathbf{f}^v = (\mathbf{f}_u^v)_{u \in \mathcal{V}} \in \mathcal{H}_v$ is given by

$$\mathbf{f}_u^v = (\mathbf{f}_{u,\vec{e}}^v)_{\vec{e} \in \vec{\mathcal{E}}_u}, \quad \mathbf{f}_{u,\vec{e}}^v = \begin{cases} \sqrt{r(e)}, & u = v, \\ 0, & u \neq v. \end{cases} \quad (3.25)$$

By construction, $\mathbf{f}^v \perp \mathbf{f}^u$ whenever $v \neq u$ and

$$\|\mathbf{f}^v\|^2 = \sum_{\vec{e} \in \vec{\mathcal{E}}_v} r(e) = m(v) \quad (3.26)$$

for all $v \in \mathcal{V}$.

Let us now show that $\mathbf{f}^v \in \text{dom}(\Theta_\alpha^0)$ for every $v \in \mathcal{V}$. It is straightforward to calculate that

$$(P_u C \mathbf{f}^v)_u = (P_u (\tilde{C} - \tilde{D} Q_{\mathcal{V}}) R_{\mathcal{V}}^{-1} \mathbf{f}^v)_u = \begin{cases} \underbrace{\left(0, 0, \dots, 0, \alpha(v) + \sum_{w \in \mathcal{V}} b(v, w)\right)}_{\text{deg}(v)}, & u = v, \\ \underbrace{\left(0, 0, \dots, 0, -b(u, v)\right)}_{\text{deg}(u)}, & u \neq v, u \sim v, \\ 0, & u \neq v, u \not\sim v, \end{cases}$$

where $b: \mathcal{V} \times \mathcal{V} \rightarrow [0, \infty)$ is the weight function given by (3.6). For $g \in \mathcal{H}_{\mathcal{V},c}$ we have

$$(P_u D g)_u = (P_u \tilde{D} R_{\mathcal{V}} g)_u = \underbrace{\left(0, 0, \dots, 0, \sum_{\tilde{e} \in \tilde{\mathcal{E}}_u} \sqrt{r(\tilde{e})} g_{u, \tilde{e}}\right)}_{\text{deg}(u)}.$$

Therefore, define $\mathbf{g}^v = (\mathbf{g}_u^v)_{u \in \mathcal{V}} \in \mathcal{H}_{\mathcal{V}}^{\text{op}}$ by

$$\mathbf{g}_u^v = (\sqrt{r(\tilde{e})})_{\tilde{e} \in \tilde{\mathcal{E}}_u} \times \begin{cases} \frac{1}{m(v)} \left(\alpha(v) + \sum_{w \sim v} b(v, w) \right), & u = v, \\ -\frac{b(u, v)}{m(u)}, & u \neq v, u \sim v, \\ 0, & u \neq v, u \not\sim v. \end{cases} \quad (3.27)$$

Clearly, this implies the equality

$$C \mathbf{f}^v = D \mathbf{g}^v,$$

and hence $\mathbf{f}^v \in \text{dom}(\Theta'_\alpha) \subseteq \text{dom}(\Theta_\alpha^0)$. Moreover, (3.27) immediately implies that

$$\mathbf{g}^v = \frac{1}{m(v)} \left(\alpha(v) + \sum_{u \sim v} b(u, v) \right) \mathbf{f}^v - \sum_{u \sim v} \frac{b(u, v)}{m(u)} \mathbf{f}^u =: \Theta_{\text{op}}^0 \mathbf{f}^v.$$

Noting that by construction the family $(\mathbf{f}^v)_{v \in \mathcal{V}}$ is an orthogonal basis in $\mathcal{H}_{\mathcal{V}}^{\text{op}}$ and taking into account (3.26), the above equality implies that the operator part Θ_{op}^0 of Θ_α^0 is unitarily equivalent to the minimal operator $\tilde{\mathbf{h}}_\alpha^0$ defined in $\ell^2(\mathcal{V})$ by

$$(\tilde{\tau} f)(v) = \frac{1}{\sqrt{m(v)}} \left(\sum_{u \in \mathcal{V}} b(v, u) \left(\frac{f(v)}{\sqrt{m(v)}} - \frac{f(u)}{\sqrt{m(u)}} \right) + \frac{\alpha(v)}{\sqrt{m(v)}} f(v) \right) \quad (3.28)$$

