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Heat-kernel and resolvent asymptotics for Schrödinger operators on metric graphs

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Abstract: We consider Schrödinger operators on compact and non-compact (finite) metric graphs. For such operators we analyse their spectra, prove that their resolvents can be represented as integral operators and introduce trace-class regularisations of the resolvents. Our main result is a complete asymptotic expansion of the trace of the (regularised) heat-semigroup generated by the Schrödinger operator. We also determine the leading coefficients in the expansion explicitly.

KEY WORDS Quantum graph, Schrödinger operator, resolvent, heat kernel

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1 Introduction

A quantum graph is a metric graph with a differential operator acting on functions defined on the edges of the graph. (Although one may also consider infinite networks, in the following we shall always focus on graphs with finitely many edges and vertices.) Often the quantum graph operator is taken to be a Laplacian, $-\Delta$. More generally, however, Schrödinger operators of the form $H = -\Delta + V$ with a potential V defined on the edges are of interest. Quantum graph models are used in many applications where a one-dimensional (wave-) motion in a structure with non-trivial connectivity is studied, see [GS06, EKK+08] for reviews. They are also used as models in quantum chaos [KS99b] and bear many similarities with problems in spectral geometry. In the latter area heat-trace asymptotics are an important tool to gain geometric and topological information on a manifold from the spectral data of a suitable operator. The same is achieved in quantum graph models using Laplace operators.

Spectral properties of quantum graph Laplacians are well understood. This is mainly due to the fact that exact trace formulae exist [Rot84, KS99b, KPS07, BE09]. They express spectral functions of the Laplacian in terms of a sum over periodic walks on the graph. Often the spectral function will be the trace of the heat-semigroup, so that the trace formula implies a complete asymptotic expansion for the heat trace as well as an exponential bound for the remainder.

The spectral information available for Schrödinger operators $H = -\Delta + V$ on graphs is less detailed. This can be seen from the fact that a trace formula for H is only known for spectral functions supported away from low eigenvalues [RS12]. The determination of the contribution of low eigenvalues is complicated by the fact that the potential may lead to trapped orbits, corresponding to resonances of H. Therefore, independent studies of heat-trace asymptotics will complement the spectral information for Schrödinger operators on graphs. Such heat-kernel expansions were first determined in [Rue12] for Schrödinger operators on compact graphs under certain (rather stringent) conditions on the behaviour of the potential in the vertices. The method used in [Rue12] is based on a parametrix construction for the heat-semigroup, which requires sufficient regularity of the symbol of H in the singular points of the graph (i.e., the vertices).

In this paper we generalise the results of [Rue12] in two major ways: We drop the conditions on the behaviour of the potential in the vertices and we allow for external edges, turning the graph into a non-compact graph. This is possible since our approach does not rely on parametrices but rather uses resolvent kernels very much in the spirit of [KS06, KPS07], where the standard Laplacian is considered. We also allow for general, self-adjoint boundary conditions in the vertices, while in [Rue12] only the case of Kirchhoff conditions was considered.

The paper is organised as follows: In Section 2 we review the construction of quantum graphs. The following Section 3 is devoted to an analysis of the point spectrum of H and the associated eigenfunctions. Here we introduce a secular equation that allows to characterise eigenvalues. The secular equation involves a matrix

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$\mathfrak{S}(k)$ that encodes the boundary conditions in the vertices. In Section 4 we represent the resolvent of H as an integral operator and express its kernel in terms of $\mathfrak{S}(k)$. We also introduce a regularisation of the resolvent that in the case of a non-compact graph leads to a trace-class operator. Asymptotic expansions of the matrix $\mathfrak{S}(k)$ are developed in Section 5, and further asymptotic expansions are performed in Section 6. A complete asymptotic expansion for the trace of the regularised resolvent is proven in Section 7. The result is presented in Theorem 7.3. Our main result is contained in Section 8. In Theorem 8.2 we prove a complete asymptotic expansion for the trace of a regularised heat-semigroup generated by a Schrödinger operator on a general (non-compact) metric graph.

2 Quantum graphs

A metric graph Γ is a finite, connected, combinatorial graph with a metric structure. It consists of a finite set $\mathcal{V}$ of vertices and a finite set $\mathcal{E} = \mathcal{E}_{\text{int}} \cup \mathcal{E}_{\text{ex}}$ of edges. Edges $e \in \mathcal{E}$ are either internal, $e \in \mathcal{E}_{\text{int}}$, or external, $e \in \mathcal{E}_{\text{ex}}$. Internal edges link two vertices, which are identified with the edge ends, and external edges are connected to a single vertex. We set $\mathfrak{V} := |\mathcal{V}|$, $E_{\text{int}} := |\mathcal{E}_{\text{int}}|$, $E_{\text{ex}} := |\mathcal{E}_{\text{ex}}|$ and $E := E_{\text{ex}} + 2E_{\text{int}}$. When an edge end is connected to a vertex we say that the edge e is adjacent to the vertex v, denoted as $e \sim v$. The number of edges adjacent to a vertex v is its degree d_v. Tadpoles, i.e., internal edges that are only adjacent to a single vertex, are allowed. However, this case will later become irrelevant when we introduce additional vertices.

A metric structure is defined by assigning intervals to edges. Each internal edge $e \in \mathcal{E}_{\text{int}}$ is assigned an interval $I_e = [0, l_e]$ of finite length l_e, whereas each external edge is assigned a half-infinite interval $I_e = [0, \infty)$. For convenience we then sometimes write $l_e = \infty$. We also introduce the vector $\boldsymbol{l} := (l_1, \ldots, l_{E_{\text{int}}})^T \in \mathbb{R}_+^{E_{\text{int}}}$ of (finite) edge lengths. The volume $\mathcal{L}$ of the interior part of the metric graph is $\mathcal{L} := \sum_{e \in \mathcal{E}_{\text{int}}} l_e$. Given two points x, y on Γ, a path from x to y is a succession of edges, connected in vertices, such that x is on the initial edge and y is on the final edge. The distance $d(x, y)$ of the points is the minimum of the lengths of all paths from x to y.

Functions on Γ are collections of functions on the intervals associated with edges, so that we can introduce the quantum graph Hilbert space

$$L^2(\Gamma) = \bigoplus_{e \in \mathcal{E}} L^2(0, l_e). \tag{2.1}$$

Similarly, other function spaces such as Sobolev spaces $H^m(\Gamma)$ and spaces of smooth functions are defined. A Schrödinger operator is a linear operator on a dense domain $\mathcal{D} \subset L^2(\Gamma)$, acting on a function on edge e as

$$(H\psi)_e := -\psi_e'' + V_e \psi_e. \tag{2.2}$$

Here $\psi_e'(x) = \frac{\mathrm{d}\psi_e}{\mathrm{d}x}(x)$, $x \in (0, l_e)$, and

$$V_e \in C^\infty(0, l_e), \quad e \in \mathcal{E}_{\text{int}}, \quad \text{or} \quad V_e \in C_0^\infty[0, \infty), \quad e \in \mathcal{E}_{\text{ex}}, \tag{2.3}$$

is a potential on the edge e, where the second requirement means that the potential has a compact support on an external edge but need not vanish at the vertex. Hence,

$$H = -\Delta + V, \tag{2.4}$$

where V is to be understood as a diagonal matrix with entries V_e as in (2.3) on the diagonal.

In order to determine domains of self-adjointness for the Schrödinger operator H the Laplacian $-\Delta$ has to be realised as a self-adjoint operator on a suitable domain $\mathcal{D}$. Then H will be self-adjoint on the same domain. Classifications of self-adjoint realisations of the Laplacian are well known [KS99a, Kuc04]. They require boundary values of functions and their (inward) derivatives,

$$\begin{aligned}
\underline{\psi} &= \left(\{\psi_e(0)\}_{e \in \mathcal{E}_{\text{ex}}}, \{\psi_e(0)\}_{e \in \mathcal{E}_{\text{int}}}, \{\psi_e(l_e)\}_{e \in \mathcal{E}_{\text{int}}} \right)^T \in \mathbb{C}^E, \\
\underline{\psi'} &= \left(\{\psi_e'(0)\}_{e \in \mathcal{E}_{\text{ex}}}, \{\psi_e'(0)\}_{e \in \mathcal{E}_{\text{int}}}, \{-\psi_e'(l_e)\}_{e \in \mathcal{E}_{\text{int}}} \right)^T \in \mathbb{C}^E,
\end{aligned} \tag{2.5}$$

which are well defined for $\psi \in H^2(\Gamma)$. Following [Kuc04], a parametrisation of self-adjoint realisations can be achieved in terms of orthogonal projectors P on $\mathbb{C}^E$ and self-adjoint maps L on $\mathbb{C}^E$ satisfying $P^\perp L P^\perp = L$: Every self-adjoint realisation of the Laplacian has a unique representation of the form

$$\mathcal{D}(P, L) := \left\{ \psi \in H^2(\Gamma); \quad (P + L)\underline{\psi} + P^\perp \underline{\psi'} = 0 \right\}. \tag{2.6}$$

The boundary conditions imposed on functions in $\mathcal{D}(P,L)$ via (2.6) do not necessarily reflect the connectivity of the graph. This will only be the case if

$$P = \bigoplus_{v\in\mathcal{V}} P_v \quad \text{and} \quad L = \bigoplus_{v\in\mathcal{V}} L_v \tag{2.7}$$

in such a way that P_v, L_v act on the space $\mathbb{C}^{d_v}$ of boundary values related to the d_v edge ends adjacent to v. We call such boundary conditions *local*. The focus on local boundary conditions becomes important in the Sections 7 and 8 where we derive the first two leading contributions of the resolvent kernel and the heat kernel for two points that are distinct on Γ but possess zero distance (ends of different edges connected in a vertex).

Examples of local boundary conditions would be Kirchhoff (or standard) conditions. Introducing coordinates such that v corresponds to $x = 0$ on every edge adjacent to v, this means $\psi_e(0) = \psi_{e'}(0)$ if e, e' are both adjacent to v, and

$$\sum_{\substack{e\in\mathcal{E},\\ e\sim v}} \psi_e'(0) = 0. \tag{2.8}$$

Notice that a vertex v with degree $d_v = 2$ and with Kirchhoff conditions (2.8) can be removed since the functions and their derivatives are continuous across the vertex.

The same fact can be used to add vertices of degree two with Kirchhoff conditions without changing the operator H. This allows us to make a few simplifying assumptions without losing generality: We first exclude potentials on external edges. When $e \in \mathcal{E}_{\rm ex}$ with non-vanishing $V_e \in C_0^\infty(0,\infty)$ we add a vertex v of degree $d_v = 2$ on e outside of the support of V_e. Secondly, we remove tadpoles by introducing an additional vertex on that edge. This procedure may change the underlying graph, but not the operator H.

The above conventions allow us to denote the boundary values of edge-potentials as $V_e(v)$ when $e \sim v$. Furthermore, the outward derivative of V_e at v is denoted as $V'(v)_e$, i.e., either $V'(v)_e = V_e'(0)$ or $V'(v)_e = -V_e'(l_e)$, depending on which edge end is adjacent to v.

3 Eigenvalues and eigenfunctions

An eigenfunction of the Schrödinger operator H is a function $\varphi = \{\varphi_e\}_{e\in\mathcal{E}} \in \mathcal{D}(P,L)$ such that there exists $\lambda \in \mathbb{R}$ with

$$H\varphi = \lambda\varphi. \tag{3.1}$$

It is convenient to set $\lambda = k^2$ with $k \in \mathbb{C}$. Self-adjointness of H then implies that either $k \in \mathbb{R}$, when $\lambda \geq 0$, or $k = \mathrm{i}\kappa$ with $\kappa \in \mathbb{R}$, when $\lambda < 0$.

On an external edge $e \in \mathcal{E}_{\rm ex}$, where $V_e = 0$, a fundamental system of solutions is given by the functions e^{ikx} and e^{-ikx} when $k^2 \neq 0$. The condition $\varphi \in L^2(\Gamma)$ then implies for $k \in \mathbb{R}$ (i.e., $\lambda > 0$) that the eigenfunction ϕ has to vanish on external edges. When $\lambda < 0$ only one of the functions is permitted, depending on the sign of $\operatorname{Im} k$. We here always choose

$$\varphi_e(x) = c_e\, \mathrm{e}^{ikx}, \quad \operatorname{Im} k > 0, \quad c_e \in \mathbb{C}. \tag{3.2}$$

On an internal edge $e \in \mathcal{E}_{\rm int}$ the equation implied by (3.1) reads

$$-\varphi_e'' + V_e\varphi_e - k^2\varphi_e = 0, \tag{3.3}$$

where $k \in \mathbb{C}$ such that $k^2 = \lambda$. We shall need a certain type of fundamental solutions on the internal edges. Below two more specific classes will be used in (3.21) and in Lemma 5.1.

Definition 3.1. *A pair $\{u_e^+(k;\cdot), u_e^-(k;\cdot)\}$ of functions in $C^\infty(I_e)$ is said to be a system of admissible fundamental solutions on an internal edge $e \in \mathcal{E}_{\rm int}$, if the functions $u_e^\pm(k;x)$ are solutions of the equation* (3.3)*, are analytic in $k \in S_\delta$, where*

$$S_\delta := \{z \in \mathbb{C};\quad 0 < |z| < \infty, \quad |\arg(-z)| > \delta\}, \tag{3.4}$$

for some (small) $\delta > 0$ and satisfy the condition

$$\overline{u_e^+(k;x)} = u_e^-(\bar{k};x), \tag{3.5}$$

for all $k \in S_\delta$. We also fix the normalisation $u_e^+(k;0) = 1 = u_e^-(k;0)$.

Remark 3.1. *Set*

$$u_e^+(k;x) = r_e(k;x)\,\mathrm{e}^{\mathrm{i}\phi_e(k;x)}, \tag{3.6}$$

with smooth, real-valued functions $r_e(k;\cdot)$ and $\phi_e(k;\cdot)$, such that $r_e(k;\cdot)$ is non-negative. Then

$$u_e^-(k;x) = r_e(\overline{k};x)\,\mathrm{e}^{-\mathrm{i}\phi_e(\overline{k};x)}. \tag{3.7}$$

If k is real, the Wronskian of this fundamental system takes the form

$$W_e(k) = {u_e^+}'(k;x)u_e^-(k;x) - u_e^+(k;x){u_e^-}'(k;x) = 2\mathrm{i}{\phi_e}'(k;x)\,r_e(k;x)^2. \tag{3.8}$$

This relation, in particular, implies that $u_e^\pm(k;x) \neq 0$ and ${u_e^\pm}'(k;x) \neq 0$ for all $k \in \mathbb{R}$ and all $x \in I_e$. As the functions $u_e^\pm(k;\cdot)$ are analytic in $k \in S_\delta$, this also implies that they, and their derivatives, are non-zero for all $x \in I_e$ with k in a neighbourhood of the positive half-line.

