HEAT KERNELS ON METRIC GRAPHS AND A TRACE FORMULA

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Dedicated to Jean-Michel Combes on the occasion of his 65-th birthday

ABSTRACT. We study heat semigroups generated by self-adjoint Laplace operators on metric graphs characterized by the property that the local scattering matrices associated with each vertex of the graph are independent from the spectral parameter. For such operators we prove a representation for the heat kernel as a sum over all walks with given initial and terminal edges. Using this representation a trace formula for heat semigroups is proven. Applications of the trace formula to inverse spectral and scattering problems are also discussed.

1. INTRODUCTION

Metric graphs or networks are one-dimensional piecewise linear spaces with singularities at the vertices. Alternatively, a metric graph is a metric space which can be written as a union of finitely many intervals, which are either compact or $[0,\infty)$; any two of these intervals are either disjoint or intersect only in one or both of their endpoints. It is natural to call the metric graph compact if all its edges have finite length.

The increasing interest in the theory of differential operators on metric graphs is motivated mainly by two reasons. The first reason is that such operators arise in a variety of applications. We refer the reader to the review [34], where a number of models arising in physics, chemistry, and engineering is discussed. The second reason is purely mathematical: It is intriguing to study the interrelation between the spectra of these operators and topological or combinatorial properties of the underlying graph. Similar interrelations are studied in spectral geometry for differential operators on Riemannian manifolds (see, e.g. [7], [15]) and in spectral graph theory for difference operators on combinatorial graphs (see, e.g. [9]). Metric graphs take an intermediate position between manifolds and combinatorial graphs.

In the present work we continue the study of heat semigroups on metric graphs initiated in [28]. There we provided sufficient conditions for a self-adjoint Laplace operator to generate a contractive semigroup. Moreover, we proved a criterion guaranteeing that this semigroup is positivity preserving. For earlier work on heat semigroups generated by Laplace operators on metric graphs and their application to spectral analysis we refer to [3], [13], [14], [40], [41], [46], [47].

In this article we study heat semigroups generated by self-adjoint Laplace operators which are characterized by the property that the local scattering matrices associated with each vertex of the graph are independent of the spectral parameter. All boundary conditions leading to such operators are described in Proposition 2.4 below. In particular, Neumann, Dirichlet, and the so called standard boundary conditions are in this class.

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Our main technical tool to study heat semigroups on metric graphs are *walks* on edges of the graph, a concept developed in [28], [29]. We will revisit this concept in Section 3 below. Furthermore, we will provide a representation for the heat kernel as a sum over all walks with given initial and terminal edges. This representation relates the topology of the graph to analytic properties of the heat semigroup.

In Section 4 we prove a trace formula for heat semigroups on arbitrary (compact as well as noncompact) metric graphs, an analog of the celebrated Selberg formula for differential operators on Riemannian manifolds (see [38], [48] for the case of compact manifolds and [22], [37] for the noncompact case). A discrete analog of the Selberg trace formula on k-regular trees is discussed in [49].

The trace formula expresses the trace of the semigroup difference as the sum over all *cycles* on the graph, that is, equivalence classes of closed walks. In the particular case of compact graphs and standard boundary conditions our result recovers the well-known trace formula obtained by Roth [46], [47]. Related results can be found in [35], [40], [41], [50]. In the physical literature trace formulas for Laplace operators on metric graphs have been discussed in [2], [31], [32], [33]. Their applications to quantum chaos and spectral statistics are reviewed in the recent article [16].

As an application of the trace formula, in Section 5 we discuss inverse spectral and scattering problems. The inverse problems considered here consist of determining the graph and its metric structure (i.e. the lengths of its edges) from the spectrum of the Laplace operator and the scattering phase (that is, half the phase of the determinant of the scattering matrix), under the condition that the boundary conditions at all vertices of the graph are supposed to be known. Another kind of the inverse scattering problem, the reconstruction of the graph and the boundary conditions from the scattering matrix, has been solved recently in [29].

The results of Section 5 provide a mathematically rigorous solution of the inverse scattering problem as proposed by Gutkin and Smilansky in [19]. Also these result extend the solution of the inverse spectral problem on compact graphs given by Kurasov and Nowaszyk in [35] to more general boundary conditions.

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2. BACKGROUND

A finite graph is a 4-tuple $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$, where V is a finite set of *vertices*, $\mathcal{I}$ is a finite set of *internal edges*, $\mathcal{E}$ is a finite set of *external edges*. Elements in $\mathcal{I} \cup \mathcal{E}$ are called *edges*. The map ∂ assigns to each internal edge $i \in \mathcal{I}$ an ordered pair of (possibly equal) vertices $\partial(i) := \{v_1, v_2\}$ and to each external edge $e \in \mathcal{E}$ a single vertex v. The vertices $v_1 =: \partial^-(i)$ and $v_2 =: \partial^+(i)$ are called the *initial* and *terminal* vertex of the internal edge i, respectively. The vertex $v = \partial(e)$ is the initial vertex of the external edge e. If $\partial(i) = \{v, v\}$, that is, $\partial^-(i) = \partial^+(i)$ then i is called a *tadpole*. A graph is called *compact* if $\mathcal{E} = \emptyset$, otherwise it is *noncompact*.

Two vertices v and v' are called *adjacent* if there is an internal edge $i \in \mathcal{I}$ such that $v \in \partial(i)$ and $v' \in \partial(i)$. A vertex v and the (internal or external) edge $j \in \mathcal{I} \cup \mathcal{E}$ are *incident* if $v \in \partial(j)$.

We do not require the map ∂ to be injective. In particular, any two vertices are allowed to be adjacent to more than one internal edge and two different external edges may be incident with the same vertex. If ∂ is injective and $\partial^-(i) \neq \partial^+(i)$ for all $i \in \mathcal{I}$, the graph $\mathcal{G}$ is called *simple*.

The *degree* $\deg(v)$ of the vertex v is defined as

$$\deg(v) = |\{e \in \mathcal{E} \mid \partial(e) = v\}| + |\{i \in \mathcal{I} \mid \partial^-(i) = v\}| + |\{i \in \mathcal{I} \mid \partial^+(i) = v\}|,$$

that is, it is the number of (internal or external) edges incident with the given vertex v by which every tadpole is counted twice.

It is easy to extend the First Theorem of Graph Theory (see, e.g. [11]) to the case of noncompact graphs:

$$\sum_{v\in V} \deg(v) = |\mathcal{E}| + 2|\mathcal{I}|. \tag{2.1}$$

A vertex is called a *boundary vertex* if it is incident with some external edge. The set of all boundary vertices will be denoted by ∂V. The vertices not in ∂V, that is in $V \setminus \partial V$ are called *internal vertices*.

The compact graph $\mathcal{G}_{\mathrm{int}} = (V, \mathcal{I}, \emptyset, \partial|_{\mathcal{I}})$ will be called the *interior* of the graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$. It is obtained from $\mathcal{G}$ by eliminating the external edges.

The *star* $\mathcal{S}(v) \subseteq \mathcal{E} \cup \mathcal{I}$ of the vertex $v \in V$ is the set of the edges adjacent to v.

Throughout the whole work we will assume that the graph $\mathcal{G}$ is connected, that is, for any $v, v' \in V$ there is an ordered sequence of vertices $\{v_1 = v, v_2, \ldots, v_{n-1}, v_n = v'\}$ such that any two successive vertices in this sequence are adjacent. In particular, this assumption implies that any vertex of the graph $\mathcal{G}$ has nonzero degree, i.e., for any vertex there is at least one edge with which it is incident.

We will endow the graph with the following metric structure. Any internal edge $i \in \mathcal{I}$ will be associated with an interval $[0, a_i]$ with $a_i > 0$ such that the initial vertex of i corresponds to $x = 0$ and the terminal one to $x = a_i$. Any external edge $e \in \mathcal{E}$ will be associated with a semiline $[0, +\infty)$. We call the number a_i the length of the internal edge i. The set of lengths $\{a_i\}_{i\in\mathcal{I}}$, which will also be treated as an element of $\mathbb{R}^{|\mathcal{I}|}$, will be denoted by $\underline{a}$. A compact or noncompact graph $\mathcal{G}$ endowed with a metric structure is called a *metric graph* and is written as $(\mathcal{G}, \underline{a})$.

Given a finite graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ with a metric structure $\underline{a} = \{a_i\}_{i\in\mathcal{I}}$ consider the Hilbert space

$$\mathcal{H} \equiv \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}, \qquad \mathcal{H}_{\mathcal{E}} = \bigoplus_{e\in\mathcal{E}} \mathcal{H}_e, \qquad \mathcal{H}_{\mathcal{I}} = \bigoplus_{i\in\mathcal{I}} \mathcal{H}_i, \tag{2.2}$$

where $\mathcal{H}_j = L^2(I_j)$ with

$$I_j = \begin{cases} [0, a_j] & \text{if} \quad j \in \mathcal{I}, \\ [0, \infty) & \text{if} \quad j \in \mathcal{E}. \end{cases}$$

Let $\overset{o}{I}_j$ be the interior of I_j, that is, $\overset{o}{I}_j = (0, a_j)$ if $j \in \mathcal{I}$ and $\overset{o}{I}_j = (0, \infty)$ if $j \in \mathcal{E}$.