for each vertex $v \in \mathcal{V}$. More specifically, as usual we define the operator $\tilde{\mathbf{h}}_\alpha^0$ in $\ell^2(\mathcal{V})$ as the closure in $\ell^2(\mathcal{V})$ of the pre-minimal operator

$$\begin{aligned} \tilde{\mathbf{h}}'_\alpha: \text{dom}(\tilde{\mathbf{h}}'_\alpha) &\rightarrow \ell^2(\mathcal{V}), \\ f &\mapsto \tilde{\tau} f, \end{aligned}$$

where $\text{dom}(\tilde{\mathbf{h}}'_\alpha) := C_c(\mathcal{V})$. It remains to notice that the operators $\tilde{\mathbf{h}}_\alpha^0$ and \mathbf{h}_α^0 are unitarily equivalent. Indeed, it is easy to verify that $\tilde{\mathbf{h}}'_\alpha = \mathcal{U}^{-1} \tilde{\mathbf{h}}_\alpha^0 \mathcal{U}$, where

$$\begin{aligned} \mathcal{U}: \ell^2(\mathcal{V}; m) &\rightarrow \ell^2(\mathcal{V}), \\ f &\mapsto \sqrt{m} f, \end{aligned} \tag{3.29}$$

is an isometric isomorphism. ■

Remark 3.12. In fact, one can write down explicitly the isometric isomorphism $\Phi: \ell^2(\mathcal{V}; m) \rightarrow \mathcal{H}_\mathcal{V}^{\text{op}}$ relating $\Theta_\alpha^{\text{op}}$ and \mathbf{h}_α^0 . Indeed, we proved that the collection of vectors $(\mathbf{f}^v)_{v \in \mathcal{V}}$ given by (3.25) forms an orthogonal basis in $\mathcal{H}_\mathcal{V}^{\text{op}}$. Moreover, their norms are given by (3.26), which immediately implies that the map

$$\begin{aligned} \Phi: \ell^2(\mathcal{V}; m) &\rightarrow \mathcal{H}_\mathcal{V}^{\text{op}}, \\ a &\mapsto \sum_{v \in \mathcal{V}} a_v \mathbf{f}^v, \end{aligned} \tag{3.30}$$

is an isometric isomorphism. In particular, this implies the following representation:

$$\Theta_\alpha^{\text{op}} = \{(\Phi f, \Phi \mathbf{h}_\alpha^0 f) : f \in \text{dom}(\mathbf{h}_\alpha^0)\}. \tag{3.31}$$

3.2.4 Proof of Theorem 3.1

Now we have all the ingredients to finish the proof of the main result of this section. It is analogous to the proof of [68, Theorem 2.9] and we provide the details for the sake of completeness.

Proof of Theorem 3.1. Consider the vertex-based boundary triplet $\Pi_\mathcal{V}$. Using Proposition 3.11, item (i) follows from Theorem A.4 (iii).

Next, observe that

$$\mathbf{H}_{e, \max} \upharpoonright \ker(\Gamma_{0,e}) =: \mathbf{H}_e^F$$

is the Friedrichs extension of $\mathbf{H}_{e, \min} = (\mathbf{H}_{e, \max})^*$, and hence we conclude that

$$\mathbf{H}_{\max} \upharpoonright \ker(\Gamma_0) = \bigoplus_{e \in \mathcal{E}} \mathbf{H}_e^F \tag{3.32}$$

is the Friedrichs extension of $\mathbf{H}_{\min} = (\mathbf{H}_{\max})^*$. Moreover,

$$\sigma(\mathbf{H}_e^F) = \left\{ \frac{\pi^2 n^2}{\eta(e)^2} : n \in \mathbb{Z}_{\geq 1} \right\}, \tag{3.33}$$

and hence

$$\inf \sigma(\mathbf{H}^F) = \inf_{e \in \mathcal{E}} \inf \sigma(\mathbf{H}_e^F) = \inf_{e \in \mathcal{E}} \frac{\pi^2}{\eta(e)^2} = \frac{\pi^2}{(\sup_{e \in \mathcal{E}} \eta(e))^2}. \quad (3.34)$$

Now item (ii) follows from Theorem A.9 and Corollary 3.9; items (iii)–(iv) as well as items (vi) and (viii) follow from Theorem A.7 by taking into account Corollary 3.9; item (vii) follows from Theorem A.10.