Note that these conditions do not uniquely determine a system of admissible fundamental solutions. Examples of admissible fundamental solutions can be found in [Fed93] as well as in [PT87]. In the former case the functions possess asymptotic expansions in k, a fact that we shall use below.

In order to characterise eigenvalues and eigenfunctions (3.1) of H we follow the method devised in [KS06]. For this we need to introduce the following matrices, using any (fixed) system of admissible fundamental solutions.

$$\begin{aligned} X(k;\boldsymbol{l}) &:= \begin{pmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & \mathbb{1} \\ 0 & \boldsymbol{u}_+(k;\boldsymbol{l}) & \boldsymbol{u}_-(k;\boldsymbol{l}) \end{pmatrix}, \\ Y(k;\boldsymbol{l}) &:= \begin{pmatrix} \mathrm{i}k\mathbb{1} & 0 & 0 \\ 0 & \boldsymbol{u}_+'(k;\boldsymbol{0}) & \boldsymbol{u}_-'(k;\boldsymbol{0}) \\ 0 & -\boldsymbol{u}_+'(k;\boldsymbol{l}) & -\boldsymbol{u}_-'(k;\boldsymbol{l}) \end{pmatrix}, \end{aligned} \tag{3.9}$$

where $\boldsymbol{u}_\pm(k;\boldsymbol{x})$ are diagonal $E_{\mathrm{int}} \times E_{\mathrm{int}}$ matrices with diagonal entries $u_e^\pm(k;x_e)$. We then define

$$Z(k;P,L,\boldsymbol{l}) := (P+L)X(k;\boldsymbol{l}) + P^\perp Y(k;\boldsymbol{l}), \tag{3.10}$$

which can be used to set up a characteristic equation.

Lemma 3.1. *Let $k^2 \neq 0$ be an eigenvalue of the Schrödinger operator H. Then one can choose $k \in S_\delta$, and for this choice*

$$\det Z(k;P,L,\boldsymbol{l}) = 0. \tag{3.11}$$

Furthermore, the pure point spectrum $\sigma_{pp}(H)$ of H consists of eigenvalues of finite multiplicities, bounded by E, and has no finite accumulation point.

Proof. The proof follows [KS06]. For every $k \in S_\delta$ and every $e \in \mathcal{E}_{\mathrm{int}}$ the functions $u_e^+(k;\cdot)$ and $u_e^-(k;\cdot)$ that are used to define Z form a complete system of solutions for (3.3). Moreover, one can choose δ such that every eigenvalue $k^2 \neq 0$ has a root $k \in S_\delta$, and either $k \in \mathbb{R}$ or k is of the form $k = \mathrm{i}\kappa$, $\kappa > 0$. Together with (3.2) this implies that an eigenfunction (3.1) can be represented as

$$\varphi_e(x) = \begin{cases} \gamma_e \mathrm{e}^{\mathrm{i}kx}, & e \in \mathcal{E}_{\mathrm{ex}}, \\ \alpha_e u_e^+(k;x) + \beta_e u_e^-(k;x), & e \in \mathcal{E}_{\mathrm{int}}, \end{cases} \tag{3.12}$$

where $\alpha_e, \beta_e, \gamma_e$ are complex coefficients. The boundary condition implied by (2.6) can be rearranged to yield

$$Z(k;P,L,\boldsymbol{l}) \begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix} = 0, \tag{3.13}$$

where $\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}$ are vectors with entries $\alpha_e, \beta_e, \gamma_e$, respectively. Hence, every eigenvalue k^2 of H leads to a zero of $\det Z(k;P,L,\boldsymbol{l})$.

Conversely, every zero of $\det Z(k;P,L,\boldsymbol{l})$ is associated with a non-trivial solution vector $\boldsymbol{\alpha}, \boldsymbol{\beta}, \boldsymbol{\gamma}$, from which a function (3.12) can be constructed that is in $C^\infty(\Gamma)$ and satisfies the vertex conditions. If $k = \mathrm{i}\kappa$, $\kappa > 0$, this function is in $L^2(\Gamma)$ and thus is an eigenfunction of H, corresponding to the eigenvalue $k^2 < 0$. When $k^2 > 0$, however, the function (3.12) is in $L^2(\Gamma)$, iff $\gamma = \boldsymbol{0}$. Thus the multiplicities of the eigenvalues are bounded by E.

Due to the assumptions made in Definition 3.1 the matrix entries of $Z(k;P,L,\boldsymbol{l})$ are analytic in $k \in S_\delta$, hence the same holds for $\det Z(k)$. Since $\det Z(k)$ is not identically zero, its zeros in S_δ form a countable set and do not have an accumulation point in S_δ. Hence the set of non-zero eigenvalues is countable and has no finite, non-zero accumulation point.

We denote the countable subset of $k \in S_\delta$ for which $Z(k; P, L, \boldsymbol{l})$ is not invertible as

$$\Sigma_Z := \{k \in S_\delta;\ \det Z(k; P, L, \boldsymbol{l}) = 0\}. \tag{3.14}$$

Using this notation, Lemma 3.1 states that $\sigma_{pp}(H) \subseteq \{k^2 \in \mathbb{R};\ k \in \Sigma_Z\} \cup \{0\}$.

In the case of the Laplacian one often uses an alternative characteristic equation for its eigenvalues involving an $\mathfrak{S}$-matrix, see [KS99b, KS06]. For a Schrödinger operator we now define an analogous quantity,

$$\mathfrak{S}(k; P, L) := -\left(P + L + P^\perp \overline{D\left(\overline{k}\right)}\right)^{-1} \left(P + L + P^\perp D(k)\right), \tag{3.15}$$

for $k \in S_\delta$, where

$$D(k) := R_2(k; \boldsymbol{l}) R_1(k; \boldsymbol{l})^{-1}, \tag{3.16}$$

with

$$\begin{aligned} R_1(k; \boldsymbol{l}) &:= \begin{pmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & 0 & \boldsymbol{u}_+(k; \boldsymbol{l}) \end{pmatrix}, \\ R_2(k; \boldsymbol{l}) &:= \begin{pmatrix} -\mathrm{i}k\mathbb{1} & 0 & 0 \\ 0 & \boldsymbol{u}'_-(k; \boldsymbol{0}) & 0 \\ 0 & 0 & -\boldsymbol{u}'_+(k; \boldsymbol{l}) \end{pmatrix}. \end{aligned} \tag{3.17}$$

When the boundary conditions are local in the sense of (2.7) the $\mathfrak{S}$-matrix decomposes as

$$\mathfrak{S}(k; P, L) = \bigoplus_{v \in \mathcal{V}} \mathfrak{S}_v(k; P, L). \tag{3.18}$$

We also set

$$T(k; \boldsymbol{l}) := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \boldsymbol{u}_-(k; \boldsymbol{l})^{-1} \\ 0 & \boldsymbol{u}_+(k; \boldsymbol{l}) & 0 \end{pmatrix}. \tag{3.19}$$

We can now rewrite the expression (3.10) as follows

$$\begin{aligned} Z(k; P, L, \boldsymbol{l}) &= (P + L)\left(\mathbb{1} + T(k; \boldsymbol{l})\right) \overline{R_1(\overline{k}; \boldsymbol{l})} \\ &\quad + P^\perp \left(\overline{R_2(\overline{k}; \boldsymbol{l})}\, \overline{R_1(\overline{k}; \boldsymbol{l})}^{-1} + R_2(k; \boldsymbol{l}) R_1(k; \boldsymbol{l})^{-1} T(k; \boldsymbol{l}) \right) \overline{R_1(\overline{k}; \boldsymbol{l})} \\ &= \left(P + L + P^\perp \overline{D(\overline{k})} + \left(P + L + P^\perp D(k)\right) T(k; \boldsymbol{l}) \right) \overline{R_1(\overline{k}; \boldsymbol{l})} \\ &= \left(P + L + P^\perp \overline{D(\overline{k})} \right) \left(\mathbb{1} - \mathfrak{S}(k; P, L) T(k; \boldsymbol{l})\right) \overline{R_1(\overline{k}; \boldsymbol{l})}, \end{aligned} \tag{3.20}$$

where we used (3.5).

We remark that in contrast to the case of the Laplacian covered in [KS06], neither of the matrices (3.15) and (3.19) are, in general, unitary when $k \in \mathbb{R}$. However, choosing a particular system of admissible fundamental solutions $u_e^\pm(k; \cdot)$ we can construct a matrix $U(k)$ that is unitary for $k \in \mathbb{R}$ such that the positive eigenvalues of H correspond to the zeros of $\det(\mathbb{1} - U(k))$. For this purpose we choose fundamental solutions on the internal edges that satisfy

$$u_e^{+\prime}(k; 0) = \mathrm{i}k, \qquad u_e^{-\prime}(k; 0) = -\mathrm{i}k, \tag{3.21}$$

and hence $W_e(k) = 2\mathrm{i}k$. Such a pair of fundamental solutions can be easily generated from the one in [PT87] through a linear combination. Using these fundamental solutions we define

$$U(k) := R(k)^{-1} \mathfrak{S}(k; P, L) T(k; \boldsymbol{l}) R(k), \tag{3.22}$$

with

$$R(k) := \begin{pmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & 0 & \boldsymbol{r}(k; \boldsymbol{l}) \end{pmatrix}. \tag{3.23}$$

Here $\boldsymbol{r}(k; \boldsymbol{l})$ is an invertible, diagonal matrix with entries $r_e(k; l_e) \neq 0$ on the diagonal, see Remark 3.1.

Lemma 3.2. *The matrix $U(k)$ is unitary for $k \in \mathbb{R}$.*

Proof. Let $k \in \mathbb{R}$, then

$$R(k)^{-1}T(k;\boldsymbol{l})R(k) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\boldsymbol{\phi}(k;\boldsymbol{l})} \\ 0 & \mathrm{e}^{\mathrm{i}\boldsymbol{\phi}(k;\boldsymbol{l})} & 0 \end{pmatrix} \tag{3.24}$$

is unitary. Here $\mathrm{e}^{\mathrm{i}\boldsymbol{\phi}(k;\boldsymbol{l})}$ is a diagonal matrix with diagonal entries $\mathrm{e}^{\mathrm{i}\phi_e(k;\boldsymbol{l})}$, see Remark 3.1. Furthermore, it follows from (3.15) that

$$\begin{aligned} R(k)^{-1}\mathfrak{S}(k;P,L)R(k) = &-\Big((P+L)R(k) + P^{\perp}\overline{D(\overline{k})}R(k)\Big)^{-1} \\ &\Big((P+L)R(k) + P^{\perp}D(k)R(k)\Big). \end{aligned} \tag{3.25}$$

Moreover,

$$D(k) = \begin{pmatrix} -\mathrm{i}k & 0 & 0 \\ 0 & -\mathrm{i}k & 0 \\ 0 & 0 & -\boldsymbol{r}'(k;\boldsymbol{l})\boldsymbol{r}(k;\boldsymbol{l})^{-1} - \mathrm{i}k\boldsymbol{r}(k;\boldsymbol{l})^{-2} \end{pmatrix}, \tag{3.26}$$

where we used the expression for the Wronskian in Remark 3.1 and the fact that $W_e(k) = 2\mathrm{i}k = 2\mathrm{i}{\phi_e}'(k;x)\,r_e(k;x)^2$ for the particular system of fundamental solutions we have chosen. This means that $R(k)^2\,\mathrm{Im}\,D(k) = -\mathrm{i}k\mathbb{1}$. With

$$\begin{aligned} K_1 &:= (P+L)R(k) + P^{\perp}\overline{D(k)}R(k), \\ K_2 &:= (P+L)R(k) + P^{\perp}D(k)R(k), \end{aligned} \tag{3.27}$$

the fact that $P+L$ and $P^{\perp}$ are self-adjoint, and $k \in \mathbb{R}$, the right-hand side of (3.25) is $-K_1^{-1}K_2$. This is unitary, if and only if $K_1K_1^* = K_2K_2^*$. A straight-forward calculation confirms that this is indeed the case.

We are now in a position to characterise the positive eigenvalues of H.

Proposition 3.1. *Let $k > 0$. Then the following statements are equivalent:*

(i) $\det Z(k;P,L,\boldsymbol{l}) = 0$,
(ii) $\det(\mathbb{1} - U(k)) = 0$,
(iii) *k^2 is an eigenvalue of H.*

Proof. From Lemma 3.1 we know that (iii) implies (i). We now first show the equivalence of (i) and (ii), using that (3.20) implies

$$Z(k;P,L,\boldsymbol{l}) = \Big((P+L)R(k) + P^{\perp}\overline{D(\overline{k})}R(k)\Big)\,(\mathbb{1} - U(k))\,R(k)^{-1}\overline{R_1(\overline{k};\boldsymbol{l})}. \tag{3.28}$$

Thus we need to show that the determinants of $(P+L)R(k) + P^{\perp}\overline{D(\overline{k})}R(k)$ and of $R(k)^{-1}\overline{R_1(\overline{k};\boldsymbol{l})}$ do not vanish when $k > 0$. For the second expression we simply note that both $R(k)$ and $R_1(k;\boldsymbol{l})$ are invertible for real k. Next, assume that $\det((P+L)R(k) + P^{\perp}\overline{D(\overline{k})}R(k)) = 0$. Then there exists $\boldsymbol{a} \in \mathbb{C}^E \setminus \{\boldsymbol{0}\}$ such that $(P+L+P^{\perp}\overline{D(\overline{k})})\boldsymbol{a} = \boldsymbol{0}$ or, equivalently, $P\boldsymbol{a} = \boldsymbol{0}$ and $(L + P^{\perp}D(k)P^{\perp})\boldsymbol{a} = \boldsymbol{0}$. Hence,

$$\big\langle \boldsymbol{a}, \big(L + P^{\perp}D(k)P^{\perp}\big)\,\boldsymbol{a}\big\rangle_{\mathbb{C}^E} = \langle \boldsymbol{a}, (L + D(k))\,\boldsymbol{a}\rangle_{\mathbb{C}^E} = 0, \tag{3.29}$$

which is equivalent to

$$\langle \boldsymbol{a}, L\boldsymbol{a}\rangle_{\mathbb{C}^E} = -\,\langle \boldsymbol{a}, \mathrm{Re}(D(k))\boldsymbol{a}\rangle_{\mathbb{C}^E} - \mathrm{i}\,\langle \boldsymbol{a}, \mathrm{Im}(D(k))\boldsymbol{a}\rangle_{\mathbb{C}^E}\,. \tag{3.30}$$

Since L is self-adjoint, the left-hand side is real, whereas (3.26) implies that the right-hand side has a non-vanishing imaginary part when $k \in \mathbb{R}$. This proves $\det\Big((P+L)R(k) + P^{\perp}\overline{D(\overline{k})}R(k)\Big) \neq 0$ for $k > 0$.