In the sequel the letters x and y will denote arbitrary elements of the product set $\times_{j\in\mathcal{E}\cup\mathcal{I}} I_j$.

By $\mathcal{D}_j$ with $j \in \mathcal{E} \cup \mathcal{I}$ denote the set of all $\psi_j \in \mathcal{H}_j$ such that $\psi_j(x)$ and its derivative $\psi_j'(x)$ are absolutely continuous and $\psi_j''(x)$ is square integrable. Let $\mathcal{D}_j^0$ denote the set of those elements $\psi_j \in \mathcal{D}_j$ which satisfy

$$\begin{matrix} \psi_j(0) = 0 \\ \psi_j'(0) = 0 \end{matrix} \quad \text{for} \quad j \in \mathcal{E} \qquad \text{and} \qquad \begin{matrix} \psi_j(0) = \psi_j(a_j) = 0 \\ \psi_j'(0) = \psi_j'(a_j) = 0 \end{matrix} \quad \text{for} \quad j \in \mathcal{I}.$$

Let Δ^0 be the differential operator

$$\left(\Delta^0\psi\right)_j(x) = \frac{d^2}{dx^2}\psi_j(x), \qquad j \in \mathcal{I}\cup\mathcal{E} \tag{2.3}$$

with domain

$$\mathcal{D}^0 = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j^0 \subset \mathcal{H}.$$

It is straightforward to verify that Δ^0 is a closed symmetric operator with deficiency indices equal to $|\mathcal{E}| + 2|\mathcal{I}|$.

We introduce an auxiliary finite-dimensional Hilbert space

$$\mathcal{K} \equiv \mathcal{K}(\mathcal{E},\mathcal{I}) = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)} \tag{2.4}$$

with $\mathcal{K}_{\mathcal{E}} \cong \mathbb{C}^{|\mathcal{E}|}$ and $\mathcal{K}_{\mathcal{I}}^{(\pm)} \cong \mathbb{C}^{|\mathcal{I}|}$. Let ${}^d\mathcal{K}$ denote the "double" of $\mathcal{K}$, that is, ${}^d\mathcal{K} = \mathcal{K}\oplus\mathcal{K}$.

For any $\psi \in \mathcal{D} := \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j$ we set

$$[\psi] := \underline{\psi} \oplus \underline{\psi}' \in {}^d\mathcal{K}, \tag{2.5}$$

with $\underline{\psi}$ and $\underline{\psi}'$ defined by

$$\underline{\psi} = \begin{pmatrix} \{\psi_e(0)\}_{e\in\mathcal{E}} \\ \{\psi_i(0)\}_{i\in\mathcal{I}} \\ \{\psi_i(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}, \qquad \underline{\psi}' = \begin{pmatrix} \{\psi_e'(0)\}_{e\in\mathcal{E}} \\ \{\psi_i'(0)\}_{i\in\mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}. \tag{2.6}$$

Let J be the canonical symplectic matrix on ${}^d\mathcal{K}$,

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{2.7}$$

with $\mathbb{I}$ being the identity operator on $\mathcal{K}$. Consider the non-degenerate Hermitian symplectic form

$$\omega([\phi],[\psi]) := \langle [\phi], J[\psi]\rangle, \tag{2.8}$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product in ${}^d\mathcal{K} \cong \mathbb{C}^{2(|\mathcal{E}|+2|\mathcal{I}|)}$.

A linear subspace $\mathcal{M}$ of ${}^d\mathcal{K}$ is called *isotropic* if the form ω vanishes identically on $\mathcal{M}$. An isotropic subspace is called *maximal* if it is not a proper subspace of a larger isotropic subspace. Every maximal isotropic subspace has complex dimension equal to $|\mathcal{E}| + 2|\mathcal{I}|$.

Let A and B be linear maps of $\mathcal{K}$ onto itself. By (A,B) we denote the linear map from ${}^d\mathcal{K} = \mathcal{K}\oplus\mathcal{K}$ to $\mathcal{K}$ defined by the relation

$$(A,B)\,(\chi_1\oplus\chi_2) := A\,\chi_1 + B\,\chi_2,$$

where $\chi_1,\chi_2\in\mathcal{K}$. Set

$$\mathcal{M}(A,B) := \operatorname{Ker}(A,B). \tag{2.9}$$

Theorem 2.1 ([24])**.** *A subspace $\mathcal{M}\subset {}^d\mathcal{K}$ is maximal isotropic if and only if there exist linear maps $A,\ B:\ \mathcal{K}\to\mathcal{K}$ such that $\mathcal{M} = \mathcal{M}(A,B)$ and*

$$\begin{aligned} &\text{(i) the map } (A,B):\ {}^d\mathcal{K}\to\mathcal{K} \text{ has maximal rank equal to } |\mathcal{E}|+2|\mathcal{I}|, \\ &\text{(ii) } AB^\dagger \text{ is self-adjoint, } AB^\dagger = BA^\dagger. \end{aligned} \tag{2.10}$$

Under the conditions (2.10) both $A \pm \mathrm{i}\mathsf{k}B$ are invertible for all $\mathsf{k} > 0$.

Definition 2.2. *Two boundary conditions (A, B) and (A', B') satisfying* (2.10) *are equivalent if the corresponding maximal isotropic subspaces coincide, that is, $\mathcal{M}(A, B) = \mathcal{M}(A', B')$.*

The boundary conditions (A, B) and (A', B') satisfying (2.10) are equivalent if and only if there is an invertible map $C : \mathcal{K} \to \mathcal{K}$ such that $A' = CA$ and $B' = CB$ (see Proposition 3.6 in [29]).

By Lemma 3.3 in [29], a subspace $\mathcal{M}(A, B) \subset {}^d\mathcal{K}$ is maximal isotropic if and only if

$$\mathcal{M}(A, B)^{\perp} = \mathcal{M}(B, -A). \tag{2.11}$$

We mention also the equalities

$$\begin{aligned} \mathcal{M}(A, B)^{\perp} &= \left[\operatorname{Ker}(A, B)\right]^{\perp} = \operatorname{Ran}(A, B)^{\dagger}, \\ \mathcal{M}(A, B) &= \operatorname{Ran}(-B, A)^{\dagger}. \end{aligned}$$

There is an alternative parametrization of maximal isotropic subspaces of ${}^d\mathcal{K}$ by unitary transformations in $\mathcal{K}$ (see [28] and Proposition 3.6 in [29]). A subspace $\mathcal{M}(A, B) \subset {}^d\mathcal{K}$ is maximal isotropic if and only if for an arbitrary $\mathsf{k} \in \mathbb{R} \setminus \{0\}$ the operator $A + \mathrm{i}\mathsf{k}B$ is invertible and

$$\mathfrak{S}(\mathsf{k}; A, B) := -(A + \mathrm{i}\mathsf{k}B)^{-1}(A - \mathrm{i}\mathsf{k}B) \tag{2.12}$$

is unitary. Moreover, given any $\mathsf{k} \in \mathbb{R}\setminus\{0\}$ the correspondence between maximal isotropic subspaces $\mathcal{M} \subset {}^d\mathcal{K}$ and unitary operators $\mathfrak{S}(\mathsf{k}; A, B) \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ on $\mathcal{K}$ is one-to-one, a result dating back to Bott [6] and rediscovered in [4], [21], and [25]. Therefore, we will use the notation $\mathfrak{S}(\mathsf{k}; \mathcal{M})$ for $\mathfrak{S}(\mathsf{k}; A, B)$ with $\mathcal{M}(A, B) = \mathcal{M}$.

Under the duality transformation $\mathcal{M} \mapsto \mathcal{M}^{\perp}$, as a direct consequence of (2.11) and (2.12), the operators (2.12) transform as follows (see Corollary 2.2 in [24]):

$$\mathfrak{S}(\mathsf{k}; \mathcal{M}^{\perp}) = -\mathfrak{S}(\mathsf{k}^{-1}; \mathcal{M}). \tag{2.13}$$

There is a one-to-one correspondence between all self-adjoint extensions of Δ^0 and maximal isotropic subspaces of ${}^d\mathcal{K}$ (see [24], [29]). In explicit terms, any self-adjoint extension of Δ^0 is the differential operator defined by (2.3) with domain

$$\operatorname{Dom}(\Delta) = \{\psi \in \mathcal{D} |\ [\psi] \in \mathcal{M}\}, \tag{2.14}$$

where $\mathcal{M}$ is a maximal isotropic subspace of ${}^d\mathcal{K}$. Conversely, any maximal isotropic subspace $\mathcal{M}$ of ${}^d\mathcal{K}$ defines through (2.14) a self-adjoint operator $\Delta(\mathcal{M}, \underline{a})$. If $\mathcal{I} = \emptyset$, we will simply write $\Delta(\mathcal{M})$. In the sequel we will call the operator $\Delta(\mathcal{M}, \underline{a})$ a Laplace operator on the metric graph $(\mathcal{G}, \underline{a})$. From the discussion above it follows immediately that any self-adjoint Laplace operator on $\mathcal{H}$ equals $\Delta(\mathcal{M}, \underline{a})$ for some maximal isotropic subspace $\mathcal{M}$. Moreover, $\Delta(\mathcal{M}, \underline{a}) = \Delta(\mathcal{M}', \underline{a})$ if and only if $\mathcal{M} = \mathcal{M}'$.