Finally, (3.32) and (3.33) imply that the spectrum of \mathbf{H}^F is purely discrete if and only if $\#\{e \in \mathcal{E} : \eta(e) > \varepsilon\}$ is finite for every $\varepsilon > 0$. Moreover, \mathcal{H}_F can be written in the form (3.19) with $\Theta_{\text{mul}} = \{0\} \times \mathcal{H}_{\mathcal{V}}$. By Theorem A.4 (iv), the difference of resolvents satisfies

$$(\mathbf{H}_\alpha - i)^{-1} - (\mathbf{H}^F - i)^{-1} \in \mathfrak{S}_\infty$$

exactly when $(\Theta_\alpha - i)^{-1} - (\Theta_{\text{mul}} - i)^{-1}$ is a compact operator. It remains to notice that $(\Theta_{\text{mul}} - i)^{-1} = \mathbb{O}_{\mathcal{H}_{\mathcal{V}}}$. ■

We finish this section with the following remark.

Remark 3.13. Notice that (3.19) establishes a bijective correspondence between the set $\text{Ext}(\mathbf{H}_{\text{min}})$ of proper extensions of \mathbf{H}_{min} and the set of all linear relations in $\mathcal{H}_{\mathcal{V}}$. In fact, Theorem 3.1 extends to all operators \mathbf{H}_Θ and it relates basic spectral properties of the self-adjoint extension \mathbf{H}_Θ and the corresponding boundary relation Θ (see, e.g., [68, Theorem 2.9]). In particular, this would be helpful in the treatment of the case when \mathbf{H}^0 has non-trivial deficiency indices (cf. Theorem 3.1 (ii)–(viii)) and this will be done in the next section.

Remark 3.14. Remark 3.13 indicates that the machinery developed in this section enables us to consider all possible (self-adjoint) vertex conditions (for instance, two other important families are δ' -couplings and symmetrized δ' -couplings). Moreover, one may include more general differential expressions including magnetic Schrödinger operators. However, the main difficulty is the search for a suitable boundary operator, which usually requires separate considerations, and then the study of its properties (cf., e.g., [143, Section 5-6]). Let us mention that there are strong indications that one may connect spectral properties (in the sense of Theorem 3.1) of magnetic Schrödinger operators on metric graphs with those of weighted magnetic Schrödinger operators on graphs (see [35, Section 3.5]). Moreover, it seems to us that one may also establish similar connections between Laplacians with δ' -couplings and symmetrized δ' -couplings and “weighted” Hodge Laplacians on graphs, respectively, signless Laplacians on graphs (cf. [181]). However, all these require separate considerations and will be done elsewhere.

3.3 Spectral properties: Metric graphs and models

We restrict ourselves to the case $\alpha \equiv 0$, that is, in this section we shall consider Kirchhoff Laplacians only. Our main aim now is to look at Corollary 3.2 from the continuous-to-discrete perspective. Let (\mathcal{G}, μ, ν) be a given weighted metric graph, that is, \mathcal{G} is a locally finite metric graph (as a metric space) and μ, ν are two edge weights on \mathcal{G} . With each model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of (\mathcal{G}, μ, ν) we can associate a weighted graph Laplacian

$$(\tau f)(v) = \frac{1}{m(v)} \sum_{u \in \mathcal{V}} b(v, u)(f(v) - f(u)), \quad v \in \mathcal{V}, \quad (3.35)$$

where m and b are defined by (3.5) and (3.6), respectively. Thus we have the minimal Kirchhoff Laplacian \mathbf{H}^0 on \mathcal{G} and the family of minimal graph Laplacians \mathbf{h}^0 associated with the models of (\mathcal{G}, μ, ν) . In this situation Corollary 3.2 (i) immediately implies the following results.