Finally, we have to show that (i) implies (iii). For this assume that $k > 0$ is a zero of $\det Z(k)$. Any solution vector $(\boldsymbol{\gamma}, \boldsymbol{\alpha}, \boldsymbol{\beta})^T$ from (3.13) can be used to construct a function (3.12). This is an eigenfunction, iff $\boldsymbol{\gamma} = \boldsymbol{0}$. By (3.28), the corresponding solution $\boldsymbol{v} = (\boldsymbol{c}, \boldsymbol{a}, \boldsymbol{b})^T$ of $(\mathbb{1} - U(k))\boldsymbol{v} = \boldsymbol{0}$ is of the form

$$\boldsymbol{v} = \begin{pmatrix} \boldsymbol{c} \\ \boldsymbol{a} \\ \boldsymbol{b} \end{pmatrix} = R(k)^{-1}\overline{R_1(\overline{k};\boldsymbol{l})}\begin{pmatrix} \boldsymbol{\gamma} \\ \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{pmatrix}, \tag{3.31}$$

such that $\boldsymbol{\gamma} = \boldsymbol{0}$, iff $\boldsymbol{c} = \boldsymbol{0}$.

Due to Lemma 3.2 the proof of Theorem 3.1 in [KS99a] can be applied to the current case, leading to $\boldsymbol{c} = \boldsymbol{0}$. Hence there exists an eigenfunction corresponding to the eigenvalue k^2.

Altogether, the spectrum of H has the following structure.

Proposition 3.2. *The spectrum of H is bounded from below and we have*

$$\sigma(H) = \begin{cases} \sigma_{pp}(H), & \mathcal{E}_{\text{ex}} = \emptyset, \\ \sigma_{ess}(H) \cup \sigma_{pp}(H), & \textit{otherwise}, \end{cases} \tag{3.32}$$

where $\sigma_{ess}(H) = [0, \infty)$ is the essential spectrum and $\sigma_{pp}(H)$ is the pure point spectrum of H, respectively. The eigenvalues in $\sigma_{pp}(H)$ have finite multiplicities that are bounded by E.

Proof. Since the multiplication operator V is bounded in $L^2(\Gamma)$ and $-\Delta$ is bounded from below, the semi-boundedness from below of the spectrum of H follows immediately.

If $\mathcal{E}_{\text{ex}} = \emptyset$ the operator H has compact resolvent and hence the spectrum is pure point and the eigenvalues have finite multiplicities.

From now on we consider $\mathcal{E}_{\text{ex}} \neq \emptyset$. The fact that then $\sigma_{ess}(H) = [0, \infty)$ follows from noticing that V is bounded and vanishes at infinity and, therefore, is relatively compact with respect to $-\Delta$. This is shown in complete analogy to [Wei03, Satz 17.2]. Hence $\sigma_{ess}(H) = \sigma_{ess}(-\Delta)$, and the latter is well known to be $[0, \infty)$.

The point spectrum is already characterised in Lemma 3.1 and in Proposition 3.1.

In order to characterise the spectrum of H fully the only remaining task is to prove the absence of a singularly continuous spectrum. This will follow from an analysis of the resolvent and will be given in the next section.

4 Resolvents

Our first goal is to identify the resolvent of H as an integral operator.

Definition 4.1 ([KS06])**.** *An operator $K : \mathcal{D}_K \subset L^2(\Gamma) \to L^2(\Gamma)$ is an integral operator, if for all $e, e' \in \mathcal{E}$ there exist functions $K_{ee'}(\cdot, \cdot) : I_e \times I_{e'} \to \mathbb{C}$ such that*

1. *$K_{ee'}(x, \cdot)\psi_{e'}(\cdot) \in L^1(I_{e'})$ for almost all $x \in I_e$ and all $\psi = \{\psi_e\}_{e \in \mathcal{E}} \in \mathcal{D}_K$,*
2. *$\phi = K\psi$ with $\psi \in \mathcal{D}_K$ and*

$$\phi_e(x) = \sum_{e' \in \mathcal{E}} \int_0^{l_{e'}} K_{ee'}(x, y)\, \psi_{e'}(y)\; \mathrm{d}y. \tag{4.1}$$

As a shorthand, we sometimes also denote the integral kernel of an integral operator K as $K(\boldsymbol{x}, \boldsymbol{y}) = \{K_{ee'}(x_e, y_{e'})\}_{e,e' \in \mathcal{E}}$ and its action (4.1) as

$$\phi(\boldsymbol{x}) = \int_\Gamma K(\boldsymbol{x}, \boldsymbol{y})\, \psi(\boldsymbol{y})\; \mathrm{d}\boldsymbol{y}. \tag{4.2}$$

We now show that the resolvent

$$R_H(k^2) = \left(H - k^2\right)^{-1} \tag{4.3}$$

of the Schrödinger operator H is an integral operator. Here we follow [KS06] closely, where the same was proven for the resolvent of the Laplacian.

We require some definitions, the first one being the 'free' resolvent kernel

$$r^{(0)}_{ee'}(k; x, y) := \frac{\delta_{ee'}}{W_e(k)} \begin{cases} \mathrm{e}^{ik|x-y|}, & e \in \mathcal{E}_{\text{ex}}, \\ u_e^+(k; x) u_e^-(k; y), & x \geq y, e \in \mathcal{E}_{\text{int}}, \\ u_e^-(k; x) u_e^+(k; y), & x \leq y, e \in \mathcal{E}_{\text{int}}, \end{cases} \tag{4.4}$$

where W_e is the Wronskian (3.8) when $e \in \mathcal{E}_{\text{int}}$ and $W_e(k) = 2\mathrm{i}k$ when $e \in \mathcal{E}_{\text{ex}}$. We also need the matrix

$$\Phi(k; \boldsymbol{x}) := \begin{pmatrix} \mathrm{e}^{\mathrm{i}k\boldsymbol{x}} & 0 & 0 \\ 0 & \boldsymbol{u}_+(k; \boldsymbol{x}) & \boldsymbol{u}_-(k; \boldsymbol{x}) \end{pmatrix}, \tag{4.5}$$

where $\mathrm{e}^{\mathrm{i}k\boldsymbol{x}}$ is a diagonal matrix with diagonal entries $\mathrm{e}^{\mathrm{i}kx_e}$, as well as the diagonal matrix

$$\boldsymbol{W}(k) := \begin{pmatrix} \boldsymbol{W}_{\text{ex}}(k) & 0 & 0 \\ 0 & \boldsymbol{W}_{\text{int}}(k) & 0 \\ 0 & 0 & \boldsymbol{W}_{\text{int}}(k) \end{pmatrix}, \tag{4.6}$$

where $\boldsymbol{W}_{\text{ex/int}}(k)$ are diagonal matrices with the Wronskians $W_e(k)$, $e \in \mathcal{E}_{\text{ex/int}}$, on the diagonal.

Theorem 4.1. *Let $k \in S_\delta \setminus \Sigma_Z$. Then $R_H(k^2)$ is an integral operator with integral kernel*

$$
\begin{aligned}
r_H(k^2;\boldsymbol{x},\boldsymbol{y}) = r^{(0)}(k;\boldsymbol{x},\boldsymbol{y}) + \Phi(k;\boldsymbol{x})\overline{R_1(\overline{k},\boldsymbol{l})}^{-1} &\left(\mathbb{1} - \mathfrak{S}(k;P,L)T(k;\boldsymbol{l})\right)^{-1} \\
&\cdot \mathfrak{S}(k;P,L)R_1(k;\boldsymbol{l})\boldsymbol{W}^{-1}(k)\Phi(k;\boldsymbol{y})^T.
\end{aligned}
\tag{4.7}
$$

Proof. In order to prove that (4.7) is the resolvent kernel we first rewrite it as

$$
\begin{aligned}
r_H\left(k^2;\boldsymbol{x},\boldsymbol{y}\right) = r^{(0)}\left(k;\boldsymbol{x},\boldsymbol{y}\right) - \Phi(k;\boldsymbol{x})&Z(k;P,L,\boldsymbol{l})^{-1} \\
&\cdot\left((P+L)R_1(k;\boldsymbol{l}) + P^\perp R_2(k;\boldsymbol{l})\right)\boldsymbol{W}^{-1}(k)\Phi(k;\boldsymbol{y})^T,
\end{aligned}
\tag{4.8}
$$

making use of the relation (3.20). We then have to show that for any $k \in S_\delta \setminus \Sigma_Z$ and for every $\psi \in L^2(\Gamma)$ the function

$$
\phi(\boldsymbol{x}) = \int_\Gamma r_H(k^2;\boldsymbol{x},\boldsymbol{y})\,\psi(\boldsymbol{y})\;\mathrm{d}\boldsymbol{y} \tag{4.9}
$$

is in the domain of H and satisfies

$$
(H-k^2)\phi = \psi. \tag{4.10}
$$

We now assume that $k \notin \Sigma_Z$, so that $Z(k)$ is invertible, and that k^2 is not in the spectrum $\sigma(H)$ of H, hence $R_H(k^2)$ is a bounded operator. Also, the explicit form of (4.8) ensures that the components ϕ_e of (4.9) are twice differentiable, hence one can apply $H-k^2$.

Suppose now that every component ψ_e is continuous on $(0,l_e)$. Direct calculations for $e \in \mathcal{E}_{\mathrm{int}}$ as well as for $e \in \mathcal{E}_{\mathrm{ex}}$ yield

$$
\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_e(x) - k^2\right)\int_0^{l_e} r_{ee}^{(0)}(k;x,y)\,\psi_e(y)\;\mathrm{d}y = \psi_e(x). \tag{4.11}
$$

Moreover, the matrix entries of $\Phi(k;\boldsymbol{x})$ are eigenfunctions of H (as a formal differential operator), so that $(H-k^2)\Phi(k;\boldsymbol{x}) = 0$. This proves (4.10) for ψ in a dense subset of $L^2(\Gamma)$. As the resolvent is bounded the result can be extended to $L^2(\Gamma)$.

In order to prove that (4.9) is in the domain of H we first observe that the explicit form (3.17) of $r_H^{(0)}$ as well as that of Φ (4.6) imply that $\phi \in H^2(\Gamma)$. Hence it remains to verify the vertex conditions.

We again assume that $\psi_e \in C(0,l_e)$ and find, when $e \in \mathcal{E}_{\mathrm{ex}}$ and x is close to zero, that

$$
\int_0^{l_e} r_{ee}^{(0)}(k;x,y)\psi_e(y)\;\mathrm{d}y = \frac{\mathrm{e}^{-\mathrm{i}kx}}{W_e(k)}\int_0^{l_e}\mathrm{e}^{\mathrm{i}ky}\psi_e(y)\;\mathrm{d}y. \tag{4.12}
$$

When $e \in \mathcal{E}_{\mathrm{int}}$ and x is close to zero, then

$$
\int_0^{l_e} r_{ee}^{(0)}(k;x,y)\psi_e(y)\;\mathrm{d}y = \frac{u_e^-(k;x)}{W_e(k)}\int_0^{l_e} u_e^+(k;y)\psi_e(y)\;\mathrm{d}y, \tag{4.13}
$$

and when x is close to l_e,

$$
\int_0^{l_e} r_{ee}^{(0)}(k;x,y)\psi_e(y)\;\mathrm{d}y = \frac{u_e^+(k;x)}{W_e(k)}\int_0^{l_e} u_e^-(k;y)\psi_e(y)\;\mathrm{d}y. \tag{4.14}
$$

With the abbreviation

$$
G(k) := -Z(k;P,L,\boldsymbol{l})^{-1}\left((P+L)R_1(k;\boldsymbol{l}) + P^\perp R_2(k;\boldsymbol{l})\right) \tag{4.15}
$$

this finally yields

$$
\begin{aligned}
\underline{\phi} &= R_1(k;\boldsymbol{l})\boldsymbol{W}^{-1}(k)\int_\Gamma \Phi(k;\boldsymbol{y})^T\psi(\boldsymbol{y})\;\mathrm{d}\boldsymbol{y} \\
&\quad + X(k;\boldsymbol{l})G(k)\boldsymbol{W}^{-1}(k)\int_\Gamma \Phi(k;\boldsymbol{y})^T\psi(\boldsymbol{y})\;\mathrm{d}\boldsymbol{y}, \\
\underline{\phi'} &= R_2(k;\boldsymbol{l})\boldsymbol{W}^{-1}(k)\int_\Gamma \Phi(k;\boldsymbol{y})\psi(\boldsymbol{y})\;\mathrm{d}\boldsymbol{y} \\
&\quad + Y(k;\boldsymbol{l})G(k)\boldsymbol{W}^{-1}(k)\int_\Gamma \Phi(k;\boldsymbol{y})^T\psi(\boldsymbol{y})\;\mathrm{d}\boldsymbol{y}.
\end{aligned}
\tag{4.16}
$$

Thus,

$$\begin{aligned}(P+L)\underline{\phi}+P^{\perp}\underline{\phi'} &= \big((P+L)R_1(k;\boldsymbol{l})+P^{\perp}R_2(k;\boldsymbol{l})\big)\,\boldsymbol{W}^{-1}(k)\int_{\Gamma}\Phi(k;\boldsymbol{y})^T\psi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\\ &\quad + Z(k;P,L,\boldsymbol{l})G(k)\boldsymbol{W}^{-1}(k)\int_{\Gamma}\Phi(k;\boldsymbol{y})^T\psi(\boldsymbol{y})\,\mathrm{d}\boldsymbol{y}\\ &= \mathbf{0}\end{aligned} \tag{4.17}$$

This proves the claim for a dense subset of $L^2(\Gamma)$. Since the resolvent is bounded the result extends to all of $L^2(\Gamma)$.

The right-hand side of (4.8) is analytic for $k\in S_\delta\setminus\Sigma_Z$ with poles in Σ_Z due to the zeros of $\det Z(k)$. Hence, the representation (4.8) for the resolvent kernel can be extended to $k\in S_\delta\setminus\Sigma_Z$.