From Theorem 2.1 it follows that the domain of the Laplace operator $\Delta(\mathcal{M}, \underline{a})$ consists of functions $\psi \in \mathcal{D}$ satisfying the boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0, \tag{2.15}$$

with (A, B) subject to (2.9) and (2.10). Here $\underline{\psi}$ and $\underline{\psi}'$ are defined by (2.6).

With respect to the orthogonal decomposition $\mathcal{K} = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)}$ any element χ of $\mathcal{K}$ can be represented as a vector

$$\chi = \begin{pmatrix} \{\chi_e\}_{e\in\mathcal{E}} \\ \{\chi_i^{(-)}\}_{i\in\mathcal{I}} \\ \{\chi_i^{(+)}\}_{i\in\mathcal{I}} \end{pmatrix}. \tag{2.16}$$

Consider the orthogonal decomposition

$$\mathcal{K} = \bigoplus_{v\in V} \mathcal{L}_v \tag{2.17}$$

with $\mathcal{L}_v$ the linear subspace of dimension $\deg(v)$ spanned by those elements (2.16) of $\mathcal{K}$ which satisfy

$$\begin{aligned} \chi_e &= 0 \quad \text{if} \quad e \in \mathcal{E} \quad \text{is not incident with the vertex} \quad v, \\ \chi_i^{(-)} &= 0 \quad \text{if} \quad v \quad \text{is not an initial vertex of} \quad i \in \mathcal{I}, \\ \chi_i^{(+)} &= 0 \quad \text{if} \quad v \quad \text{is not a terminal vertex of} \quad i \in \mathcal{I}. \end{aligned} \tag{2.18}$$

Obviously, the subspaces $\mathcal{L}_{v_1}$ and $\mathcal{L}_{v_2}$ are orthogonal if $v_1 \neq v_2$.

Set ${}^d\mathcal{L}_v := \mathcal{L}_v \oplus \mathcal{L}_v \cong \mathbb{C}^{2\deg(v)}$. Obviously, each ${}^d\mathcal{L}_v$ inherits a symplectic structure from ${}^d\mathcal{K}$ in a canonical way, such that the orthogonal decomposition

$$\bigoplus_{v\in V} {}^d\mathcal{L}_v = {}^d\mathcal{K}$$

holds.

Definition 2.3. *Given the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$, boundary conditions (A, B) satisfying* (2.10) *are called* local on $\mathcal{G}$ *if the maximal isotropic subspace $\mathcal{M}(A, B)$ of ${}^d\mathcal{K}$ has an orthogonal symplectic decomposition*

$$\mathcal{M}(A, B) = \bigoplus_{v\in V} \mathcal{M}_v, \tag{2.19}$$

with $\mathcal{M}_v$ maximal isotropic subspaces of ${}^d\mathcal{L}_v$. Otherwise the boundary conditions are called non-local.

By Proposition 4.2 in [29], given the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$, the boundary conditions (A, B) satisfying (2.10) are local on $\mathcal{G}$ if and only if there is an invertible map $C: \mathcal{K} \to \mathcal{K}$ and linear transformations $A(v)$ and $B(v)$ in $\mathcal{L}_v$ such that the simultaneous orthogonal decompositions

$$CA = \bigoplus_{v\in V} A(v) \quad \text{and} \quad CB = \bigoplus_{v\in V} B(v) \tag{2.20}$$

are valid. From the equality $\mathcal{M}(A, B) = \mathcal{M}(CA, CB)$ it follows that the subspaces $\mathcal{M}_v$ in (2.19) are equal to $\mathcal{M}(A(v), B(v))$.

Boundary conditions $(A(v), B(v))$ induce local boundary conditions (A, B) on the graph $\mathcal{G}$ with

$$A = \bigoplus_{v\in V} A(v) \quad \text{and} \quad B = \bigoplus_{v\in V} B(v). \tag{2.21}$$

From (2.20) we get that

$$\mathfrak{S}(\mathsf{k}; A, B) = \mathfrak{S}(\mathsf{k}; CA, CB) = \bigoplus_{v\in V} \mathfrak{S}(\mathsf{k}; A(v), B(v)) \tag{2.22}$$

holds with respect to the orthogonal decomposition (2.17).

The following proposition is taken from [29].

Proposition 2.4. *Let $\mathcal{M} = \mathcal{M}(A, B)$ be a maximal isotropic subspace. The following conditions are equivalent:*

(i) $\mathfrak{S}(\mathsf{k}; \mathcal{M})$ *is* k*-independent,*

(ii) $\mathfrak{S}(\mathsf{k};\mathcal{M})$ *is self-adjoint for some* $\mathsf{k} > 0$,
(iii) *for some* $\mathsf{k} > 0$ *there is an orthogonal projection* P *such that* $\mathfrak{S}(\mathsf{k};\mathcal{M}) = \mathbb{I} - 2P$,
(iv) $AB^{\dagger} = 0$.

Since this proposition will be crucial in what follows, we recall the

Proof. **(i)** $\Leftrightarrow$ **(ii).** Assume that $\mathfrak{S}(\mathsf{k};\mathcal{M})$ is k-independent. Then, by (2.12), for any eigenvector $\chi \in \mathcal{K}$ with eigenvalue λ the equality

$$(\lambda+1)A\chi + \mathrm{i}\mathsf{k}(\lambda-1)B\chi = 0$$

holds for all $\mathsf{k} > 0$. Under the conditions (2.10) we have $\operatorname{Ker} A \perp \operatorname{Ker} B$ (see Lemma 3.4 in [29]). Hence, $\lambda \in \{-1, 1\}$. Thus, $\mathfrak{S}(\mathsf{k};\mathcal{M})$ is self-adjoint for all $\mathsf{k} > 0$.

Conversely, assume that $\mathfrak{S}(\mathsf{k};\mathcal{M})$ is self-adjoint for some $\mathsf{k}_0 > 0$. Due to the obvious equality

$$\mathfrak{S}(\mathsf{k};\mathcal{M}) = \big((\mathsf{k}-\mathsf{k}_0)\mathfrak{S}(\mathsf{k}_0;\mathcal{M}) + (\mathsf{k}+\mathsf{k}_0)\big)^{-1}\big((\mathsf{k}+\mathsf{k}_0)\mathfrak{S}(\mathsf{k}_0;\mathcal{M}) + (\mathsf{k}-\mathsf{k}_0)\big), \tag{2.23}$$

it is self-adjoint for all $\mathsf{k} > 0$. Let $\chi \in \mathcal{K}$ be an arbitrary eigenvector of $\mathfrak{S}(\mathsf{k}_0;\mathcal{M})$ corresponding to the eigenvalue $\lambda \in \{-1, 1\}$. Observing that

$$\frac{(\mathsf{k}+\mathsf{k}_0)\lambda + \mathsf{k} - \mathsf{k}_0}{(\mathsf{k}-\mathsf{k}_0)\lambda + \mathsf{k} + \mathsf{k}_0} = \lambda,$$

again by (2.23), we conclude that χ is an eigenvector of $\mathfrak{S}(\mathsf{k};\mathcal{M})$ corresponding to the same eigenvalue λ for all $\mathsf{k} > 0$. Thus, $\mathfrak{S}(\mathsf{k};\mathcal{M})$ does not depend on $\mathsf{k} > 0$.

The equivalence **(ii)** $\Leftrightarrow$ **(iii)** is obvious.

The equivalence **(iv)** $\Leftrightarrow$ **(ii)** follows directly from the identity

$$\begin{aligned}
&\mathfrak{S}(\mathsf{k};\mathcal{M}) - \mathfrak{S}(\mathsf{k};\mathcal{M})^{\dagger}\\
&\qquad = 2\mathrm{i}\mathsf{k}(A + \mathrm{i}\mathsf{k}B)^{-1}\big[B(A^{\dagger} - \mathrm{i}\mathsf{k}B^{\dagger}) + (A + \mathrm{i}\mathsf{k}B)B^{\dagger}\big](A^{\dagger} - \mathrm{i}\mathsf{k}B^{\dagger})^{-1}\\
&\qquad = 4\mathrm{i}\mathsf{k}(A + \mathrm{i}\mathsf{k}B)^{-1}AB^{\dagger}(A^{\dagger} - \mathrm{i}\mathsf{k}B^{\dagger})^{-1}.
\end{aligned}$$

□

We will write $\mathfrak{S}(\mathcal{M})$ instead of $\mathfrak{S}(\mathsf{k};\mathcal{M})$, whenever any of the equivalent conditions of Proposition 2.4 is met. Analogously we will drop the k-dependence in (2.22):

$$\mathfrak{S}(\mathcal{M}) = \bigoplus_{v\in V}\mathfrak{S}(A(v), B(v)) = \bigoplus_{v\in V}\mathfrak{S}(\mathcal{M}_v).$$

From Proposition 3.5 in [28] it follows that for any maximal isotropic subspace $\mathcal{M}$ satisfying any of the conditions of Proposition 2.4, the Laplace operator $-\Delta(\mathcal{M}, \underline{a})$ is nonnegative.