Corollary 3.15. *Let (\mathcal{G}, μ, ν) be a weighted metric graph and let \mathbf{H}^0 be the corresponding minimal Kirchhoff Laplacian. Then:*

- (i) *For each model of (\mathcal{G}, μ, ν) , the deficiency indices of \mathbf{H}^0 and \mathbf{h}^0 are equal,*

$$n_{\pm}(\mathbf{H}^0) = n_{\pm}(\mathbf{h}^0). \quad (3.36)$$

- (ii) *If \mathbf{H}^0 is self-adjoint, then \mathbf{h}^0 is self-adjoint for each model. And conversely, \mathbf{H}^0 is self-adjoint exactly when \mathbf{h}^0 is self-adjoint for one (and hence for all) models of (\mathcal{G}, μ, ν) .*

In order to preserve the equivalences further, the next results require a careful choice of a model, which motivates the following definition.

Definition 3.16. For a given model $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ of (\mathcal{G}, μ, ν) , the quantity $\eta^*(\mathcal{E})$ defined by (3.2) is called *the intrinsic size of the model*. A model has *finite intrinsic size* if $\eta^*(\mathcal{E}) < \infty$. Otherwise, $(\mathcal{V}, \mathcal{E}, |\cdot|, \mu, \nu)$ is called a model of *infinite intrinsic size*.

A weighted metric graph (\mathcal{G}, μ, ν) has *finite intrinsic size* if all its models are of finite intrinsic size. Otherwise, (\mathcal{G}, μ, ν) has *infinite intrinsic size*.

We define the *essential intrinsic size* of a given model with edge set \mathcal{E} by

$$\eta_{\text{ess}}^*(\mathcal{E}) := \inf_{\tilde{\mathcal{E}}} \sup_{e \in \mathcal{E} \setminus \tilde{\mathcal{E}}} \eta(e),$$

where the infimum is taken over all finite subsets $\tilde{\mathcal{E}}$ of \mathcal{E} .

Remark 3.17. A few remarks are in order.

- (i) The above definition becomes transparent when $\mu = \nu$. Indeed, in this case $\eta(e) = |e|$ for all $e \in \mathcal{E}$ and the intrinsic size of a model is simply the length

of its “longest” edge, that is, $\eta^*(\mathcal{E}) = \ell^*(\mathcal{E})$, where

$$\ell^*(\mathcal{E}) = \sup_{e \in \mathcal{E}} |e|.$$

In particular, such a model has infinite intrinsic size exactly when there is an arbitrarily long edge. Similarly,

$$\eta_{\text{ess}}^*(\mathcal{E}) = \ell_{\text{ess}}^*(\mathcal{E}) := \inf_{\tilde{\mathcal{E}}} \sup_{e \in \mathcal{E} \setminus \tilde{\mathcal{E}}} |e|,$$

where the infimum is taken over all finite subsets $\tilde{\mathcal{E}}$ of \mathcal{E} .

- (ii) The function r in (3.5) is given by (3.3) if the model has finite size and by (3.4) if it has infinite size.
- (iii) The definition of essential intrinsic size can be understood as follows. For any compact subgraph $\tilde{\mathcal{G}} \subset \mathcal{G}$ and every $\varepsilon > 0$, one can always find an edge in $\mathcal{E} \setminus \tilde{\mathcal{E}}$ whose intrinsic length is at least $\eta_{\text{ess}}^*(\mathcal{E}) - \varepsilon$. Moreover, for any $\varepsilon > 0$, there is a compact subgraph $\tilde{\mathcal{G}}$ such that the intrinsic length of every edge $e \in \mathcal{E} \setminus \tilde{\mathcal{E}}$ is smaller than $\eta_{\text{ess}}^*(\mathcal{E}) + \varepsilon$. In particular, $\eta_{\text{ess}}^*(\mathcal{E}) = 0$ means that for any $\varepsilon > 0$ there is a compact subgraph $\tilde{\mathcal{G}}$ such that all edges in $\mathcal{E} \setminus \tilde{\mathcal{E}}$ have intrinsic length less than ε .