The explicit form (4.7) of the resolvent kernel allows us to prove the absence of a singular continuous spectrum in a way similar to the case of Laplacians on graphs [Ong06].

Proposition 4.1. *Let $\phi\in C_0^\infty(\Gamma)$. Then the function $\langle\phi,(R_H(\lambda)-R_H(\lambda)^*)\,\phi\rangle$ can be extended from the upper half-plane $\operatorname{Im}\lambda>0$ through $\mathbb{R}_+$ into the lower half-plane, except for a discrete subset of $\mathbb{R}_+$. In particular, the singular continuous spectrum of H is empty. Hence, $\sigma(H)=\sigma_{ac}(H)\cup\sigma_{pp}(H)$.*

Proof. We choose $\phi\in C_0^\infty(\Gamma)$ and consider

$$\langle\phi,\operatorname{Im}R_H\,(\lambda+\mathrm{i}\varepsilon)\,\phi\rangle\,,\quad \lambda>0,\quad \varepsilon\to 0^+, \tag{4.18}$$

where

$$\operatorname{Im}R_H(\lambda):=\frac{1}{2\mathrm{i}}\left(R_H(\lambda)-R_H(\lambda)^*\right),\quad \lambda\in\mathbb{C}\setminus\sigma(H). \tag{4.19}$$

Representing $\lambda+\mathrm{i}\varepsilon=k^2$, the limit required in (4.18) can be achieved by keeping $\mathrm{Re}k>0$ fixed and taking $\operatorname{Im}k\to 0^+$. We remark that $R_H(k^2)^*$ is an integral operator whose kernel is the complex conjugate of (4.7).

We now fix two consecutive zeros $0<k_n<k_{n+1}$ of $\det Z(k)$ (corresponding to consecutive eigenvalues $0<k_n^2<k_{n+1}^2$ of H) and choose $0<a<b$ such that $(a,b)\subset(k_n,k_{n+1})$. The contribution to (4.18) involving the matrix-valued integral kernel $r^{(0)}\left(k^2;\cdot,\cdot\right)$ in (4.7) is uniformly bounded in λ taken from a suitable neighbourhood of (a^2,b^2).

Now choosing the representation (4.8) for the resolvent kernel one obtains that all contributions safe of $r^{(0)}\left(k^2;\cdot,\cdot\right)$ depend on $k\in S_\delta$ through the fundamental solutions $u_e^{\pm}$, or e^{ikx}. Hence, their contribution to (4.18) is analytic in k except for poles at $k\in\Sigma_Z$ and at $k=0$. Since Σ_Z is discrete with no finite accumulation point, and all positive $k\in\Sigma_Z$ lead to eigenvalues k^2 of H, the contribution in question is also uniformly bounded in λ taken from a suitable neighbourhood of (a^2,b^2).

Altogether this confirms that there exists a constant $C_\phi\geq 0$ such that

$$\liminf_{\varepsilon\to 0^+}\sup_{\lambda\in(a,b)}\langle\phi,\operatorname{Im}R_H\,(\lambda+\mathrm{i}\varepsilon)\,\phi\rangle_{L^2(\Gamma)}\leq C_\phi. \tag{4.20}$$

Hence [CFKS87, Proposition 4.1] applies, implying that H has (at most) purely absolutely continuous spectrum in (a,b). Since $(a,b)\subset(k_n,k_{n+1})$ can be chosen arbitrarily we conclude that the singularly continuous spectrum of H is empty.

In Proposition 3.2 it was shown that H has a purely discrete spectrum if and only if the graph is compact. Hence, for non-compact graphs the heat-semigroup e^{-Ht}, $t>0$, is not trace class and, therefore, no heat-trace asymptotics exists. In that case we subtract a 'free' contribution in such a way that the difference is a trace-class operator. As

$$\mathrm{e}^{-Ht}=\frac{\mathrm{i}}{2\pi}\int_\gamma \mathrm{e}^{-\lambda t}\,R_H(\lambda)\,\mathrm{d}\lambda, \tag{4.21}$$

where γ is a contour encircling the spectrum of H with positive orientation, the relevant difference can be achieved by subtracting a 'free' resolvent from R_H in (4.21). This procedure follows [Yaf92, KPS07, DP11].

The 'free' comparison operator is constructed using a graph Γ_{ex} by removing all internal edges from Γ and linking all external edges of Γ in a single vertex. Thus Γ_{ex} is an infinite star graph with E_{ex} edges. The associated Hilbert space is then

$$L^2(\Gamma_{\mathrm{ex}})=\bigoplus_{e\in\mathcal{E}_{\mathrm{ex}}}L^2(0,\infty), \tag{4.22}$$

which is embedded in $L^2(\Gamma)$ in an obvious way, using the embedding operator $J_{\mathrm{ex}} : L^2(\Gamma_{\mathrm{ex}}) \to L^2(\Gamma)$,

$$J_{\mathrm{ex}}(\psi)_e := \begin{cases} \psi_e, & e \in \mathcal{E}_{\mathrm{ex}}, \\ 0, & e \in \mathcal{E}_{\mathrm{int}}. \end{cases} \tag{4.23}$$

On Γ_{ex} the two comparison operators are the Dirichlet-Laplacian, $-\Delta_D$, and the Neumann-Laplacian, $-\Delta_N$. Their domains (in $L^2(\Gamma_{\mathrm{ex}})$) are given in analogy to (2.6) and (2.5), with $P_D = \mathbb{1}_{E_{\mathrm{ex}}}, L_D = 0$ and $P_N = 0, L_N = 0$, respectively.

Both operators, $-\Delta_{D/N}$, are non-negative and self-adjoint. Their resolvents, $R_{D/N}\left(k^2\right) := \left(-\Delta_{D/N} - k^2\right)^{-1}$, and heat-semigroups, $\exp(t\Delta_{D/N})$, $t > 0$, are operators acting on $L^2(\Gamma_{\mathrm{ex}})$. They can be compared to the resolvent, respectively to the heat-semigroup, of H in terms of the operators $J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*$ and $J_{\mathrm{ex}} \exp(t\Delta_{D/N}) J_{\mathrm{ex}}^*$ acting on $L^2(\Gamma)$. By construction, $R_{D/N}$ is the direct sum of the resolvents of Dirichlet-, respectively Neumann-, Laplacians on a half-line. Hence, they are integral operators with well-known integral kernels from which one immediately obtains the integral kernels for $J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*$, as

$$r_{D/N,ee'}\left(k^2; x, y\right) = \delta_{ee'} \frac{\mathrm{i}}{2k} \begin{cases} \mathrm{e}^{\mathrm{i}k|x-y|} \pm \mathrm{e}^{\mathrm{i}k(x+y)}, & e \in \mathcal{E}_{\mathrm{ex}} \\ 0, & e \in \mathcal{E}_{\mathrm{int}} \end{cases}, \tag{4.24}$$

when $\operatorname{Im} k > 0$ (see also [KPS07]).

Proposition 4.2. *The difference of resolvents, $R_H\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*$, is a trace-class operator and is self-adjoint for $k \in \mathrm{i}\mathbb{R}_+ \cup \mathbb{R}_0$. It is an integral operator with kernel*

$$\begin{aligned} r_H\left(k^2; \boldsymbol{x}, \boldsymbol{y}\right) - r_{D/N}\left(k^2; \boldsymbol{x}, \boldsymbol{y}\right) = r^{(0)}\left(k^2; \boldsymbol{x}, \boldsymbol{y}\right) - r_{D/N}\left(k^2; \boldsymbol{x}, \boldsymbol{y}\right) \\ + \Phi(k; \boldsymbol{x}) \overline{R_1(\bar{k}, \boldsymbol{l})}^{-1} \left(\mathbb{1} - \mathfrak{S}(k; P, L) T(k; \boldsymbol{l})\right)^{-1} \\ \cdot \mathfrak{S}(k; P, L) R_1(k; \boldsymbol{l}) \boldsymbol{W}^{-1}(k) \Phi(k; \boldsymbol{y})^T. \end{aligned} \tag{4.25}$$

The trace of $R_H\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*$ can be expressed as

$$\begin{aligned} \int_\Gamma \left[r_H\left(k^2; \boldsymbol{x}, \boldsymbol{x}\right) - r_{D/N}\left(k^2; \boldsymbol{x}, \boldsymbol{x}\right)\right] \, \mathrm{d}\boldsymbol{x} \\ = \sum_{e \in \mathcal{E}} \int_0^{l_e} \left[r_{H,ee}\left(k^2; x, x\right) - r_{D/N,ee}\left(k^2; x, x\right)\right] \, \mathrm{d}x. \end{aligned} \tag{4.26}$$

Proof. Self-adjointness is clear since by assumption $k^2 \in \mathbb{R}$ and the operators H and $-\Delta_{D/N}$ are self-adjoint.

In order to prove the trace-class property we introduce the auxiliary graph Γ_{int}, obtained by removing the external edges from Γ. Hence, Γ_{int} is a compact graph with edge set $\mathcal{E}_{\mathrm{int}}$. We then define the Hilbert space $L^2(\Gamma_{\mathrm{int}})$ and the embedding operator $J_{\mathrm{int}} : L^2(\Gamma_{\mathrm{int}}) \to L^2(\Gamma)$ in analogy to (4.22) and (4.23), respectively, interchanging $\mathcal{E}_{\mathrm{ex}}$ with $\mathcal{E}_{\mathrm{int}}$. We also require the auxiliary operators $H_{D/N}$ and $H_{\mathrm{int},D/N}$, both acting as the Schrödinger operator H. The domain of $H_{D/N}$ consists of functions in $H^2(\Gamma)$ with Dirichlet/Neumann conditions in the vertices and, analogously, the domain of $H_{\mathrm{int},D/N}$ comprises of functions in $H^2(\Gamma_{\mathrm{int}})$ with Dirichlet/Neumann conditions. Since $H_{D/N}$ is a finite rank perturbation of H we infer that $R_H\left(k^2\right) - R_{H_{D/N}}\left(k^2\right)$ is trace class. Moreover, $H_{\mathrm{int},D/N}$ acts on a compact graph and can be bounded from above and below (in the sense of quadratic forms) by $-\Delta_{\mathrm{int},D/N} + V_{\min/\max}$, where $V_{\min/\max}$ is the minimal/maximal value taken by the potential V on the compact graph Γ_{int}. The operators $-\Delta_{\mathrm{int},D/N} + V_{\min/\max}$ have compact resolvents (see [Kuc04]) and their eigenvalue asymptotics follow a Weyl law (in one dimension). Hence their resolvents are trace class. This implies that $J_{\mathrm{int}} R_{H_{\mathrm{int},D/N}}\left(k^2\right) J_{\mathrm{int}}^*$ is also trace class. Moreover, by construction $R_{H_{D/N}}\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^* = J_{\mathrm{int}} R_{H_{\mathrm{int},D/N}}\left(k^2\right) J_{\mathrm{int}}^*$. Hence, the difference of resolvents,

$$\begin{aligned} R_H\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^* = \left[R_H\left(k^2\right) - R_{H_{D/N}}\left(k^2\right)\right] \\ + \left[R_{H_{D/N}}\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*\right], \end{aligned} \tag{4.27}$$

is trace class.

By construction, and using Theorem 4.1, the kernel of the difference $R_H\left(k^2\right) - J_{\mathrm{ex}} R_{D/N}\left(k^2\right) J_{\mathrm{ex}}^*$ is given by (4.25), where

$$r_{ee'}^{(0)}\left(k^2; x, y\right) - r_{D/N,ee'}\left(k^2; x, y\right) = \frac{\delta_{ee'}}{W_e(k)} \begin{cases} \mp \mathrm{e}^{ik(x+y)}, & e \in \mathcal{E}_{\mathrm{ex}}, \\ u_e^+(k; x) u_e^-(k; y), & x \geq y, \ e \in \mathcal{E}_{\mathrm{int}}, \\ u_e^-(k; x) u_e^+(k; y), & x \leq y, \ e \in \mathcal{E}_{\mathrm{int}}. \end{cases} \tag{4.28}$$

Since the functions $u_e^{\pm}(k;x)$ are smooth on every compact interval I_e, $e \in \mathcal{E}_{\mathrm{int}}$, and $\mathrm{e}^{ik(x+y)}$ is smooth and square integrable on $\mathbb{R}^+ \times \mathbb{R}^+$ when $\operatorname{Im} k > 0$, the relation (4.26) follows from [KPS07, p. 15] and [GK69, p. 117].

5 Asymptotics of the $\mathfrak{S}$-matrix

In order to prove heat-kernel asymptotics for small t we employ the relation (4.21) and first determine the behaviour of the resolvent kernel for large $|k|$. Following Theorem 4.1 this requires the asymptotics of the $\mathfrak{S}$-matrix.

For the purpose of asymptotic expansions we now choose a particular systems of admissible fundamental solutions, see Definition 3.1.

Lemma 5.1 ([Fed93, HKT12])**.** *On each internal edge $e \in \mathcal{E}_{\mathrm{int}}$ and for each $k \in S_\delta$ the equation*

$$-u_e'' + V_e u_e - k^2 u_e = 0 \tag{5.1}$$

possesses two linearly independent solutions $u_e^{\pm}$ such that, for fixed $x \in (0, l_e)$, the functions $u_e^{\pm}(k;x)$ are analytic in $k \in S_\delta$, and for fixed k they are smooth in x. Moreover, for $|k| \to \infty$, $k \in S_\delta$, these solutions possess asymptotic expansions

$$u_e^{\pm}(k;x) \sim \exp\left(\sum_{l=-1}^{\infty} k^{-l} \int_0^x \beta_{e,l,\pm}(y)\ \mathrm{d}y\right), \tag{5.2}$$

that are uniform in $x \in (0, l_e)$. The derivatives $u_e^{\pm\prime}$ (with respect to x) possess asymptotic expansions in the same domain that are given as the derivatives of the right-hand side of (5.2).

The coefficient functions $\beta_{e,l,\pm}(x)$ are determined by the recursion relations

$$\beta_{e,l+1,\pm}(x) = \pm\frac{\mathrm{i}}{2}\left(\beta_{e,l,\pm}'(x) + \sum_{j=0}^{l} \beta_{e,j,\pm}(x)\beta_{e,l-j,\pm}(x)\right) \tag{5.3}$$

with $\beta_{e,-1,\pm}(x) = \pm\mathrm{i}$, $\beta_{e,0,\pm}(x) = 0$ and $\beta_{e,1,\pm}(x) = \mp\frac{\mathrm{i}}{2}V_e(x)$.