Remark 2.5. *Assume that the maximal isotropic subspace* $\mathcal{M} \subset {}^d\mathcal{K}$ *satisfies any of the conditions of Proposition 2.4. By* (2.11) *the orthogonal maximal isotropic subspace* $\mathcal{M}^{\perp} \subset {}^d\mathcal{K}$ *then also satisfies the conditions of Proposition 2.4. From* (2.13) *it follows that* $\mathfrak{S}(\mathcal{M}^{\perp}) = -\mathfrak{S}(\mathcal{M})$.

Obviously, Dirichlet $A = \mathbb{I}$, $B = 0$ and Neumann $A = 0$, $B = \mathbb{I}$ boundary conditions satisfy the conditions of Proposition 2.4 with $\mathfrak{S}(\mathbb{I}, 0) = -\mathbb{I}$ and $\mathfrak{S}(0, \mathbb{I}) = \mathbb{I}$, respectively. We now provide two important examples of boundary conditions satisfying the conditions referred to in Proposition 2.4.

Example 2.6 (Standard boundary conditions)**.** *Given a graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$ for each vertex $v \in V$ with* $\deg(v) \geq 2$ *define the boundary conditions* $(A(v), B(v))$ *the* $\deg(v) \times \deg(v)$ *matrices*

$$A(v) = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -1 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}, \quad B(v) = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 1 & 1 & 1 & \dots & 1 & 1 \end{pmatrix}.$$

Clearly, $A(v)B(v)^\dagger = 0$ *and* $(A(v), B(v))$ *has maximal rank. The corresponding unitary matrices* (2.12) *are given by*

$$[\mathfrak{S}(A(v), B(v))]_{e,e'} = \frac{2}{\deg(v)} - \delta_{e,e'} \tag{2.24}$$

with $\delta_{e,e'}$ *Kronecker symbol. If* $\deg(v) = 1$*, we set* $A(v) = 0$*,* $B(v) = 1$ *(Neumann boundary conditions) such that* (2.24) *remains valid.*

The local boundary conditions (A, B) *on the graph* $\mathcal{G}$ *defined by* (2.21) *will be called* standard *boundary conditions. We use the notation* $\mathcal{M}_{\mathrm{st}}$ *for the corresponding maximal isotropic subspace.*

Remark 2.7. *Consider a graph with no internal lines* $\mathcal{G} = (\{v\}, \varnothing, \mathcal{E}, \partial)$ *and* $|\mathcal{E}| \geq 2$*. By Proposition 2.1 in* [12]*, the set of all isotropic subspaces satisfying any of the equivalent conditions of Proposition 2.4, contains precisely four spaces, which correspond to the boundary conditions invariant with respect to permutations of edges:* $\mathcal{M}(\mathbb{I}, 0)$ *(Dirichlet),* $\mathcal{M}(0, \mathbb{I})$ *(Neumann), standard* $\mathcal{M}_{\mathrm{st}}$*, and co-standard* $\mathcal{M}_{\mathrm{st}}^\perp$*.*

Furthermore, by a result in [30]*, in the set of all isotropic subspaces satisfying any of the equivalent conditions of Proposition 2.4,* $\mathcal{M}_{\mathrm{st}}$ *is the only one with the property that every function in the domain of* $\Delta(\mathcal{M})$ *is continuous at the vertex* v*.*

Example 2.8 (Magnetic perturbations of standard boundary conditions)**.** *If the maximal isotropic subspace* $\mathcal{M}(A, B)$ *satisfies any of the equivalent conditions of Proposition 2.4, then for any unitary* U *we have*

$$AU(BU)^\dagger = AB^\dagger = 0.$$

Thus, the maximal isotropic subspace $\mathcal{M}^U := \mathcal{M}(AU, BU)$ *also satisfies the conditions of Proposition 2.4. In particular, since*

$$\mathfrak{S}(\mathcal{M}^U) = U^\dagger \mathfrak{S}(\mathcal{M}) U,$$

we have the relation

$$\operatorname{tr}_{\mathcal{K}} \mathfrak{S}(\mathcal{M}^U) = \operatorname{tr}_{\mathcal{K}} \mathfrak{S}(\mathcal{M}). \tag{2.25}$$

A special choice of unitary matrices U *corresponds to magnetic perturbations of the Laplace operator* $\Delta(\mathcal{M}, \underline{a})$*. By a result in* [27] *any magnetic perturbation of the Laplace operator* $\Delta(\mathcal{M}, \underline{a})$ *is unitarily equivalent to* $\Delta(\mathcal{M}^U, \underline{a})$ *with some* $U = \bigoplus_{v \in V} U_v$*, where every* U_v *is unitary and diagonal with respect to the canonical basis in* $\mathcal{L}_v$*,*

$$U_v = \operatorname{diag}\left(\{\mathrm{e}^{\mathrm{i}\varphi_j(v)}\}_{j \in \mathcal{S}(v)}\right).$$

In particular, any magnetic perturbation of standard boundary conditions (see Example 2.6) satisfies the conditions of Proposition 2.4.

3. HEAT KERNEL AND WALKS ON THE GRAPH

3.1. **The Resolvent.** The structure of the underlying Hilbert space $\mathcal{H}$ (2.2) gives naturally rise to the following definition of integral operators.

Definition 3.1. *The operator K on the Hilbert space $\mathcal{H}$ is called* integral operator *if for all $j, j' \in \mathcal{E} \cup \mathcal{I}$ there are measurable functions $K_{j,j'}(\cdot,\cdot) : I_j \times I_{j'} \to \mathbb{C}$ with the following properties*

(i) $K_{j,j'}(x_j,\cdot)\varphi_{j'}(\cdot) \in L^1(I_{j'})$ *for almost all* $x_j \in I_j$,
(ii) $\psi = K\varphi$ *with*

$$\psi_j(x_j) = \sum_{j' \in \mathcal{E}\cup\mathcal{I}} \int_{I_{j'}} K_{j,j'}(x_j, y_{j'})\varphi_{j'}(y_{j'})dy_{j'}. \tag{3.1}$$

The $(|\mathcal{I}| + |\mathcal{E}|) \times (|\mathcal{I}| + |\mathcal{E}|)$ *matrix-valued function* $(x,y) \mapsto K(x,y)$ *with*

$$[K(x,y)]_{j,j'} = K_{j,j'}(x_j, y_{j'})$$

is called the integral kernel *of the operator* K.

Below we will use the following shorthand notation for (3.1):

$$\psi(x) = \int^{\mathcal{G}} K(x,y)\varphi(y)dy.$$

We denote

$$R(\mathsf{k};\underline{a}) := \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix}, \tag{3.2}$$

and

$$T(\mathsf{k};\underline{a}) := \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & 0 \end{pmatrix} \tag{3.3}$$

with respect to the orthogonal decomposition (2.4). The diagonal $|\mathcal{I}| \times |\mathcal{I}|$ matrices $\mathrm{e}^{\pm\mathrm{i}\mathsf{k}\underline{a}}$ are given by

$$[\mathrm{e}^{\pm\mathrm{i}\mathsf{k}\underline{a}}]_{jk} = \delta_{jk}\mathrm{e}^{\pm\mathrm{i}\mathsf{k}a_j} \quad \text{for} \quad j,k \in \mathcal{I}. \tag{3.4}$$

Lemma 3.2. *For any maximal isotropic subspace $\mathcal{M} \subset {}^d\mathcal{K}$ the resolvent*

$$(-\Delta(\mathcal{M};\underline{a}) - \mathsf{k}^2)^{-1} \quad \textit{for} \quad \mathsf{k}^2 \in \mathbb{C} \setminus \operatorname{spec}(-\Delta(\mathcal{M};\underline{a})) \quad \textit{with} \quad \det(A + \mathrm{i}\mathsf{k}B) \neq 0$$

is the integral operator with the $(|\mathcal{I}| + |\mathcal{E}|) \times (|\mathcal{I}| + |\mathcal{E}|)$ *matrix-valued integral kernel* $r_{\mathcal{M}}(x,y;\mathsf{k},\underline{a})$, $\operatorname{Im}\mathsf{k} > 0$, *admitting the representation*

$$\begin{aligned} r_{\mathcal{M}}(x,y;\mathsf{k},\underline{a}) &= r^{(0)}(x,y,\mathsf{k}) \\ &+ \frac{\mathrm{i}}{2\mathsf{k}}\Phi(x,\mathsf{k})R(\mathsf{k};\underline{a})^{-1}[\mathbb{I} - \mathfrak{S}(\mathsf{k};\mathcal{M})T(\mathsf{k};\underline{a})]^{-1}\mathfrak{S}(\mathsf{k};\mathcal{M})R(\mathsf{k};\underline{a})^{-1}\Phi(y,\mathsf{k})^T, \end{aligned} \tag{3.5}$$

where $R(\mathsf{k};\underline{a})$ is defined in (3.2)*, the matrix $\Phi(x,\mathsf{k})$ is given by*

$$\Phi(x,\mathsf{k}) := \begin{pmatrix} \phi(x,\mathsf{k}) & 0 & 0 \\ 0 & \phi_+(x,\mathsf{k}) & \phi_-(x,\mathsf{k}) \end{pmatrix}$$

with diagonal matrices $\phi(x,\mathsf{k}) = \operatorname{diag}\{\mathrm{e}^{\mathrm{i}\mathsf{k}x_j}\}_{j\in\mathcal{E}}$, $\phi_\pm(x,\mathsf{k}) = \operatorname{diag}\{\mathrm{e}^{\pm\mathrm{i}\mathsf{k}x_j}\}_{j\in\mathcal{I}}$, *and*

$$[r^{(0)}(x,y,\mathsf{k})]_{j,j'} = \mathrm{i}\delta_{j,j'}\frac{\mathrm{e}^{\mathrm{i}\mathsf{k}|x_j - y_j|}}{2\mathsf{k}}, \quad x_j, y_j \in I_j.$$