Corollary 3.18. *Let (\mathcal{G}, μ, ν) be a weighted metric graph such that the corresponding minimal Kirchhoff Laplacian \mathbf{H}^0 is self-adjoint, $\mathbf{H}^0 = \mathbf{H}$. Then:*

- (i) *The operator \mathbf{H} is positive definite, $\lambda_0(\mathbf{H}) > 0$, if and only if there is a model of finite intrinsic size such that the corresponding operator \mathbf{h} is positive definite, $\lambda_0(\mathbf{h}) > 0$.*
- (ii) *We have $\lambda_0^{\text{ess}}(\mathbf{H}) > 0$ exactly when there is a model of finite intrinsic size such that $\lambda_0^{\text{ess}}(\mathbf{h}) > 0$.*
- (iii) *If (\mathcal{G}, μ, ν) has infinite intrinsic size, then $\lambda_0(\mathbf{H}) = \lambda_0^{\text{ess}}(\mathbf{H}) = 0$ and, moreover, $\lambda_0(\mathbf{h}) = \lambda_0^{\text{ess}}(\mathbf{h}) = 0$ for all models with finite intrinsic size.*
- (iv) *The spectrum of \mathbf{H} is purely discrete if and only if there is a model with zero essential intrinsic size, $\eta_{\text{ess}}^*(\mathcal{E}) = 0$ and the spectrum of the corresponding graph Laplacian \mathbf{h} is purely discrete.*
- (v) *If there is a model with $\eta_{\text{ess}}^*(\mathcal{E}) > 0$, then the essential spectrum of \mathbf{H} is not empty and, moreover, so is the essential spectrum of \mathbf{h} for each model with $\eta_{\text{ess}}^*(\tilde{\mathcal{E}}) = 0$.*

Proof. By Corollary 3.15, \mathbf{h} is self-adjoint, $\mathbf{h} = \mathbf{h}^0$ for each model of a given weighted metric graph. Moreover, the operators \mathbf{H} and \mathbf{h} are both non-negative. Then (i) and (ii) follow immediately from Corollary 3.2 (iii)–(iv) since one can always find a model with finite intrinsic size. The same argument together with Theorem 3.1 (v) proves (iv)–(v).

Thus it remains to show (iii). In fact, we only need to prove the first claim that

$$\lambda_0(\mathbf{H}) = \lambda_0^{\text{ess}}(\mathbf{H}) = 0$$

if there is a model of infinite size. However, the Friedrichs extension \mathbf{H}^F has zero spectral gap, see (3.34), and hence so does every non-negative self-adjoint restriction of \mathbf{H}_{\max} .² ■

Remark 3.19. Notice that one can always find a model with $\eta_{\text{ess}}^*(\mathcal{E}) = 0$ by refining (even if (\mathcal{G}, μ, ν) has infinite intrinsic size). Indeed, for each model the edge set \mathcal{E} is countable and hence one can obtain a new model satisfying $\eta_{\text{ess}}^*(\tilde{\mathcal{E}}) = 0$ by “cutting” an edge into equally short pieces; then the next edge into shorter ones, and so on.

Let us stress the following fact. The above results demonstrate that a Kirchhoff Laplacian shares some properties with the corresponding graph Laplacians for each model (e.g., self-adjointness), however, for some properties the class of models must be sufficiently good in a certain sense. For instance, strict positivity of spectra/essential spectra requires models having finite intrinsic size, $\eta^*(\mathcal{E}) < \infty$. Discreteness (that is, compactness of resolvents) requires even a more refined choice (essential intrinsic size must be zero, $\eta_{\text{ess}}^*(\mathcal{E}) = 0$). On the other hand, Corollary 3.18 demonstrates that if the set of models is in a certain sense too wide (for instance, there are models having infinite size), then the corresponding Kirchhoff Laplacian cannot have the required property (e.g., positive spectral gap). However, in the latter case the absence of a required property is shared with all graph Laplacians arising from all reasonable models.

We would like to finish with a result which sheds light on the situation when the deficiency indices of \mathbf{H}^0 are non-trivial. However, first we need the following useful fact.