Proof. The existence of the fundamental solutions possessing the asymptotic behaviour (5.2) is proven in [Fed93, p. 37,38]. The recursion relations (5.3) for the coefficients are deduced in [HKT12, p. 12].

Remark 5.1. *We note that the leading asymptotic behaviour implied by (5.3) is*

$$u_e^{\pm}(k;x) = \mathrm{e}^{\pm\mathrm{i}kx + O(k^{-1})}. \tag{5.4}$$

Similarly [Fed93],

$$(u_e^{\pm})'(k;x) = \left(\pm\mathrm{i}k + O(k^{-1})\right) u_e^{\pm}(k;x). \tag{5.5}$$

Hence, asymptotically for large wave numbers, the solutions $u_e^{\pm}$ are left- and right-moving, complex, plane waves.

The recursion relations (5.3) imply for the next coefficients that

$$\begin{aligned}
\beta_{e,2,\pm}(x) &= \frac{1}{4}V_e'(x) \\
\beta_{e,3,\pm}(x) &= \pm\frac{\mathrm{i}}{8}V_e''(x) \mp \frac{\mathrm{i}}{8}V_e(x)^2 \\
\beta_{e,4,\pm}(x) &= -\frac{1}{16}V_e^{(3)}(x) + \frac{1}{4}V_e'(x)V_e(x).
\end{aligned} \tag{5.6}$$

Using a simple induction on l we also observe that

$$\beta_{e,l,+}(x) = (-1)^l \beta_{e,l,-}(x) \tag{5.7}$$

and

$$\beta_{e,l,\pm}(x) \in \begin{cases} \mathbb{R}, & l \quad \text{even} \\ \mathrm{i}\mathbb{R}, & l \quad \text{odd}. \end{cases} \tag{5.8}$$

We note that the condition $u_e^{\pm}(k;x) = \overline{u_e^{\mp}(\overline{k};x)}$ required by Definition 3.1 is consistent with equation (5.7).

If one adds further restrictions such as (3.21), an asymptotic expansion as in Lemma 5.1 need not hold.

The goal of this section is to prove an asymptotic expansion for the $\mathfrak{S}$-matrix (3.15) for large $|k|$. We first notice that by setting $V \equiv 0$ the $\mathfrak{S}$-matrix (3.15) becomes the well-known expression

$$\mathfrak{S}_{-\Delta}(k;P,L) = -\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}\left(P+L-\mathrm{i}kP^{\perp}\right) \tag{5.9}$$

for the Laplacian (see [KS06]).

Definition 5.1. *Let*

$$\boldsymbol{\beta}_j := \begin{pmatrix} 0 & 0 & 0 \\ 0 & \beta_{e,j,-}(\mathbf{0}) & 0 \\ 0 & 0 & -\beta_{e,j,+}(\boldsymbol{l}) \end{pmatrix}. \tag{5.10}$$

We then set

$$\Lambda_m := \sum_{\substack{j,n\in\mathbb{N}_0,\\ n+j=m}} (\mathrm{i}L)^n P^{\perp}\overline{\boldsymbol{\beta}_{j+1}}. \tag{5.11}$$

Let $\boldsymbol{m} = (m_1,\ldots,m_n) \in {\mathbb{N}_0}^n$ be a multi-index. Let

$$\Lambda_{n,r} := \sum_{|\boldsymbol{m}|=r}\prod_{j=1}^{n}\Lambda_{m_j}, \tag{5.12}$$

where $|\boldsymbol{m}| := \sum_{j=1}^{n} m_i$ is the length of the multi-index. Finally set

$$\Omega_j := \sum_{\substack{n\geq 1,\ r\geq 0,\\ r+2n=j}} \mathrm{i}^n\Lambda_{n,r} \tag{5.13}$$

with the convention that $\Omega_0 = 1$.

Our main result in this section is the following.

Theorem 5.2. *The $\mathfrak{S}$-matrix for a Schrödinger operator admits the asymptotic expansion*

$$\mathfrak{S}\left(k;P,L\right) \sim \mathfrak{S}_{\infty} + \sum_{m=1}^{\infty} k^{-m}\mathfrak{S}_m, \quad |k|\to\infty,\ k\in S_{\delta}, \tag{5.14}$$

where the matrix $\mathfrak{S}_{\infty}$ is defined as the large-k limit of the $\mathfrak{S}$-matrix of the Laplacian and is given by

$$\mathfrak{S}_{\infty} := \mathbb{1} - 2P = \lim_{|k|\to\infty}\mathfrak{S}(k,P,L) = \lim_{|k|\to\infty}\mathfrak{S}_{-\Delta}(k,P,L). \tag{5.15}$$

The perturbative terms are given by

$$\mathfrak{S}_m := \Omega_m\mathfrak{S}_{\infty} + 2\sum_{\substack{l\geq 0,\ n\geq 1,\\ l+n=m}}\Omega_l(\mathrm{i}L)^n + \mathrm{i}\sum_{\substack{r,n,l\in\mathbb{N}_0,\\ r+n+l=m-2}}\Omega_l(\mathrm{i}L)^r P^{\perp}\boldsymbol{\beta}_{n+1}. \tag{5.16}$$

In order to prove Theorem 5.2 we need some auxiliary results. We compute the asymptotics of the $\mathfrak{S}$-matrix by comparing it to the case of the Laplacian with the help of the following lemma.

Lemma 5.3. *The $\mathfrak{S}$-matrix for the operator H can be written as a perturbation of the $\mathfrak{S}$-matrix of the Laplacian by*

$$\mathfrak{S}(k;P,L) = \Omega(k)\mathfrak{S}_{-\Delta}(k;P,L) - \Omega(k)\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(D(k)+\mathrm{i}k\right), \tag{5.17}$$

where the matrix-valued function $\Omega(k)$ is given by

$$\Omega(k) := \left(\mathbb{1} + \left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(\overline{D\left(\overline{k}\right)} - \mathrm{i}k\right)\right)^{-1}. \tag{5.18}$$

Proof. A direct calculation using the definitions (3.15) and (5.9) shows that

$$\begin{aligned}
&\Omega(k)\mathfrak{S}_{-\Delta}(k;P,L) - \Omega(k)\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(D(k)+\mathrm{i}k\right)\\
&\quad= -\Omega(k)\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}\left(\left(P+L-\mathrm{i}kP^{\perp}\right)+P^{\perp}\left(D(k)+\mathrm{i}k\right)\right)\\
&\qquad-\left(\left(P+L+\mathrm{i}kP^{\perp}\right)+P^{\perp}\left(\overline{D\left(\overline{k}\right)}-\mathrm{i}k\right)\right)^{-1}\left(P+L+P^{\perp}D(k)\right)\\
&\quad=\mathfrak{S}(k;P,L).
\end{aligned} \tag{5.19}$$

From Remark 5.1 one concludes that $\overline{D\left(\overline{k}\right)} \to \mathrm{i}k$ when $|k|\to\infty$ in S_δ, and thus $\Omega(k)\to\mathbb{1}$ as well as $\mathfrak{S}(k;P,L)\sim\mathfrak{S}_{-\Delta}(k;P,L)$, cf. (5.15). In order to arrive at an asymptotic expansion of the $\mathfrak{S}$-matrix more is needed.

Lemma 5.4. *The function $\Omega(k)$ possesses an asymptotic expansion*

$$\Omega(k)\sim\sum_{l=0}^{\infty}k^{-l}\Omega_l, \tag{5.20}$$

for $|k|\to\infty$, $k\in S_\delta$.

Proof. We have

$$D(k)\sim-\mathrm{i}k+\sum_{l=1}^{\infty}k^{-l}\boldsymbol{\beta}_l,\qquad |k|\to\infty \tag{5.21}$$

from the definition of $D(k)$ in equation (3.16) and of $\boldsymbol{\beta}_l$ in equation (5.10). This implies $\left(\overline{D\left(\overline{k}\right)}-\mathrm{i}k\right)=O(k^{-1})$, so that we can expand $\Omega(k)$ in a power series,

$$\Omega(k)=\sum_{n=0}^{\infty}(-1)^n\left(\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(\overline{D\left(\overline{k}\right)}-\mathrm{i}k\right)\right)^n. \tag{5.22}$$

With

$$\begin{aligned}
\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}&=P+(\mathrm{i}k)^{-1}P^{\perp}\left(\mathbb{1}+(\mathrm{i}k)^{-1}L\right)^{-1}P^{\perp}\\
&=P-\mathrm{i}k^{-1}\sum_{r=0}^{\infty}k^{-r}P^{\perp}(\mathrm{i}L)^rP^{\perp}.
\end{aligned} \tag{5.23}$$

Each term in (5.22) can be expanded as $|k|\to\infty$ (see [BH75]),

$$\begin{aligned}
&(-1)^n\left(\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(\overline{D\left(\overline{k}\right)}-\mathrm{i}k\right)\right)^n\\
&\quad\sim\mathrm{i}^nk^{-2n}\left(\sum_{l,r=0}^{\infty}k^{-(l+r)}(\mathrm{i}L)^rP^{\perp}\overline{\boldsymbol{\beta}_{l+1}}\right)^n\\
&\quad=\mathrm{i}^nk^{-2n}\left(\sum_{m=0}^{\infty}k^{-m}\Lambda_m\right)^n=\mathrm{i}^n\sum_{j=0}^{\infty}k^{-j-2n}\Lambda_{n,j}.
\end{aligned} \tag{5.24}$$

Hence, as $|k|\to\infty$,

$$\begin{aligned}
&\sum_{n=0}^{\infty}(-1)^n\left(\left(P+L+\mathrm{i}kP^{\perp}\right)^{-1}P^{\perp}\left(\overline{D\left(\overline{k}\right)}-\mathrm{i}k\right)\right)^n\\
&\qquad\sim\mathbb{1}+\sum_{\substack{n=1,\\ j=0}}^{\infty}\mathrm{i}^nk^{-j-2n}\Lambda_{n,j}=\sum_{l=0}^{\infty}k^{-l}\Omega_l.
\end{aligned} \tag{5.25}$$

Proof. [Proof of Theorem 5.2] We finally have all the necessary input to prove Theorem 5.2. We use Lemma 5.3 and for $\mathfrak{S}_{-\Delta}(k;P,L)$ we employ a result from [BE09],

$$\mathfrak{S}_{-\Delta}(k;P,L)\sim\mathfrak{S}_{\infty}+2\sum_{n=1}^{\infty}k^{-n}(\mathrm{i}L)^n,\quad |k|\to\infty. \tag{5.26}$$

For the first term on the right-hand side of (5.17) we obtain

$$\Omega(k)\mathfrak{S}(k;P,L) \sim \sum_{l=0}^{\infty} k^{-l}\Omega_l\mathfrak{S}_\infty + \sum_{\substack{n=1,\\ l=0}}^{\infty} k^{-(n+l)}\Omega_l 2(\mathrm{i}L)^n, \tag{5.27}$$

as $|k| \to \infty$. Moreover, by Lemma 5.4 and equation (5.23) the second term in (5.17) gives,

$$\begin{aligned}
&\Omega(k)\left(P + L + \mathrm{i}kP^\perp\right)^{-1} P^\perp\left(D(k) + ik\right)\\
&\sim -\mathrm{i}k^{-2}\left(\sum_{l=0}^{\infty} k^{-l}\Omega_l\right)\left(\sum_{r=0}^{\infty} k^{-r}(\mathrm{i}L)^r\right) P^\perp \left(\sum_{n=0}^{\infty} k^{-n}\boldsymbol{\beta}_{n+1}\right)\\
&= -\mathrm{i}k^{-2}\sum_{l,r,n=0}^{\infty} k^{-l-r-n}\Omega_l(\mathrm{i}L)^r P^\perp\boldsymbol{\beta}_{n+1}, \quad |k| \to \infty,
\end{aligned} \tag{5.28}$$

Collecting all the terms finally yields Theorem 5.2.

Corollary 5.1. *The first terms of the asymptotic expansion* (5.14) *read*

$$\begin{aligned}
\mathfrak{S}\left(k;P,L\right) = \mathfrak{S}_\infty &+ 2k^{-1}\mathrm{i}L + 2k^{-2}\left(\mathrm{i}P^\perp\boldsymbol{\beta}_1 P - L^2\right)\\
&+ 2k^{-3}\left(P^\perp\boldsymbol{\beta}_1 L - L\boldsymbol{\beta}_1 P + \mathrm{i}P^\perp\boldsymbol{\beta}_2 P^\perp - \mathrm{i}L^3\right) + O\left(k^{-4}\right),
\end{aligned} \tag{5.29}$$

as $|k| \to \infty$.

Proof. The claim follows by Theorem 5.2 and Definition 5.1. Using (5.16) we find

$$\begin{aligned}
\Omega_2 &= \mathrm{i}\Lambda_{1,0} = \mathrm{i}P^\perp\overline{\boldsymbol{\beta}_1}\\
\Omega_3 &= \mathrm{i}\Lambda_{1,1} = \mathrm{i}(\mathrm{i}L)P^\perp\overline{\boldsymbol{\beta}_1} + \mathrm{i}P^\perp\overline{\boldsymbol{\beta}_2}.
\end{aligned} \tag{5.30}$$

Then, using $\mathfrak{S}_\infty = 1 - 2P$ and that $\boldsymbol{\beta}_1$ is a purely imaginary-valued matrix as well as that $\boldsymbol{\beta}_2$ is a real-valued matrix we get

$$\begin{aligned}
\mathfrak{S}_1 &= 2\mathrm{i}L\\
\mathfrak{S}_2 &= \Omega_2\mathfrak{S}_\infty + 2(\mathrm{i}L)^2 + \mathrm{i}P^\perp\boldsymbol{\beta}_1\\
&= \mathrm{i}P^\perp\overline{\boldsymbol{\beta}_1} - 2\mathrm{i}P^\perp\overline{\boldsymbol{\beta}_1}P - 2L^2 + \mathrm{i}P^\perp\boldsymbol{\beta}_1\\
\mathfrak{S}_3 &= \Omega_3\mathfrak{S}_\infty + 2(\mathrm{i}L)^3 + \Omega_2 2(\mathrm{i}L) + \mathrm{i}(\mathrm{i}L)P^\perp\boldsymbol{\beta}_1 + \mathrm{i}P^\perp\boldsymbol{\beta}_2\\
&= -LP^\perp\overline{\boldsymbol{\beta}_1} + 2LP^\perp\overline{\boldsymbol{\beta}_1}P + \mathrm{i}P^\perp\overline{\boldsymbol{\beta}_2} - 2\mathrm{i}P^\perp\overline{\boldsymbol{\beta}_2}P\\
&\quad - 2\mathrm{i}L^3 - 2P^\perp\overline{\boldsymbol{\beta}_1}L - LP^\perp\boldsymbol{\beta}_1 + \mathrm{i}P^\perp\boldsymbol{\beta}_2.
\end{aligned} \tag{5.31}$$

We will also need the asymptotic behaviour of $\mathfrak{S}(k;P,L)T(k;\boldsymbol{l})$.