If $\mathcal{I} = \emptyset$, this representation simplifies to

$$r_{\mathcal{M}}(x, y, \mathsf{k}) = r^{(0)}(x, y, \mathsf{k}) + \frac{\mathrm{i}}{2\mathsf{k}} \phi(x, \mathsf{k}) \mathfrak{S}(\mathsf{k}; \mathcal{M}) \phi(y, \mathsf{k}).$$

The integral kernel $r_{\mathcal{M}}(x, y; \mathsf{k}, \underline{a})$ is called *Green's function* or *Green's matrix*.

The proof of Lemma 3.2 is given in [28].

3.2. **Walks on Graphs and Cycles.** We recall the following definitions from [28]. A nontrivial walk $\mathbf{w}$ on the graph $\mathcal{G}$ from $j \in \mathcal{E} \cup \mathcal{I}$ to $j' \in \mathcal{E} \cup \mathcal{I}$ is an ordered sequence formed out of edges and vertices

$$\{j, v_0, j_1, v_1, \ldots, j_n, v_n, j'\} \tag{3.6}$$

such that

(i) $j_1, \ldots, j_n \in \mathcal{I}$;
(ii) the vertices $v_0 \in V$ and $v_n \in V$ satisfy $v_0 \in \partial(j)$, $v_0 \in \partial(j_1)$, $v_n \in \partial(j')$, and $v_n \in \partial(j_n)$;
(iii) for any $k \in \{1, \ldots, n-1\}$ the vertex $v_k \in V$ satisfies $v_k \in \partial(j_k)$ and $v_k \in \partial(j_{k+1})$;
(iv) $v_k = v_{k+1}$ for some $k \in \{0, \ldots, n-1\}$ if and only if j_k is a tadpole.

If $j, j' \in \mathcal{E}$ this definition is equivalent to that given in [29].

The number n is the *combinatorial length* $|\mathbf{w}|_{\mathrm{comb}}$ and the number

$$|\mathbf{w}| = \sum_{k=1}^{n} a_{j_k} > 0$$

is the *metric length* of the walk $\mathbf{w}$.

A *trivial* walk on the graph $\mathcal{G}$ from $j \in \mathcal{E} \cup \mathcal{I}$ to $j' \in \mathcal{E} \cup \mathcal{I}$ is a triple $\{j, v, j'\}$ such that $v \in \partial(j)$ and $v \in \partial(j')$. Otherwise the walk is called nontrivial. In particular, if $\partial(j) = \{v_0, v_1\}$, then $\{j, v_0, j\}$ and $\{j, v_1, j\}$ are trivial walks, whereas $\{j, v_0, j, v_1, j\}$ and $\{j, v_1, j, v_0, j\}$ are nontrivial walks of combinatorial length 1 and of metric length a_j. Both the combinatorial and metric length of a trivial walk are zero.

We will say that the walk (3.6) leaves the edge j through the vertex v_0 and enters the edge j' through the vertex v_n. A trivial walk $\{j, v, j'\}$ leaves j and enters j' through the same vertex v.

For any given walk $\mathbf{w}$ from $j \in \mathcal{E} \cup \mathcal{I}$ to $j' \in \mathcal{E} \cup \mathcal{I}$ we denote by $v_-(\mathbf{w})$ the vertex through which the walk leaves the edge j and by $v_+(\mathbf{w})$ the vertex through which the walk enters the edge j'. For trivial walks one has $v_-(\mathbf{w}) = v_+(\mathbf{w})$.

Assume that the edges $j, j' \in \mathcal{E} \cup \mathcal{I}$ are not tadpoles. For a walk $\mathbf{w}$ from j to j' we set

$$\operatorname{dist}(x_j, v_-(\mathbf{w})) := \begin{cases} x_j & \text{if} \quad v_-(\mathbf{w}) = \partial^-(j), \\ a_j - x_j & \text{if} \quad v_-(\mathbf{w}) = \partial^+(j), \end{cases}$$

and

$$\operatorname{dist}(x_{j'}, v_+(\mathbf{w})) := \begin{cases} x_{j'} & \text{if} \quad v_+(\mathbf{w}) = \partial^-(j), \\ a_j - x_j & \text{if} \quad v_+(\mathbf{w}) = \partial^+(j). \end{cases}$$

A walk $\mathbf{w} = \{j, v_0, j_1, v_1, \ldots, j_n, v_n, j'\}$ *traverses* an internal edge $i \in \mathcal{I}$ if $j_k = i$ for some $1 \le k \le n$. It *visits* the vertex v if $v_k = v$ for some $0 \le k \le n$. The *score* $\underline{n}(\mathbf{w})$

of a walk $\mathbf{w}$ is the set $\{n_i(\mathbf{w})\}_{i\in\mathcal{I}}$ with $n_i(\mathbf{w}) \geq 0$ being the number of times the walk $\mathbf{w}$ traverses the internal edge $i \in \mathcal{I}$. In particular,

$$|\mathbf{w}| = \sum_{i\in\mathcal{I}} a_i n_i(\mathbf{w}).$$

We say that the walk is *transmitted* at the vertex v_k if either $v_k = \partial(e)$ or $v_k = \partial(e')$ or $v_k \in \partial(i_k)$, $v_k \in \partial(i_{k+1})$, and $i_k \neq i_{k+1}$. We say that a trivial walk from e' to e is transmitted at the vertex $v = \partial(e) = \partial(e')$ if $e \neq e'$. Otherwise the walk is said to be *reflected*.

Let $\mathcal{W}_{j,j'}$, $j, j' \in \mathcal{E} \cup \mathcal{I}$ be the (infinite if $\mathcal{I} \neq \emptyset$) set of all walks $\mathbf{w}$ on $\mathcal{G}$ from j to j'. By $\mathcal{W}_{j,j'}(\underline{n})$, $\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ we denote set of all walks $\mathbf{w}$ on $\mathcal{G}$ from j to j' with score $\underline{n}$.

A walk

$$\mathbf{w} = \{j, v_0, j_1, v_1, \ldots, j_n, v_n, j'\} \tag{3.7}$$

is called *closed* if $j = j'$. It is called *properly closed* if it is closed and $v_-(\mathbf{w}) \equiv v_0 \neq v_n \equiv v_+(\mathbf{w})$. For any closed walk $\mathbf{w}$ we denote by $j(\mathbf{w})$ its initial edge, that is, $j(\mathbf{w}) = j = j'$.

For instance, let j be an arbitrary internal edge with $\partial(j) = \{v_0, v_1\}$, $v_0 \neq v_1$. Then, the walk $\{j, v_0, j\}$ is not properly closed, whereas $\{j, v_0, j, v_1, j\}$ is. Any closed walk from an external edge is not properly closed.

We will say that two properly closed walks $\mathbf{w}$ and $\mathbf{w}'$ are equivalent, if they can be obtained from each other by successive application of the transformation of the form

$$\{j, v_0, j_1, v_1, \ldots, j_n, v_n, j\} \to \{j_1, v_1, \ldots, j_n, v_n, j, v_0, j_1\}.$$

A *cycle* is an equivalence class of properly closed walks. We will say that the cycle $\mathfrak{c}$ is associated with a walk $\mathbf{w}$ and write $\mathfrak{c}(\mathbf{w})$, if $\mathbf{w}$ is in the equivalence class $\mathfrak{c}$.

The number

$$|\mathfrak{c}| := |\mathbf{w}| + a_j, \tag{3.8}$$

where $\mathbf{w}$ is an arbitrary walk in the equivalence class $\mathfrak{c}$ and $j = j(\mathbf{w})$, will be called the *metric length* of the cycle $\mathfrak{c}$. Obviously, this definition does not depend on the particular choice of the walk $\mathbf{w}$ in $\mathfrak{c}$. The set of all cycles on the graph $\mathcal{G}$ will be denoted by $\mathfrak{C}$.

We call a cycle $\mathfrak{c}$ *primitive* if for any $\mathbf{w}$ in $\mathfrak{c}$ there is no integer $p \geq 2$ such that $\{p^{-1}n_i(\mathbf{w})\}_{i\in\mathcal{I}}$ is a score of a properly closed walk. For instance, if $j \in \mathcal{I}$, $\partial(j) = \{v_0, v_1\}$, $v_0 \neq v_1$, the cycle associated with the properly closed walk $\{j, v_0, j, v_1, j\}$ is primitive, whereas the cycle associated with the properly closed walk $\{j, v_0, j, v_1, j, v_0, j, v_1, j\}$ is not.