Lemma 3.20. *Let (\mathcal{G}, μ, ν) be a weighted metric graph together with the minimal Kirchhoff Laplacian \mathbf{H}^0 . If $n_{\pm}(\mathbf{H}^0) > 0$, then for each model the map*

$$\begin{aligned} \tilde{\mathbf{h}} \mapsto \tilde{\mathbf{H}} = \mathbf{H}_{\tilde{\Theta}} &:= \mathbf{H}_{\max} \upharpoonright \{f \in \text{dom}(\mathbf{H}_{\max}) : (\Gamma_0^{\mathcal{V}} f, \Gamma_1^{\mathcal{V}} f) \in \tilde{\Theta}\}, \\ \tilde{\Theta} &:= \Theta_{\text{mul}} \oplus \{(\Phi f, \Phi \tilde{\mathbf{h}} f) : f \in \text{dom}(\tilde{\mathbf{h}})\} \end{aligned} \quad (3.37)$$

is a bijection between the sets $\text{Ext}_S(\mathbf{h}^0)$ and $\text{Ext}_S(\mathbf{H}^0)$ of self-adjoint extensions of \mathbf{h}^0 and \mathbf{H}^0 . Here $\{\mathcal{H}_{\mathcal{V}}, \Gamma_0^{\mathcal{V}}, \Gamma_1^{\mathcal{V}}\}$ is the vertex-based boundary triplet defined in Section 3.2.2, the map Φ and the multivalued part Θ_{mul} are given by (3.30) and, respectively, (3.23).

Proof. The existence of a bijection is a trivial consequence of von Neumann’s formulas in view of (3.36), however, we would like to give another proof based on the use

²In fact, following line by line the argument of M. Solomyak in [196, Theorem 5.1], one can show in this case that the whole semi-axis $[0, \infty)$ belongs to the spectrum of \mathbf{H} .

of the boundary triplets approach, which enables us to connect self-adjoint extensions of \mathbf{H}^0 and \mathbf{h}^0 in a rather transparent way.

Take a self-adjoint extension $\tilde{\mathbf{H}} \in \text{Ext}(\mathbf{H}^0)$ of \mathbf{H}^0 . Then for a chosen model it admits the representation (3.19), that is, there exists a self-adjoint linear relation $\tilde{\Theta}$ in \mathcal{H}_ν such that³

$$\text{dom}(\tilde{\mathbf{H}}) = \{f \in \text{dom}(\mathbf{H}_{\max}) : (\Gamma_0^\nu f, \Gamma_1^\nu f) \in \tilde{\Theta}\}. \quad (3.38)$$

By Theorem A.4 (i), $\tilde{\Theta}$ is a self-adjoint extension of the linear relation Θ^0 parameterizing \mathbf{H}^0 via (3.20). As it was mentioned in the proof of Proposition 3.11, Θ^0 admits the representation (3.24). Similarly, $\tilde{\Theta}$ admits an analogous decomposition. Moreover, the multivalued parts of Θ^0 and $\tilde{\Theta}$ coincides, that is, $\Theta_{\text{mul}} = \tilde{\Theta}_{\text{mul}}$, since both Θ_{mul} and $\tilde{\Theta}_{\text{mul}}$ are self-adjoint relations (or since $\text{mul}(\Theta^0) = \text{mul}(\Theta)$). Therefore, $\tilde{\Theta}_{\text{op}}$ is a self-adjoint extension of Θ_{op}^0 in $\mathcal{H}_\nu^{\text{op}}$. Taking into account (3.31), every self-adjoint extension of Θ^0 has the form

$$\tilde{\Theta} = \Theta_{\text{mul}} \oplus \{(\Phi f, \Phi \tilde{\mathbf{h}} f) : f \in \text{dom}(\tilde{\mathbf{h}})\},$$

where $\tilde{\mathbf{h}}$ is a self-adjoint extension of \mathbf{h}^0 . ■

Remark 3.21. In fact, one can rewrite the map (3.37) in a more convenient form and this will be done in Chapter 4 (see Lemma 4.7 below).

Lemma 3.20 provides us with a map establishing a one-to-one correspondence between self-adjoint extensions of \mathbf{H}^0 and \mathbf{h}^0 . It turns out that their spectral properties are closely connected as well:

Theorem 3.22. *Let (\mathcal{G}, μ, ν) be a weighted metric graph together with a fixed model. Suppose*

$$n_{\pm}(\mathbf{H}^0) > 0,$$

and $\tilde{\mathbf{H}} \in \text{Ext}_S(\mathbf{H}_0)$. If $\tilde{\mathbf{h}} \in \text{Ext}_S(\mathbf{h}_0)$ is the self-adjoint extension corresponding to $\tilde{\mathbf{H}}$ via (3.37). Then:

- (i) $\tilde{\mathbf{H}}$ is lower semibounded if and only if $\tilde{\mathbf{h}}$ is lower semibounded.
- (ii) $\tilde{\mathbf{H}}$ is non-negative if and only if $\tilde{\mathbf{h}}$ is non-negative.
- (iii) The total multiplicities of negative spectra of $\tilde{\mathbf{H}}$ and $\tilde{\mathbf{h}}$ coincide,

$$\kappa_-(\tilde{\mathbf{H}}) = \kappa_-(\tilde{\mathbf{h}}).$$

- (iv) The spectrum of $\tilde{\mathbf{H}}$ is purely discrete if and only if the model satisfies $\eta_{\text{ess}}^*(\mathcal{E}) = 0$ and the spectrum of $\tilde{\mathbf{h}}$ is purely discrete.

If additionally the corresponding model has finite intrinsic size, $\eta^(\mathcal{E}) < \infty$, then:*

- (v) $\tilde{\mathbf{H}}$ is positive definite if and only if $\tilde{\mathbf{h}}$ is positive definite.

³Taking into account Theorem A.4, in fact $\tilde{\Theta}$ is given by $\tilde{\Theta} = \{(\Gamma_0^\nu f, \Gamma_1^\nu f) : f \in \text{dom}(\tilde{\mathbf{H}})\}$.

- (vi) *If, in addition, the extension $\tilde{\mathbf{H}}$ is lower semibounded, then $\lambda_0^{\text{ess}}(\tilde{\mathbf{H}}) > 0$ ($\lambda_0^{\text{ess}}(\tilde{\mathbf{H}}) = 0$) exactly when $\lambda_0^{\text{ess}}(\tilde{\mathbf{h}}) > 0$ (respectively, $\lambda_0^{\text{ess}}(\tilde{\mathbf{h}}) = 0$).*
- (vii) *Moreover, the equivalence*

$$\tilde{\mathbf{H}}^- \in \mathfrak{S}_p(L^2) \iff \tilde{\mathbf{h}}^- \in \mathfrak{S}_p(\ell^2)$$

holds for all $p \in (0, \infty]$. In particular, negative spectra of $\tilde{\mathbf{H}}$ and $\tilde{\mathbf{h}}$ are discrete simultaneously.

The proof is an immediate corollary of Lemma 3.20 and Remark 3.13 and we leave it to the reader.

Remark 3.23. In fact, Theorem 3.22 specifies the properties of the map (3.37) when it is further restricted to certain subclasses of self-adjoint extensions. Namely, items (i)–(iii) say that the map (3.37) is a bijection between the sets of semibounded/non-negative/self-adjoint extensions. According to items (v) and (vi), (3.37) is a bijection between self-adjoint extensions having a positive spectral gap/positive essential spectral gap, however, only if the corresponding model of a weighted metric graph has finite intrinsic size.

Remark 3.24 (Laplacians with δ -couplings). It is not difficult to notice that Lemma 3.20 extends to the operator \mathbf{H}_α^0 with $\alpha \neq 0$ in an obvious way. Taking into account that the representation (3.37) is the key to prove Theorem 3.22, it is then straightforward to see that the analog of Theorem 3.22 holds true for the operator \mathbf{H}_α with non-trivial α .

3.3.1 Historical remarks

The fact that the boundary triplets machinery is a convenient tool to investigate finite and infinite metric graphs was realized in the 2000s (the literature is enormous and we only refer to [35, 67, 182], which also contain further references). However, in all these studies it was assumed that edge lengths admit a uniform positive lower bound ($\inf_{e \in \mathcal{E}} \eta(e) > 0$ in our notation). Notice that in contrast to the finite intrinsic size assumption (which can always be achieved by subdividing edges), this “uniform positive lower bound” assumption, which is rather common in the quantum graph literature [25, 182], is indeed a restriction. The main obstacle on this way is to construct a boundary triplet for the maximal operator \mathbf{H}_{\max} . A convenient approach to construct such a triplet was proposed by M.M. Malamud and H. Neidhardt in [156] (see Theorem A.11). This technique was applied in [143] to investigate one-dimensional Schrödinger operators with local point interactions on discrete sets and then in [68] to Laplacians on unweighted metric graphs ($\mu = \nu \equiv 1$).