Corollary 5.2. *For* $|k| \to \infty$ *with* $k \in S_\delta$,

$$\mathfrak{S}(k;P,L)T(k;\boldsymbol{l}) = \mathfrak{S}_\infty T_\infty(k) + O\left(k^{-1}\right), \tag{5.32}$$

where

$$T_\infty(k;\boldsymbol{l}) := \begin{pmatrix} 0 & 0 & 0\\ 0 & 0 & e^{\mathrm{i}k\boldsymbol{l}}\\ 0 & e^{\mathrm{i}k\boldsymbol{l}} & 0 \end{pmatrix}. \tag{5.33}$$

Proof. The statement follows immediately from Theorem 5.2 together with (5.4) and the definition (3.19) of $T(k)$.

6 Asymptotics of the Wronskian and related terms

The representation (4.7) of the resolvent kernel requires the knowledge of some further quantities, among them the Wronskians (3.8) associated with internal edges $e \in \mathcal{E}_{\mathrm{int}}$. To compute the asymptotics of the inverse of the Wronskian we need a similar definition to Definition 5.1.

Definition 6.1. *(i) Let $n \in \mathbb{N}$ and let $\boldsymbol{m} \in \mathbb{N}_0^n$ be a multi-index. Then we set*

$$\beta_e^{\boldsymbol{m}}(x) := \mathrm{i}^n \prod_{j=1}^{n} \beta_{e,2m_j+1,+}(x). \tag{6.1}$$

(ii) We also define the coefficients

$$w_{e,l}(x) := \begin{cases} \sum\limits_{n=1}^{l} \sum\limits_{|\boldsymbol{m}|=l-n} \beta_e^{\boldsymbol{m}}(x), & l \in \mathbb{N}, \\ 1, & l = 0. \end{cases} \tag{6.2}$$

Lemma 6.1. *The Wronskian associated with an internal edge has the following asymptotic expansion,*

$$W_e(k) \sim -2u_e^+(k;x)u_e^-(k;x) \sum_{l=-1}^{\infty} k^{-(2l+1)} \beta_{e,2l+1,+}(x), \tag{6.3}$$

when $|k| \to \infty$ with $k \in S_\delta$.

Proof. We have

$$\begin{aligned} W_e(k) &= u_e^+(k;x)u_e^{-\prime}(k;x) - u_e^-(k;x)u_e^{+\prime}(k;x) \\ &\sim u_e^+(k;x)\left(\sum_{l=-1}^{\infty} k^{-l}\beta_{e,l,-}(x)\right)u_e^-(k;x) \\ &\qquad - u_e^-(k;x)\left(\sum_{l=-1}^{\infty} k^{-l}\beta_{e,l,+}(x)\right)u_e^+(k;x) \\ &= u_e^+(k;x)u_e^-(k;x)\sum_{l=-1}^{\infty} k^{-l}\left(\beta_{e,l,-}(x) - \beta_{e,l,+}(x)\right) \\ &= -2u_e^+(k;x)u_e^-(k;x)\sum_{l=-1}^{\infty} k^{-(2l+1)}\beta_{e,2l+1,+}(x), \end{aligned} \tag{6.4}$$

where we used the symmetry relations of the coefficients given in (5.7) and (5.8).

This result is useful to obtain another asymptotic expansion needed in the resolvent.

Lemma 6.2. *As $|k| \to \infty$ with $k \in S_\delta$ the following asymptotic expansion holds,*

$$\frac{1}{W_e(k)} u_e^+(k;x)u_e^-(k;x) \sim -\frac{1}{2\mathrm{i}k}\sum_{l=0}^{\infty} k^{-2l} w_{e,l}(x), \tag{6.5}$$

where $w_{e,l}$ is defined in (6.2).

Proof. This follows from a direct application of Lemma 6.1.

$$\begin{aligned} \frac{1}{W_e(k)} u_e^+(k;x)u_e^-(k;x) &\sim -\left(\sum_{l=-1}^{\infty} 2k^{-(2l+1)}\beta_{e,2l+1,+}(x)\right)^{-1} \\ &= -(2\mathrm{i}k)^{-1}\left(1 - \left(\sum_{l=0}^{\infty} \mathrm{i}k^{-2l-2}\beta_{e,2l+1,+}(x)\right)\right)^{-1} \\ &= -(2\mathrm{i}k)^{-1}\sum_{n=0}^{\infty}\left(\sum_{l=0}^{\infty} \mathrm{i}k^{-2l-2}\beta_{e,2l+1,+}(x)\right)^{n} \\ &= -(2\mathrm{i}k)^{-1}\sum_{l=0}^{\infty} k^{-2l} w_{e,l}(x). \end{aligned} \tag{6.6}$$

The leading terms of this expansion can be worked out explicitly. Using

$$w_{e,1}(x) = \beta_e^0(x) = \mathrm{i}\beta_{e,1,+}(x) = \frac{1}{2}V_e(x) \tag{6.7}$$

and

$$\begin{aligned} w_{e,2}(x) &= \beta_e^1(x) + \beta_e^{(0,0)}(x) = \mathrm{i}\beta_{e,3,+}(x) - \beta_{e,1,+}(x)^2 \\ &= -\frac{1}{8}V_e''(x) + \frac{3}{8}V_e^2(x), \end{aligned} \tag{6.8}$$

we find that

$$\frac{1}{W_e(k)}u_e^+(k;x)u_e^-(k;x) \sim -\frac{1}{2\mathrm{i}}k^{-1} - \frac{V_e(x)}{4\mathrm{i}}k^{-3} + \frac{V_e''(x) - 3V_e^2(x)}{16\mathrm{i}}k^{-5} + O\left(k^{-7}\right). \tag{6.9}$$

We also need the asymptotics of the following two expressions in the upper half-plane. For that purpose we introduce the sector

$$S_\delta^+ := \left\{z \in \mathbb{C};\ 0 < |z| < \infty,\ \left|\arg(z) - \frac{\pi}{2}\right| < \frac{\pi}{2} - \delta\right\} \subset S_\delta \tag{6.10}$$

for $\delta > 0$ (supposed to be small). In particular, $k \in S_\delta^+$ implies $\operatorname{Im} k > 0$.

Lemma 6.3. *Let $e \in \mathcal{E}_{\mathrm{int}}$ and let k be confined to the sector S_δ^+. Then the two expressions below possess a complete asymptotic expansion as $|k| \to \infty$, whose leading terms are*

$$\frac{1}{W_e(k)}\int_0^{l_e} u_e^+(k;x)^2\ \mathrm{d}x = -\frac{1}{4k^2} - \frac{1}{4k^4}V_e(0) + \frac{1}{8\mathrm{i}k^5}V_e(0) + O\left(k^{-6}\right), \tag{6.11}$$

and

$$\frac{1}{W_e(k)}\frac{u_e^+(k;l_e)}{u_e^-(k;l_e)}\int_0^{l_e} u_e^-(k;x)^2\ \mathrm{d}x = -\frac{1}{4k^2} - \frac{1}{4k^4}V_e(l_e) - \frac{1}{8\mathrm{i}k^5}V_e'(l_e) + O(k^{-6}). \tag{6.12}$$

Proof. In view of the asymptotic behaviour (5.4) of the fundamental system we set

$$u_e^\pm(k;x) = \mathrm{e}^{\pm\mathrm{i}kx}\, v_e^\pm(k;x) \tag{6.13}$$

and notice that for fixed x the functions $v_e^\pm(k;x)$ are bounded in k, and their derivatives are of the order $O(k^{-1})$.

Integrating by parts $(N+1)$-times and using that $\operatorname{Im} k > 0$ when $k \in S_\delta^+$ we find for (6.11) that

$$\int_0^{l_e} \mathrm{e}^{2\mathrm{i}kx}v_e^+(k;x)^2\ \mathrm{d}x = \sum_{n=0}^{N} \frac{1}{(-2\mathrm{i}k)^{n+1}}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\ \left(v_e^+(k;x)^2\right)\big|_{x=0} + O\left(k^{-N-2}\right). \tag{6.14}$$

From Lemma 5.1 we find that

$$\begin{aligned} v_e^+(k;0)^2 &= 1 \\ \frac{\mathrm{d}}{\mathrm{d}x}\ \left(v_e^+(k;x)^2\right)\big|_{x=0} &= 2k^{-1}\beta_{e,1,+}(0) + 2k^{-2}\beta_{e,2,+}(0) + O\left(k^{-3}\right) \\ \frac{\mathrm{d}^2}{\mathrm{d}x^2}\ \left(v_e^+(k;x)^2\right)\big|_{x=0} &= 2k^{-1}\beta_{e,1,+}'(0) + O\left(k^{-2}\right) \\ \frac{\mathrm{d}^3}{\mathrm{d}x^3}\ \left(v_e^+(k;x)^2\right)\big|_{x=0} &= O\left(k^{-1}\right), \end{aligned} \tag{6.15}$$

and using this in (6.14) gives

$$\begin{aligned} &\int_0^{l_e} u_e^+(k;x)^2\ \mathrm{d}x \\ &\qquad = -\frac{1}{2\mathrm{i}k} - \frac{\beta_{e,1,+}(0)}{2k^3} - \frac{1}{k^4}\left(\frac{\beta_{e,2,+}(0)}{2} + \frac{\mathrm{i}\beta_{e,1,+}'(0)}{4}\right) + O\left(k^{-5}\right). \end{aligned} \tag{6.16}$$

An expansion for $1/W_e(k)$ follows from Lemma 6.2 and (6.9) evaluated at $x=0$. Altogether this yields

$$\begin{aligned} &\frac{1}{W_e(k)}\int_0^{l_e} u_e^+(k;x)^2\ \mathrm{d}x \\ &= \left(-\frac{1}{2\mathrm{i}k}-\frac{V_e(0)}{4\mathrm{i}k^3}+O\left(k^{-5}\right)\right)\left(-\frac{1}{2\mathrm{i}k}-\frac{V_e(0)}{4\mathrm{i}k^3}-\frac{V_e'(0)}{4k^4}+O\left(k^{-5}\right)\right) \\ &= -\frac{1}{4k^2}-\frac{V_e(0)}{4k^4}+\frac{V_e'(0)}{8\mathrm{i}k^5}+O\left(k^{-6}\right). \end{aligned} \tag{6.17}$$

For (6.12) we use Lemma 6.1 evaluated at $x=l$, and then integrate by parts $(N+1)$-times as in (6.14),

$$\begin{aligned} &\frac{1}{W_e(k)}\frac{u_e^+(k;l_e)}{u_e^-(k;l_e)}\int_0^{l_e} u_e^-(k;x)^2\ \mathrm{d}x \\ &\sim \frac{1}{-2\sum\limits_{l=-1}^{\infty}k^{-(2l+1)}\beta_{e,2l+1,+}(l_e)}\int_0^{l_e}\mathrm{e}^{-2\mathrm{i}k(x-l_e)}\,\frac{v_e^-(k;x)^2}{v_e^-(k;l_e)^2}\ \mathrm{d}x \\ &\sim \frac{1}{2ik}\left(\sum_{l=0}^{\infty}k^{-2l}w_{e,l}(l_e)\right) \\ &\quad\cdot\left(\sum_{n=0}^{N}\frac{1}{(2\mathrm{i}k)^{n+1}}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\ \left(v_e^-(k;x)^2\right)\big|_{x=0}+O\left(k^{-N-2}\right)\right) \end{aligned} \tag{6.18}$$

The prefactor was computed as in (6.6). We still need

$$\begin{aligned} v_e^-(k;0)&=1 \\ \frac{\mathrm{d}}{\mathrm{d}x}\ \left(v_e^-(k;x)^2\right)\big|_{x=0}&=2k^{-1}\beta_{e,1,-}(l_e)+2k^{-2}\beta_{e,2,-}(l_e)+O(k^{-3}) \\ \frac{\mathrm{d}^2}{\mathrm{d}x^2}\ \left(v_e^-(k;x)^2\right)\big|_{x=0}&=2k^{-1}\beta_{e,1,-}'(l_e)+O(k^{-2}) \\ \frac{\mathrm{d}^3}{\mathrm{d}x^3}\ \left(v_e^-(k;x)^2\right)\big|_{x=0}&=O(k^{-1}), \end{aligned} \tag{6.19}$$

giving

$$\begin{aligned} &\sum_{n=0}^{N}\frac{1}{(2\mathrm{i}k)^{n+1}}\frac{\mathrm{d}^n}{\mathrm{d}x^n}\ \left(v_e^-(k;x)^2\right)\big|_{x=0}+O\left(k^{-N-2}\right) \\ &= \frac{1}{2ik}-\frac{1}{2k^3}\beta_{e,1,-}(l_e)-\frac{1}{4k^4}\left(2\beta_{e,2,-}(l_e)-i\beta_{e,1,-}'(l_e)\right)+O(k^{-5}) \end{aligned} \tag{6.20}$$

Now using $w_{e,0}(l_e)=1$ and (6.7) finally yields (6.12).

7 Asymptotics of the resolvent kernel

The results of the previous sections enable us to determine the precise asymptotic behaviour of the resolvent kernel for k in the sector S_δ^+. As expected, the result on the diagonal is different from that off the diagonal, and this distinction carries over to the heat kernel.

Lemma 7.1. *In the sector S_δ^+ the resolvent kernel of H satisfies the estimate*

$$r_{H,ee'}(k^2;x,y)=O\left(k^{-1}\mathrm{e}^{-\operatorname{Im}kd(x,y)}\right), \tag{7.1}$$

when $|k|\to\infty$.

Proof. For the proof we use the representation (4.7) of the resolvent kernel. The contribution of the 'free' part $r_{ee'}^{(0)}(k;x,y)$ is clearly of the form (7.1), see (4.4).