For an arbitrary cycle $\mathfrak{c}$ and any $p \in \mathbb{N}$ we denote by $p\mathfrak{c}$ the unique cycle with the following property: For any walk $\mathbf{w}$ in $p\mathfrak{c}$ there is a walk $\mathbf{w}'$ in $\mathfrak{c}$ with the score $\{p^{-1}n_i(\mathbf{w})\}_{i\in\mathcal{I}}$. The set of all primitive cycles on the graph $\mathcal{G}$ will be denoted by $\mathfrak{C}_{\mathrm{prim}}$.

The reverse of the walk $\mathbf{w}$ is the walk $\mathbf{w}_{\mathrm{rev}}$ is $\{j', v_n, j_n, \ldots, v_1, j_1, v_0, j\}$. It may happen that $\mathbf{w}_{\mathrm{rev}} = \mathbf{w}$. If $\mathbf{w}$ is a properly closed walk, then its reverse $\mathbf{w}_{\mathrm{rev}}$ is also properly closed. We will write $\mathfrak{c}_{\mathrm{rev}}$ for the equivalence class associated with $\mathbf{w}_{\mathrm{rev}}$ for $\mathbf{w}$ in $\mathfrak{c}$. Obviously, the map $\mathfrak{c} \mapsto \mathfrak{c}_{\mathrm{rev}}$ satisfies $(p\mathfrak{c})_{\mathrm{rev}} = p\mathfrak{c}_{\mathrm{rev}}$ for any $p \in \mathbb{N}$. From what has been just said, it follows that the case $\mathfrak{c} = \mathfrak{c}_{\mathrm{rev}}$ may occur.

3.3. **Combinatorial Expansion of the Resolvent.** For any $\mathsf{k} \in \mathbb{C}$ with $\operatorname{Im} \mathsf{k} > 0$, the operator $T(\mathsf{k}; \underline{a})$ defined in (3.3) is a uniform contraction. Therefore,

$$[\mathbb{I} - \mathfrak{S}(\mathsf{k}; \mathcal{M})T(\mathsf{k}; \underline{a})]^{-1}\mathfrak{S}(\mathsf{k}; \mathcal{M}) = \sum_{n=0}^{\infty} \mathfrak{S}(\mathsf{k}; \mathcal{M}) \left(T(\mathsf{k}; \underline{a})\mathfrak{S}(\mathsf{k}; \mathcal{M})\right)^n \tag{3.9}$$

converges uniformly in k for k in any of the sets $\{\mathsf{k} \in \mathbb{C} | \operatorname{Im} \mathsf{k} > \varepsilon > 0\}$. Inserting (3.9) into (3.5), we get

$$\begin{aligned} r_{\mathcal{M}}(x, y; \mathsf{k}, \underline{a}) &= r^{(0)}(x, y, \mathsf{k}) \\ &+ \frac{\mathrm{i}}{2\mathsf{k}} \sum_{n=0}^{\infty} \Phi(x, \mathsf{k}) R(\mathsf{k}; \underline{a})^{-1} \mathfrak{S}(\mathsf{k}; \mathcal{M}) \left(T(\mathsf{k}; \underline{a}) \mathfrak{S}(\mathsf{k}; \mathcal{M})\right)^n R(\mathsf{k}; \underline{a})^{-1} \Phi(y, \mathsf{k})^T. \end{aligned}$$

For maximal isotropic subspaces satisfying any of the equivalent conditions of Proposition 2.4, $\mathfrak{S}(\mathsf{k}; \mathcal{M})$ is independent of k. Thus, using (3.9) we get

Proposition 3.3. *Assume that the graph $\mathcal{G}$ has no tadpoles. For any maximal isotropic subspace $\mathcal{M}$ satisfying any of the equivalent conditions of Proposition 2.4, the Green function of the Laplace operator $\Delta(\mathcal{M}, \underline{a})$ has the absolutely converging expansion*

$$\begin{aligned} [r_{\mathcal{M}}(x, y; \mathsf{k}, \underline{a})]_{j,j'} &= \frac{\mathrm{i}}{2\mathsf{k}} \delta_{j,j'} \mathrm{e}^{\mathrm{i}\mathsf{k}|x_j - y_j|} \\ &+ \frac{\mathrm{i}}{2\mathsf{k}} \sum_{\mathbf{w} \in \mathcal{W}_{j,j'}} \mathrm{e}^{\mathrm{i}\mathsf{k}\,\mathrm{dist}(x_j, v_-(\mathbf{w}))} W_{\mathcal{M}}(\mathbf{w}) \mathrm{e}^{\mathrm{i}\mathsf{k}|\mathbf{w}|} \mathrm{e}^{\mathrm{i}\mathsf{k}\,\mathrm{dist}(y_{j'}, v_+(\mathbf{w}))}, \qquad \operatorname{Im} \mathsf{k} > 0, \end{aligned} \tag{3.10}$$

where $W_{\mathcal{M}}(\mathbf{w})$ is a (complex-valued) weight of the walk $\mathbf{w} = \{j, v_0, j_1, v_1, \ldots, j_n, v_n, j'\}$,

$$W_{\mathcal{M}}(\mathbf{w}) = \prod_{l=0}^{|\mathbf{w}|_{\mathrm{comb}}} [\mathfrak{S}(A(v_l), B(v_l))]_{i_{l+1}, i_l}. \tag{3.11}$$

3.4. **Heat Kernel.** The semigroup generated by the positive operator $-\Delta(\mathcal{M}, \underline{a})$ is related to its resolvent by the Dunford-Taylor integral (see [23, Section IX.1.6])

$$\mathrm{e}^{t\Delta(\mathcal{M}, \underline{a})} = -\frac{1}{2\pi\mathrm{i}} \int_{\gamma} \mathrm{e}^{-t\lambda} (-\Delta(\mathcal{M}, \underline{a}) - \lambda)^{-1} d\lambda,$$

where γ is any contour encircling a positive semiline counterclockwise. The integral converges in the sense of Bochner. Using the well-known identity

$$\frac{1}{2\pi} \int_{-\infty + \mathrm{i}\varepsilon}^{+\infty + \mathrm{i}\varepsilon} \mathrm{e}^{-\mathsf{k}^2 t} \mathrm{e}^{\mathrm{i}\mathsf{k}u} d\mathsf{k} = g_t(u) := \frac{1}{\sqrt{4\pi t}} \exp\left\{-u^2/4t\right\}, \qquad \varepsilon > 0,$$

we immediately get the following corollary of Proposition 3.3.

Corollary 3.4. *Assume that the maximal isotropic subspace $\mathcal{M}$ satisfies any of the equivalent conditions of Proposition 2.4 and defines local boundary conditions on the graph $\mathcal{G}$. Assume, in addition, that the graph $\mathcal{G}$ has no tadpoles. Then the heat kernel of $-\Delta(\mathcal{M}, \underline{a})$ has the absolutely convergent expansion*

$$\begin{aligned} [p_t(x, y; \mathcal{M}, \underline{a})]_{j,j'} &= \delta_{j,j'} g_t(x_j - y_j) \\ &+ \sum_{\mathbf{w} \in \mathcal{W}_{j,j'}} W_{\mathcal{M}}(\mathbf{w})\, g_t\big(\mathrm{dist}(x_j, v_-(\mathbf{w})) + |\mathbf{w}| + \mathrm{dist}(y_{j'}, v_+(\mathbf{w}))\big), \end{aligned} \tag{3.12}$$

The series converges uniformly in $x, y \in \underset{j \in \mathcal{E} \cup \mathcal{I}}{\times} I_j$.

Proof. It remains to prove that the series in (3.12) converges uniformly. This follows from the estimate

$$\begin{aligned}
&\left| \sum_{\mathbf{w}\in\mathcal{W}_{j,j'}} W_{\mathcal{M}}(\mathbf{w})\, g_t\big(\operatorname{dist}(x_j, v_-(\mathbf{w})) + |\mathbf{w}| + \operatorname{dist}(x_{j'}, v_+(\mathbf{w}))\big) \right| \\
&\qquad \leq \frac{1}{\sqrt{4\pi t}} \sum_{\mathbf{w}\in\mathcal{W}_{j,j'}} \exp\{-|\mathbf{w}|^2/4t\} \\
&\qquad \leq \frac{1}{\sqrt{4\pi t}} \sum_{\underline{n}\in(\mathbb{N}_0)^{|\mathcal{I}|}} \sum_{\mathbf{w}\in\mathcal{W}_{j,j'}(\underline{n})} \exp\{-|\mathbf{w}|^2/4t\} \\
&\qquad \leq \frac{1}{\sqrt{4\pi t}} \sum_{\underline{n}\in(\mathbb{N}_0)^{|\mathcal{I}|}} \frac{|\underline{n}|!}{\prod_{i\in\mathcal{I}} n_i!} \exp\{-|\underline{n}|^2 a_{\min}^2/4t\} \\
&\qquad \leq \frac{1}{\sqrt{4\pi t}} \sum_{n=0}^{\infty} |\mathcal{I}|^n \exp\{-n^2\, a_{\min}^2/4t\} < \infty,
\end{aligned}$$

where $a_{\min} = \min_{i\in\mathcal{I}}\{a_j\}$. □

In the particular case of a connected graph with $\mathcal{I} = \varnothing$ and standard boundary conditions, we observe that $\mathcal{W}_{j,j'}$ consists of precisely one walk. Hence, from (3.12) we get the representation (7.1) in [28], which has first been derived in [14] by different methods. In the particular case $\mathcal{M} = \mathcal{M}_{\mathrm{st}}$ for compact graphs $\mathcal{G}$ a representation similar to (3.12) has been obtained by Roth in [47].

We will now look at the situation with standard boundary conditions at all vertices in more detail. For a given walk $\mathbf{w}$ we set

$$\begin{aligned}
N_{\mathrm{refl}}(\mathbf{w}) &= \text{number of times the walk } \mathbf{w} \text{ is reflected}, \\
N_{\mathrm{trans}}(\mathbf{w}) &= \text{number of times the walk } \mathbf{w} \text{ is transmitted},
\end{aligned}$$

such that

$$N_{\mathrm{refl}}(\mathbf{w}) + N_{\mathrm{trans}}(\mathbf{w}) = |\mathbf{w}|_{\mathrm{comb}} + 1.$$

From Corollary 3.4 we obtain

Corollary 3.5. *Assume that the graph $\mathcal{G}$ is k-regular, that is, $\deg(v) = k$ for all $v \in V$, and has no tadpoles. Then for standard boundary conditions at each of the vertices the heat kernel of $-\Delta(\mathcal{M}_{\mathrm{st}}, \underline{a})$ has the absolutely convergent expansion*

$$\begin{aligned}
[p_t(x,y;\mathcal{M}_{\mathrm{st}},\underline{a})]_{j,j'} &= \delta_{j,j'}\, g_t(x_j - y_j) \\
&\quad + \sum_{\mathbf{w}\in\mathcal{W}_{j,j'}} \left(\frac{2-k}{k}\right)^{N_{\mathrm{refl}}(\mathbf{w})} \left(\frac{2}{k}\right)^{N_{\mathrm{trans}}(\mathbf{w})} \\
&\quad \cdot g_t(\operatorname{dist}(x_j, v_-(\mathbf{w})) + |\mathbf{w}| + \operatorname{dist}(y_{j'}, v_+(\mathbf{w}))).
\end{aligned} \tag{3.13}$$

4. The Trace Formula

On the exterior $\mathcal{G}_{\mathrm{ext}} = (\partial V, \varnothing, \mathcal{E}, \partial|_{\mathcal{E}})$ of the graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ we consider the Laplace operators $\Delta_+ := \Delta(A_{\mathcal{E}} = 0, B_{\mathcal{E}} = \mathbb{I})$ corresponding to Neumann boundary conditions and $\Delta_- := \Delta(A_{\mathcal{E}} = \mathbb{I}, B_{\mathcal{E}} = 0)$ corresponding to Dirichlet boundary conditions.

Let $\mathcal{J} : \mathcal{H}_{\mathcal{E}} \to \mathcal{H}$ be the embedding operator defined for any $\chi \in \mathcal{H}_{\mathcal{E}}$ by $\mathcal{J}\chi = \chi \oplus 0$, where the orthogonal sum is taken with respect to the decomposition $\mathcal{H} = \mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}$, such that $\mathcal{J}^\dagger\mathcal{J}$ is the identity on $\mathcal{H}_\mathcal{E}$ and $\mathcal{J}\mathcal{J}^\dagger$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{H}_\mathcal{E}$. If $\mathcal{E}=\emptyset$, we set $\mathcal{J}=0$.

Theorem 4.1. *Assume that the graph $\mathcal{G}$ has no tadpoles. Let the maximal isotropic subspace $\mathcal{M}$ satisfy any of the equivalent conditions of Proposition 2.4 and assume that it defines local boundary conditions on $\mathcal{G}$. Then*

$$\begin{aligned}\operatorname{tr}_\mathcal{H}\left(\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})}-\mathcal{J}\mathrm{e}^{t\Delta_\pm}\mathcal{J}^\dagger\right) &= \frac{L}{2\sqrt{\pi t}}+\frac{1}{4}\operatorname{tr}_\mathcal{K}\mathfrak{S}(\mathcal{M})\mp\frac{|\mathcal{E}|}{4}\\ &\quad+\frac{1}{2\sqrt{\pi t}}\sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}}\sum_{p\in\mathbb{N}}W_\mathcal{M}(\mathfrak{c})^p|\mathfrak{c}|\exp\left\{-\frac{p^2|\mathfrak{c}|^2}{4t}\right\},\quad t>0,\end{aligned}$$

where $L:=\sum_{j\in\mathcal{I}}a_j$ is the total metric length of the interior of the graph $\mathcal{G}$, and $W_\mathcal{M}(\mathfrak{c})$ is the weight $W_\mathcal{M}(\mathbf{w})$ associated with any walk in the cycle $\mathfrak{c}$. In particular, if the maximal isotropic subspace $\mathcal{M}$ corresponds to a magnetic perturbation of the standard boundary conditions (see Example 2.8), then

$$\begin{aligned}\operatorname{tr}_\mathcal{H}\left(\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})}-\mathcal{J}\mathrm{e}^{t\Delta_\pm}\mathcal{J}^\dagger\right) &= \frac{L}{2\sqrt{\pi t}}+\begin{cases}\frac{|V|-|\mathcal{I}|-|\mathcal{E}|}{2} & \text{for “}+\text{”}\\ \frac{|V|-|\mathcal{I}|}{2} & \text{for “}-\text{”}\end{cases}\\ &\quad+\frac{1}{2\sqrt{\pi t}}\sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}}\sum_{p\in\mathbb{N}}W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c})^p|\mathfrak{c}|\exp\left\{-\frac{p^2|\mathfrak{c}|^2}{4t}\right\}\mathrm{e}^{\mathrm{i}p\Phi(\mathfrak{c})},\quad t>0,\end{aligned}\tag{4.1}$$

where $\Phi(\mathfrak{c})$ is the magnetic flux through the cycle $\mathfrak{c}$ defined in (4.6) *below.*

Remark 4.2. *Since $\Phi(\mathfrak{c}_{\mathrm{rev}})=-\Phi(\mathfrak{c})$ and $W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c}_{\mathrm{rev}})=W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c})$ (see* (4.7) *below), the factor $\mathrm{e}^{\mathrm{i}p\Phi(\mathfrak{c})}$ in* (4.1) *can be replaced by* $\cos(p\Phi(\mathfrak{c}))$.

Before we turn to the proof of Theorem 4.1 we will briefly discuss the trace formula (4.1). The first term on its r.h.s. is a familiar Weyl term. In complete analogy with small t expansion of the trace of heat semigroups on smooth two-dimensional Riemannian manifolds [39], the second term depends solely on the topology of the graph: The number $|\mathcal{I}|-|V|$ is the Euler characteristic of the graph viewed as a simplicial complex. In the context of metric graphs the Euler characteristics has been discussed in [27] and [36]. If we interpret the quantity $\frac{1}{2}\deg(v)-1$ as the local curvature at the vertex $v\in V$, then (2.1) gives a discrete version of the Gauß-Bonnet theorem for compact graphs:

$$\sum_{v\in V}\left(\frac{1}{2}\deg(v)-1\right)=|\mathcal{I}|-|V|.$$

We emphasize that the local curvature at the vertices of the graph is not a curvature in the sense of Regge calculus [45]. Regge calculus, however, can be used to define local curvatures on piecewise flat (or piecewise linear) spaces including Lipschitz-Killing curvatures and boundary curvatures [8]. In particular, these curvatures have been used in [8] to give an alternative proof of the Chern-Gauß-Bonnet theorem for compact closed Riemannian manifolds.

In a similar vein the term $|\mathcal{I}|+|\mathcal{E}|-|V|$ appearing in (4.1) can be interpreted as the relative Euler characteristic (cf. [44]) of the graph $\mathcal{G}$ whenever $\mathcal{G}$ is noncompact, that is, when $\mathcal{E}\neq\emptyset$. In the context of exterior domains in $\mathbb{R}^d$, the relation of Laplace operators on forms with absolute and relative boundary conditions (analogs of Dirichlet and Neumann boundary conditions) to absolute and relative Euler characteristics, respectively, has been established in [5] as a relative index theorem in the spirit of [18].

The sum over primitive cycles of the graph $\mathcal{G}$ in the r.h.s. of (4.1) is an analog of the sum over primitive periodic geodesics on the manifold in the celebrated Selberg trace formula [48] (see also [10], [20], [22], [37], [38]).

The remainder of this section is devoted to the proof of Theorem 4.1.