For the remaining contributions we note that as $|k| \to \infty$ with $k \in S_\delta$,

$$
\begin{aligned}
\Phi(k;\boldsymbol{x})\overline{R_1(\overline{k},\boldsymbol{l})}^{-1} &= \begin{pmatrix} \mathrm{e}^{ik\boldsymbol{x}} & 0 & 0 \\ 0 & \boldsymbol{u}_+(k;\boldsymbol{x}) & \boldsymbol{u}_-(k;\boldsymbol{x})\boldsymbol{u}_-(k;\boldsymbol{l})^{-1} \end{pmatrix} \\
&\sim \begin{pmatrix} \mathrm{e}^{ik\boldsymbol{x}} & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k\boldsymbol{x}} & \mathrm{e}^{\mathrm{i}k(\boldsymbol{l}-\boldsymbol{x})} \end{pmatrix},
\end{aligned}
\tag{7.2}
$$

as well as

$$
\begin{aligned}
R_1(k;\boldsymbol{l})\boldsymbol{W}^{-1}(k)\Phi(k;\boldsymbol{y})^T &= \boldsymbol{W}^{-1}(k)\begin{pmatrix} \mathrm{e}^{ik\boldsymbol{y}} & 0 \\ 0 & \boldsymbol{u}_+(k;\boldsymbol{y}) \\ 0 & \boldsymbol{u}_+(k;\boldsymbol{l})\boldsymbol{u}_-(k;\boldsymbol{y}) \end{pmatrix} \\
&\sim \frac{\mathrm{i}}{2k}\begin{pmatrix} \mathrm{e}^{ik\boldsymbol{y}} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k\boldsymbol{y}} \\ 0 & \mathrm{e}^{\mathrm{i}k(\boldsymbol{l}-\boldsymbol{y})} \end{pmatrix}.
\end{aligned}
\tag{7.3}
$$

The remaining expression $\left(\mathbb{1}-\mathfrak{S}(k;P,L)T(k;\boldsymbol{l})\right)^{-1}\mathfrak{S}(k;P,L)$ has an asymptotic behaviour that follows from Theorem 5.2 and Corollary 5.2. The latter implies, in particular, that for sufficiently large $|k|$ and $\operatorname{Im} k > 0$ the matrix $\mathfrak{S}(k;P,L)T(k;\boldsymbol{l})$ has norm less than one. Moreover, for such values of k,

$$
\begin{aligned}
&\left(\mathbb{1}-\mathfrak{S}(k;P,L)T(k;\boldsymbol{l})\right)^{-1}\mathfrak{S}(k;P,L) \\
&\quad= \sum_{n=0}^{\infty}\left(\mathfrak{S}(k;P,L)T(k;\boldsymbol{l})\right)^n\mathfrak{S}(k;P,L) \\
&\quad= \sum_{n=0}^{\infty}\left(\mathfrak{S}_\infty T_\infty(k;\boldsymbol{l})\right)^n\mathfrak{S}_\infty + O\left(k^{-1}\right).
\end{aligned}
\tag{7.4}
$$

Putting (7.2)-(7.4) together according to (4.7) we notice that, asymptotically, the same expression emerges for the 'non-free' contribution to the resolvent kernel as in the case where H is a Laplacian, see [KPS07, Proposition 3.3.]. Hence, asymptotically this contribution can be represented as a sum over paths from y to x on Γ. Let $\mathcal{P}_{xy}$ the set of such paths, and let $d_p(x,y)$ be the distance of x and y along $p_{xy} \in \mathcal{P}_{xy}$, then

$$
\begin{aligned}
r_{H,ee'}\left(k^2;x,y\right) &\sim \delta_{ee'}\frac{\mathrm{i}}{2k}\,\mathrm{e}^{\mathrm{i}k|x-y|} + O\left(k^{-2}\right) \\
&\quad + \frac{\mathrm{i}}{2k}\sum_{p_{xy}\in\mathcal{P}_{xy}}\left(A_p + O\left(k^{-1}\right)\right)\mathrm{e}^{\mathrm{i}kd_p(x,y)},
\end{aligned}
\tag{7.5}
$$

when $|k| \to \infty$ with $k \in S_\delta^+$. Here the amplitudes A_p arise from multiplying matrix elements of $\mathfrak{S}_\infty$ along the path p_{xy} in the same way as in [KPS07]. As the distance $d(x,y)$ is the minimum of $d_p(x,y)$ over all $p_{xy} \in \mathcal{P}_{xy}$, the result (7.1) follows.

According to Lemma 7.1 points x, y on the graph with zero distance deserve a further investigation. When such points x, y are at edge ends, particular care has to be taken as to which edge the points belong to. We clarify this case by using the notation $x \cong (v,e) \in \mathcal{V}\times\mathcal{E}$ indicating that the point is an edge end of e and v is the vertex adjacent to e. This notation is well defined since we have excluded tadpoles in our construction. Moreover, in the following we use for the corresponding matrix elements the notation $M_{xy} := M_{ee'}$, $x \cong (v,e)$, $y \cong (v,e')$, where v has to be adjacent to e and e'. This notation is well-defined since we have assumed local boundary conditions and no tadpoles.

Lemma 7.2. *Let x, y be points on Γ with $d(x,y) = 0$. Then, for $k \in S_\delta^+$ the resolvent kernel of H possesses a complete asymptotic expansion as $|k| \to \infty$ in powers of k^{-1}. The leading terms are given by:*

(i) x is not an edge end:

$$
r_{H,ee}\left(k;x,x\right)_{ee} = \frac{\mathrm{i}}{2k} + O(k^{-3}),
\tag{7.6}
$$

(ii) $x \cong (v,e)$ and $y \cong (v,e')$ with $e \neq e'$:

$$
r_{H,ee'}\left(k;x,y\right) = \frac{\mathrm{i}\mathfrak{S}_{\infty,xy}}{2k} - \frac{L_{xy}}{k^2} + O\left(k^{-3}\right),
\tag{7.7}
$$

(iii) $x \cong (v,e)$:

$$r_{H,ee}(k;x,x) = \frac{\mathrm{i}}{2k}\left(1+\mathfrak{S}_{\infty,xx}\right) - \frac{L_{xx}}{k^2} + O\left(k^{-3}\right). \tag{7.8}$$

Proof. We use the expansion (7.4) in the representation (4.25) of the resolvent kernel. The coefficients of k^{-1} and k^{-2} in (7.6), (7.7) and (7.8) follow from the leading term, coming from $n=0$, in (7.4). For $e, e' \in \mathcal{E}_{\rm int}$ we have

$$\begin{aligned}
&\left(\Phi(k;\boldsymbol{x})\overline{R_1(\overline{k},\boldsymbol{l})}^{-1}\mathfrak{S}\left(k;P,L\right)R_1(k;\boldsymbol{l})\boldsymbol{W}^{-1}(k)\Phi(k;\boldsymbol{y})^T\right)_{ee'}\\
&\quad= u_e^+(k;x_e)\mathfrak{S}\left(k;P,L\right)_{ee'}W_{e'}{}^{-1}(k)u_{e'}^+(k;y_{e'})\\
&\qquad+ u_e^+(k;x_e)\mathfrak{S}\left(k;P,L\right)_{ee'}u_{e'}^+(k;l_{e'})W_{e'}^{-1}(k)u_{e'}^-(k;y_{e'})\\
&\qquad+ u_e^-(k;x_e)u_e^-(k;l_e)^{-1}\mathfrak{S}(k;P,L)_{ee'}W_{e'}^{-1}(k)u_{e'}^+(k;y_{e'})\\
&\qquad+ u_e^-(k;x_e)u_e^-(k;l_e)^{-1}\mathfrak{S}(k;P,L)_{ee'}u_{e'}^+(k;l_{e'})W_{e'}^{-1}(k)u_{e'}^-(k;y_{e'}).
\end{aligned} \tag{7.9}$$

Analogous results hold for the other three cases. A straightforward incorporation of the leading two coefficients with respect to k coming from (5.2), (5.29) and (6.3) in (7.9) completes the proof.

We now have all the ingredients to determine the trace of a regularised resolvent, in the sense of Proposition 4.2.

Theorem 7.3. *Let Γ be a compact or non-compact metric graph. Then the trace of the difference of resolvents, $R_H(k^2) - J_{\rm ex}R_{D/N}(k^2)J_{\rm ex}^*$, possesses an asymptotic expansion in powers of k^{-1} when $|k|\to\infty$ with k in the sector S_δ^+ of the upper half-plane,*

$$\operatorname{tr}\left(R_H(k^2) - J_{\rm ex}R_{D/N}(k^2)J_{\rm ex}^*\right) \sim \sum_{n=1}^{\infty} b_n k^{-n}. \tag{7.10}$$

The leading coefficients are given by

$$\begin{aligned}
b_1 &= -\frac{\mathcal{L}}{2\mathrm{i}}\\
b_2 &= -\frac{1}{4}\operatorname{tr}\mathfrak{S}_\infty \pm \frac{E_{\rm ex}}{4}\\
b_3 &= -\frac{1}{4\mathrm{i}}\int_{\Gamma_{\rm int}} V(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \frac{1}{2\mathrm{i}}\operatorname{tr}L\\
b_4 &= -\frac{1}{4}\sum_{v\in\mathcal{V}}\sum_{e\sim v}\mathfrak{S}_{\infty,ee}V_e(v) + \frac{1}{2}\operatorname{tr}L^2\\
b_5 &= \frac{1}{16\mathrm{i}}\int_{\Gamma_{\rm int}}\left(V''(\boldsymbol{x}) - 3V^2(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x} + \frac{1}{8\mathrm{i}}\sum_{v\in\mathcal{V}}\sum_{e\sim v}\mathfrak{S}_{\infty,ee}V_e'(v)\\
&\quad+\frac{3}{4\mathrm{i}}\sum_{v\in\mathcal{V}}\sum_{e\sim v}L_{ee}V_e(v) - \frac{1}{2\mathrm{i}}\operatorname{tr}L^3 - \frac{1}{8\mathrm{i}}\sum_{v\in\mathcal{V}}\sum_{e\sim v}P_{ee}^\perp V_e'(v).
\end{aligned} \tag{7.11}$$

Proof. By Proposition 4.2 the difference of resolvents is trace class and the trace can be obtained from the resolvent kernel as in (4.26) with the kernel (4.25).

The first contribution comes from the 'free' part (4.28),

$$\begin{aligned}
&\int_\Gamma \left(r^{(0)}\left(k^2;\boldsymbol{x},\boldsymbol{x}\right) - r_{D/N}\left(k^2;\boldsymbol{x},\boldsymbol{x}\right)\right)\mathrm{d}\boldsymbol{x}\\
&\quad= \mp\sum_{e\in\mathcal{E}_{\rm ex}}\frac{\mathrm{i}}{2k}\int_0^\infty \mathrm{e}^{2\mathrm{i}kx}\,\mathrm{d}x + \int_{\Gamma_{\rm int}}\frac{1}{\boldsymbol{W}_{\rm int}(k)}\boldsymbol{u}_+(k;\boldsymbol{x})\boldsymbol{u}_-(k;\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}.
\end{aligned} \tag{7.12}$$

For the first term on the right-hand side we use that $\operatorname{Im}k>0$. The asymptotics of the second term follow from Lemma 6.2 and (6.9),

$$\begin{aligned}
\int_\Gamma \left(r^{(0)}\left(k^2;\boldsymbol{x},\boldsymbol{x}\right) - r_{D/N}\left(k^2;\boldsymbol{x},\boldsymbol{x}\right)\right)\mathrm{d}\boldsymbol{x} &\sim \pm\frac{E_{\rm ex}}{4k^2} - \frac{\mathcal{L}}{2\mathrm{i}k} - \frac{1}{4\mathrm{i}k^3}\int_{\Gamma_{\rm int}} V(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}\\
&\quad+\frac{1}{16\mathrm{i}k^5}\int_{\Gamma_{\rm int}}\left(V''(\boldsymbol{x}) - 3V^2(\boldsymbol{x})\right)\mathrm{d}\boldsymbol{x} + O\left(k^{-7}\right).
\end{aligned} \tag{7.13}$$

The 'non-free' contribution, i.e., the second and third lines on the right-hand side of (4.25), will give the contribution at the vertices. We first observe that Corollary 5.2 implies, when $\operatorname{Im} k > 0$, that $(\mathbb{1} - \mathfrak{S}(k; P, L)T(k; \boldsymbol{l})))^{-1} = \mathbb{1} + O(k^{-\infty})$. After a cyclic permutation we hence have to determine the asymptotic expansion of

$$\operatorname{tr}\left(\int_\Gamma \mathfrak{S}\,(k; P, L)\, R_1(k; \boldsymbol{l}) \boldsymbol{W}(k)^{-1} \phi(k; \boldsymbol{x})^T \phi(k; \boldsymbol{x}) \overline{R_1\left(\overline{k}, \boldsymbol{l}\right)}^{-1} \mathrm{d}\boldsymbol{x}\right). \tag{7.14}$$

As the $\mathfrak{S}$-matrix is independent of $\boldsymbol{x}$ we only need to integrate the remaining terms. For these, a straight-forward calculation gives

$$\begin{aligned} &R_1(k; \boldsymbol{l}) \boldsymbol{W}(k)^{-1} \phi(k; \boldsymbol{x})^T \phi(k; \boldsymbol{x}) \overline{R_1\left(\overline{k}, \boldsymbol{l}\right)}^{-1} \\ &\quad = \begin{pmatrix} \mathrm{e}^{2\mathrm{i}k\boldsymbol{x}} & 0 & 0 \\ 0 & \frac{\boldsymbol{u}_+(k;\boldsymbol{x})^2}{\boldsymbol{W}_{\mathrm{int}}(k)} & \frac{\boldsymbol{u}_+(k;\boldsymbol{x})\boldsymbol{u}_-(k;\boldsymbol{x})\boldsymbol{u}_+(k;\boldsymbol{l})}{\boldsymbol{W}_{\mathrm{int}}(k)} \\ 0 & \frac{\boldsymbol{u}_-(k;\boldsymbol{x})\boldsymbol{u}_+(k;\boldsymbol{x})}{\boldsymbol{W}_{\mathrm{int}}(k)\boldsymbol{u}_-(k;\boldsymbol{l})} & \frac{\boldsymbol{u}_-(k;\boldsymbol{x})^2\boldsymbol{u}_+(k;\boldsymbol{l})}{\boldsymbol{W}_{\mathrm{int}}(k)\boldsymbol{u}_-(k;\boldsymbol{l})} \end{pmatrix}. \end{aligned} \tag{7.15}$$

We note that $\mathrm{e}^{2\mathrm{i}k\boldsymbol{x}} = O(k^{-\infty})$, and that asymptotic expansions of the integrals of the remaining diagonal blocks were determined in Lemma 6.3. Lemma 6.2 implies that $\boldsymbol{W}_{\mathrm{int}}(k)^{-1}\boldsymbol{u}_\pm(k; \boldsymbol{x})\boldsymbol{u}_\mp(k; \boldsymbol{x})$ possess asymptotic expansions in powers of k^{-1}. In the off-diagonal blocks of (7.15), however, these terms are multiplied by $\boldsymbol{u}_\pm(k; \boldsymbol{l})^{\pm 1} = O(k^{-\infty})$. Therefore, the off-diagonal blocks do not contribute to the expansion. Thus,

$$\begin{aligned} &\int_\Gamma R_1(k; \boldsymbol{l}) \boldsymbol{W}(k)^{-1} \phi(k; \boldsymbol{x})^T \phi(k; \boldsymbol{x}) \overline{R_1\left(\overline{k}, \boldsymbol{l}\right)}^{-1} \mathrm{d}\boldsymbol{x} \\ &\quad = -\frac{1}{4k^2}\begin{pmatrix} 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & 0 & \mathbb{1} \end{pmatrix} - \frac{1}{4k^4}\begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\mathbf{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}) \end{pmatrix} \\ &\qquad + \frac{1}{8\mathrm{i}k^5}\begin{pmatrix} 0 & 0 & 0 \\ 0 & V'(\mathbf{0}) & 0 \\ 0 & 0 & -V'(\boldsymbol{l}) \end{pmatrix} + O(k^{-6}) \end{aligned} \tag{7.16}$$

We still need to multiply this with the $\mathfrak{S}$-matrix whose asymptotic expansion was determined in Theorem 5.2 and in Corollary 5.1,

$$\begin{aligned} \mathfrak{S}\,(k; P, L) &= \mathfrak{S}_\infty + 2k^{-1}\mathrm{i}L + 2k^{-2}\left(\mathrm{i}P^\perp \boldsymbol{\beta}_1 P - L^2\right) \\ &\quad + 2k^{-3}\left(P^\perp \boldsymbol{\beta}_1 L - L\boldsymbol{\beta}_1 P + \mathrm{i}P^\perp \boldsymbol{\beta}_2 P^\perp - \mathrm{i}L^3\right) + O\left(k^{-4}\right) \\ &= \mathfrak{S}_\infty - \frac{2}{\mathrm{i}k}L - \frac{1}{k^2}\left(P^\perp \begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\mathbf{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}_{\boldsymbol{e}}) \end{pmatrix} P + 2L^2\right) \\ &\quad - \frac{1}{\mathrm{i}k^3}\left(P^\perp \begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\mathbf{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}_{\boldsymbol{e}}) \end{pmatrix} L - L\begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\mathbf{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}_{\boldsymbol{e}}) \end{pmatrix} P \right. \\ &\quad \left. + \frac{1}{2}P^\perp \begin{pmatrix} 0 & 0 & 0 \\ 0 & V'(\mathbf{0}) & 0 \\ 0 & 0 & -V'(\boldsymbol{l}_{\boldsymbol{e}}) \end{pmatrix} P^\perp - 2L^3\right) + O\left(k^{-4}\right) \end{aligned} \tag{7.17}$$

When taking the trace the third and the sixth term on the right-hand side vanish as they contain P and $P^\perp$, and P and L, respectively. The latter case is due to $L = P^\perp L P^\perp$.

This gives the following contribution of (7.14) to the coefficients (7.11),

$$\begin{aligned} \tilde{b}_2 &= -\frac{1}{4}\operatorname{tr}\mathfrak{S}_\infty \\ \tilde{b}_3 &= \frac{1}{2\mathrm{i}}\operatorname{tr} L \\ \tilde{b}_4 &= -\frac{1}{4}\operatorname{tr}\left(\mathfrak{S}_\infty\begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\mathbf{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}) \end{pmatrix}\right) + \frac{1}{2}\operatorname{tr} L^2 \\ &= -\frac{1}{4}\sum_{v\in\mathcal{V}}\sum_{e\sim v}\mathfrak{S}_{\infty,ee}V_e(v) + \frac{1}{2}\operatorname{tr} L^2 \end{aligned} \tag{7.18}$$

$$
\begin{aligned}
\tilde{b}_5 =& \frac{1}{8\mathrm{i}} \operatorname{tr}\left(\mathfrak{S}_\infty \begin{pmatrix} 0 & 0 & 0 \\ 0 & V'(\boldsymbol{0}) & 0 \\ 0 & 0 & -V'(\boldsymbol{l}) \end{pmatrix}\right) \\
&+ \frac{1}{2\mathrm{i}} \operatorname{tr}\left(L \begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\boldsymbol{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l}) \end{pmatrix}\right) - \frac{1}{2\mathrm{i}} \operatorname{tr} L^3 \\
&+ \frac{1}{4\mathrm{i}} \operatorname{tr}\left(P^\perp \begin{pmatrix} 0 & 0 & 0 \\ 0 & V(\boldsymbol{0}) & 0 \\ 0 & 0 & V(\boldsymbol{l_e}) \end{pmatrix} L\right) \\
&+ \frac{1}{8\mathrm{i}} \operatorname{tr}\left(P^\perp \begin{pmatrix} 0 & 0 & 0 \\ 0 & V'(\boldsymbol{0}) & 0 \\ 0 & 0 & -V'(\boldsymbol{l_e}) \end{pmatrix} P^\perp\right) \\
=& \frac{1}{8\mathrm{i}} \sum_{v\in\mathcal{V}} \sum_{e\sim v} \mathfrak{S}_{\infty,ee} V_e'(v) + \frac{3}{4\mathrm{i}} \sum_{v\in\mathcal{V}} \sum_{e\sim v} L_{ee} V_e(v) \\
&- \frac{1}{2\mathrm{i}} \operatorname{tr} L^3 - \frac{1}{8\mathrm{i}} \sum_{v\in\mathcal{V}} \sum_{e\sim v} P_{ee}^\perp V_e'(v).
\end{aligned}
$$

Combined with the contributions in (7.13) this finally proves (7.11).

8 Asymptotics of the heat kernel

We shall use the relation

$$
\mathrm{e}^{-Ht} - J_{\mathrm{ex}} \mathrm{e}^{\Delta_{D/N} t} J_{\mathrm{ex}}^* = \frac{\mathrm{i}}{2\pi} \int_\gamma \mathrm{e}^{-\lambda t} \left(R_H(k^2) - J_{\mathrm{ex}} R_{D/N}(k^2) J_{\mathrm{ex}}^*\right) \, \mathrm{d}\lambda, \tag{8.1}
$$

on the level of kernels, where the (positively oriented) contour γ encloses $\sigma(H)$, to determine an asymptotic expansion for small t of the trace of (8.1). This approach is based on the following lemma.

Lemma 8.1 ([Won01], p. 31)**.** *Let $f \in C(0,\infty)$ such that $\mathrm{e}^{-ct} f(t) \in L^1(0,\infty)$ for some $c \in \mathbb{R}^+$. Let*

$$
F(z) = \int_0^\infty \mathrm{e}^{-zt} f(t) \, \mathrm{d}t \tag{8.2}
$$

be the Laplace-transform of f. Assume that F has a complete asymptotic expansion

$$
F(z) \sim \sum_{n=0}^\infty a_n \Gamma(d_n) z^{-d_n}, \quad |z| \to \infty, \tag{8.3}
$$

uniformly in $|\arg(z-c)| \le \frac{\pi}{2}$, such that $d_n \to \infty$ when $n \to \infty$. Then f has a complete asymptotic expansion,

$$
f(t) \sim \sum_{n=0}^\infty a_n t^{d_n - 1}, \quad t \to 0^+. \tag{8.4}
$$

First, however, we establish the following.

Proposition 8.1. *Let Γ be a compact or non-compact metric graph with Schrödinger operator H. Then, for every $t > 0$, the operator e^{-Ht} is an integral operator with kernel*

$$
k_H(t;\cdot,\cdot) \in L^\infty(\Gamma\times\Gamma) \cap C^\infty(\Gamma\times\Gamma). \tag{8.5}
$$

The heat kernel (8.5) possesses a complete asymptotic expansion for $t \to 0^+$ in powers of $\sqrt{t}$. On the diagonal the leading terms are:

(i) x not an edge end:

$$
k_{H,ee}(t;x,x) = \frac{1}{2\sqrt{\pi t}} \left(1 + O(t)\right), \tag{8.6}
$$

(ii) $x \cong (v,e)$ *and* $y \cong (v,e')$ *with* $e \neq e'$*:*

$$k_{H,ee'}(t;x,y) = \frac{\mathfrak{S}_{\infty,xy}}{2\sqrt{\pi t}}\left(1 + 2\sqrt{\pi t}L_{xy} + O(t)\right), \tag{8.7}$$

(iii) $x \cong (v,e)$*:*

$$k_{H,ee}(t;x,x) = \frac{1+\mathfrak{S}_{\infty,xx}}{2\sqrt{\pi t}}\left(1 + 2\sqrt{\pi t}L_{xx} + O\left(\sqrt{t}\right)\right). \tag{8.8}$$

Proof. The fact that e^{-Ht} is an integral operator whose kernel satisfies (8.5) is proved in the same way as [KS06, Lemma 6.1]. For this one needs to know that $\sigma(H)$ is bounded from below (Proposition 3.2) and that the resolvent kernel is composed of smooth functions (Theorem 4.1 and Lemma 5.1).

The leading diagonal terms (8.6)-(8.8) follow from an application of Lemma 8.1 to Lemma 7.2.

We are now in a position to determine heat kernels from resolvent kernels. As we are eventually interested in trace asymptotics we need to consider the difference (8.1) of heat operators.

Theorem 8.2. *Let* Γ *be a compact or non-compact metric graph with Schrödinger operator* H*. Then, for every* $t > 0$*, the difference* (8.1) *of heat operators is a trace-class integral operator. Its kernel* $k_{H,D/N}(t;\cdot,\cdot)$ *satisfies*

$$k_{H,D/N}(t;\cdot,\cdot) \in L^\infty(\Gamma\times\Gamma)\cap C^\infty(\Gamma\times\Gamma). \tag{8.9}$$

The trace of (8.1) *possesses a complete asymptotic expansion for* $t \to 0^+$ *given by*

$$\operatorname{tr}\left(\mathrm{e}^{-Ht} - J_{\mathrm{ex}}\mathrm{e}^{\Delta_{D/N}t}J_{\mathrm{ex}}^*\right) = \int_\Gamma \operatorname{tr} k_{H,D/N}(t;\boldsymbol{x},\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \sim \sum_{n=1}^{\infty} a_n t^{\frac{n}{2}-1}, \tag{8.10}$$

where

$$\begin{aligned} a_{2n} &= \frac{(-1)^n}{(n-1)!}b_{2n}, \quad n\in\mathbb{N} \\ a_{2n+1} &= \mathrm{i}\frac{(-1)^{n+1}}{\Gamma\left(n+\frac{1}{2}\right)}b_{2n+1}, \quad n\in\mathbb{N}_0, \end{aligned} \tag{8.11}$$

with the coefficients b_n *from* (7.10)*.*

Proof. The fact that the difference (8.1) of heat operators is trace class is proven in complete analogy to the trace-class property of the corresponding difference of resolvents, see Proposition 4.2. The integral kernel for (8.1) is the difference of the heat kernel (8.5) and the kernel for $J_{\mathrm{ex}}\mathrm{e}^{\Delta_{D/N}t}J_{\mathrm{ex}}{}^*$ that is given in [KS06, KPS07]. Both kernel are in $L^\infty(\Gamma\times\Gamma)\cap C^\infty(\Gamma\times\Gamma)$, hence (8.9) follows.

As for the asymptotics, we apply Lemma 8.1 to

$$\operatorname{tr}\left(R_H\left(-k^2\right) - J_{\mathrm{ex}}R_{D/N}\left(-k^2\right)J_{\mathrm{ex}}^*\right) = \int_0^\infty \mathrm{e}^{-k^2t}\operatorname{tr}\left(\mathrm{e}^{-Ht} - J_{\mathrm{ex}}\mathrm{e}^{\Delta_{D/N}t}J_{\mathrm{ex}}^*\right)\,\mathrm{d}t, \tag{8.12}$$

where $k^2 > -\inf\sigma(H)$. For this we first notice that

$$\mathrm{e}^{-ct}\operatorname{tr}\left(\mathrm{e}^{-Ht} - J_{\mathrm{ex}}\mathrm{e}^{\Delta_{D/N}t}J_{\mathrm{ex}}^*\right) \in L^1(0,\infty), \tag{8.13}$$

iff $c > -\inf\sigma(H)$. Lemma 8.1 requires the left-hand side of (8.12) to posses a complete asymptotic expansion for $|k^2|\to\infty$ in the right half-plane $|\arg(k^2-c)| \le \frac{\pi}{2}$. Such an expansion is indeed given by Theorem 7.3, under the condition that $k^2 \in S_{2\delta}$ which contains the half-plane $|\arg(k^2-c)| \le \frac{\pi}{2}$. Comparing (8.3) and (7.11) we identify $d_n = \frac{n}{2}$, leading to the relations (8.11).

The first few heat-kernel coefficients can be worked out explicitly, making use of the resolvent coefficients (7.11). Using Theorems 7.3 and 8.2 we can read off the first five coefficients. A direct calculation leads to

$$\operatorname{tr}\left(\mathrm{e}^{-Ht} - J_{\mathrm{ex}}\mathrm{e}^{\Delta_{D/N}t}J_{\mathrm{ex}}^*\right) = \frac{\mathcal{L}}{\sqrt{4\pi t}} + \frac{1}{4}\left(\operatorname{tr}\mathfrak{S}_\infty \mp E_{\mathrm{ex}}\right) + \left(-\frac{1}{2}\int_{\Gamma_{\mathrm{int}}} V(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} + \operatorname{tr} L\right)\sqrt{t} + O(t)\,. \tag{8.14}$$

an one can observe that the first two terms of this expansion are independent of the potential. They indeed agree with the result [KPS07, Theorem 4.1], where the case of $V\equiv 0$ and vertex conditions such that $L=0$ is covered. From [KPS07, Theorem 4.1] it also follows that $a_n = 0$ for $n\ge 3$ in the case covered there. The terms involving the potential also agree with the ones computed in [Rue12]. The presence of the potential, and the possibility of more general boundary conditions allowing $L\neq 0$, implies that in general all heat-kernel coefficients a_n will be non-zero.

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