The heat semigroups $\mathrm{e}^{t\Delta_\pm}$ are integral operators with kernels

$$h_t^{\pm}(x_j, y_j) := g_t(x_j - y_j) \pm g_t(x_j + y_j),$$

respectively. That the difference $\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})} - \mathcal{J}\mathrm{e}^{t\Delta_\pm}\mathcal{J}^\dagger$ is trace class follows from the fact that $\Delta(\mathcal{M},\underline{a})$ is a finite rank perturbation of $\Delta_\pm$. For any trace class operator K on $\mathcal{H}$

$$\operatorname{tr}_{\mathcal{H}} K = \sum_{j\in\mathcal{I}\cup\mathcal{E}} \operatorname{tr}_{\mathcal{H}_j} P_j K P_j,$$

where P_j is the orthogonal projection in $\mathcal{H}$ onto $\mathcal{H}_j$. Observe that $P_j\left(\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})} - \mathrm{e}^{t\Delta_\pm}\right)P_j$ are integral operators on $L^2(I_j)$ with kernels jointly continuous in $x_j, y_j \in \overset{o}{I}_j$ (due to the uniform convergence of the series in (3.12)). Therefore, by Corollary III.10.2 in [17], the trace of $P_j\left(\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})} - \mathrm{e}^{t\Delta_\pm}\right)P_j$ equals the integral of its kernel over the diagonal. Hence, from Corollary 3.4, we get

$$\begin{aligned}
&\operatorname{tr}_{\mathcal{H}}\left(\mathrm{e}^{t\Delta(\mathcal{M})} - \mathcal{J}\mathrm{e}^{t\Delta_\pm}\mathcal{J}^\dagger\right)\\
&= \sum_{j\in\mathcal{I}} \int_{I_j} g_t(0)dx_j + \sum_{j\in\mathcal{E}}\int_{I_j}[g_t(0) - h_t^{\pm}(x_j,x_j)]dx_j \qquad (4.2)\\
&+ \sum_{j\in\mathcal{I}\cup\mathcal{E}}\sum_{\mathbf{w}\in\mathcal{W}_{j,j}} W(\mathbf{w})\int_{I_j} g_t(\operatorname{dist}(x_j, v_-(\mathbf{w})) + |\mathbf{w}| + \operatorname{dist}(x_j, v_+(\mathbf{w})))dx_j,
\end{aligned}$$

where the sum converges absolutely. We will evaluate the different contributions to the r.h.s. of (4.2) separately. Essentially we will follow the original ideas of Roth developed in [47].

1. We start with the terms in (4.2) not associated with any walk on the graph $\mathcal{G}$. Simple calculations yield

$$\int_0^{a_j} g_t(0)dx_j = \frac{a_j}{\sqrt{4\pi t}} \qquad \text{if} \qquad j\in\mathcal{I}$$

and

$$\int_0^{\infty}\left[g_t(0) - h_t^{\pm}(x_j,x_j)\right]dx_j = \mp\int_0^{\infty} g_t(2x_j)dx_j = \mp\frac{1}{4} \qquad \text{if} \qquad j\in\mathcal{E}.$$

Summing over all edges $j\in\mathcal{I}\cup\mathcal{E}$ we get the following contribution to (4.2)

$$\frac{1}{\sqrt{4\pi t}}\sum_{j\in\mathcal{I}} a_j \mp \frac{|\mathcal{E}|}{4}.$$

2. Next we study the contributions from properly closed walks. Let $\mathbf{w}$ be a (nontrivial) properly closed walk from $j\in\mathcal{I}$ to $j\in\mathcal{I}$. In this case $v_-(\mathbf{w}) \neq v_+(\mathbf{w})$ and, therefore, we have

$$\operatorname{dist}(x_j, v_-(\mathbf{w})) + \operatorname{dist}(x_j, v_+(\mathbf{w})) = a_j.$$

Therefore,

$$\sum_{\text{properly closed } \mathbf{w}\in\mathcal{W}_{j,j}} W_{\mathcal{M}}(\mathbf{w})\int_{I_j} g_t(|\mathbf{w}| + a_j)dx_j = a_j W_{\mathcal{M}}(\mathbf{w}) g_t(|\mathbf{w}| + a_j)$$

Summing over all walks in the cycle $\mathfrak{c} = \mathfrak{c}(\mathbf{w})$ and using (3.8) we get

$$W_{\mathcal{M}}(\mathfrak{c}) g_t(|\mathfrak{c}|) \sum_{\mathbf{w}\in\mathfrak{c}} a_{j(\mathbf{w})}.$$

Obviously, $\sum_{\mathbf{w}\in\mathfrak{c}} a_{j(\mathbf{w})} = |\mathfrak{c}'|$ if $\mathfrak{c} = p\mathfrak{c}'$ for some $p \in \mathbb{N}$ and some primitive cycle $\mathfrak{c}'$. Thus, the sum of the contributions in (4.2) from all properly closed walks equals

$$\frac{1}{2\sqrt{\pi t}} \sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}} \sum_{p\in\mathbb{N}} W_{\mathcal{M}}(p\mathfrak{c}) |\mathfrak{c}| \exp\left\{-\frac{p^2|\mathfrak{c}|^2}{4t}\right\}, \quad t > 0.$$

Obviously, the relation $W_{\mathcal{M}}(p\mathfrak{c}) = W_{\mathcal{M}}(\mathfrak{c})^p$ holds for all $p \in \mathbb{N}$.

3. We turn to the contributions which are not coming from properly closed walks. In this case $v_-(\mathbf{w}) = v_+(\mathbf{w})$ and, therefore, we have

$$\mathrm{dist}(x_j, v_-(\mathbf{w})) + \mathrm{dist}(x_j, v_+(\mathbf{w})) = \begin{cases} 2x_j & \text{if} \quad v_-(\mathbf{w}) \in \partial^-(j), \\ 2(a_j - x_j) & \text{if} \quad v_-(\mathbf{w}) \in \partial^+(j). \end{cases}$$

We will call a not properly closed walk $\mathbf{w}$ a walk of type A if it is of the form

$$\mathbf{w} = \{j_p, v_p, j_{p-1}, v_{p-1}, \ldots, j_0, v_0, j_0, \ldots, v_{p-1}, j_{p-1}, v_p, j_p\}.$$

Otherwise a not properly closed walk $\mathbf{w}$ is called a walk of type B. By $\mathcal{W}_{j,j}^A$ and $\mathcal{W}_{j,j}^B$ we denote the set of all walks from j to j of type A and B, respectively.

Obviously, any not properly closed walk is either of type A or B. Any walk of type A is invariant with respect to reversion, that is, $\mathbf{w}_{\mathrm{rev}} = \mathbf{w}$, whereas walks of type B are not.

The following two lemmas complete the proof of the first part of Theorem 4.1.

Lemma 4.3.

$$\sum_{j\in\mathcal{I}\cup\mathcal{E}} \sum_{\mathbf{w}\in\mathcal{W}_{j,j}^A} W_{\mathcal{M}}(\mathbf{w}) \int_{I_j} g_t(2x_j + |\mathbf{w}|) dx_j = \frac{1}{4} \mathrm{tr}_{\mathcal{K}}\, \mathfrak{S}(\mathcal{M}).$$

Lemma 4.4.

$$\sum_{j\in\mathcal{I}\cup\mathcal{E}} \sum_{\mathbf{w}\in\mathcal{W}_{j,j}^B} W_{\mathcal{M}}(\mathbf{w}) \int_{I_j} g_t(2x_j + |\mathbf{w}|) dx_j = 0.$$

Proof of Lemma 4.3. For an arbitrary vertex $v_0 \in V$ and arbitrary $p \in \mathbb{N}_0$ we set

$$\partial G_{v_0}^{\mathcal{I}}(p) := \{\text{walks of the form } \{j_p, v_p, j_{p-1}, \ldots, j_0, v_0, j_0, \ldots, j_{p-1}, v_p, j_p\} \text{ with } j_p \in \mathcal{I}\},$$

$$\partial G_{v_0}^{\mathcal{E}}(p) := \{\text{walks of the form } \{j_p, v_p, j_{p-1}, \ldots, j_0, v_0, j_0, \ldots, j_{p-1}, v_p, j_p\} \text{ with } j_p \in \mathcal{E}\},$$

$$\partial G_{v_0}(p) := \partial G_{v_0}^{\mathcal{I}}(p) \cup \partial G_{v_0}^{\mathcal{E}}(p), \qquad \text{and} \qquad G_{v_0}(p) := \bigcup_{q=0}^{p} \partial G_{v_0}(q).$$

We claim that

$$\begin{aligned} \sum_{\mathbf{w}\in G_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|) dx_{j(\mathbf{w})} &= \frac{1}{4} \mathrm{tr}_{\mathcal{L}_{v_0}} [\mathfrak{S}_{v_0}] \\ &- \frac{1}{4} \sum_{\mathbf{w}\in\partial G_{v_0}^{\mathcal{I}}(p)} W_{\mathcal{M}}(\mathbf{w}) \mathrm{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right) \end{aligned} \tag{4.3}$$

holds for all $p \in \mathbb{N}_0$. Here for brevity we set $\mathfrak{S}_{v_0} := \mathfrak{S}(\mathcal{M}_{v_0})$, where $\mathcal{M}_{v_0} \subset {}^d\mathcal{L}_{v_0}$ is the maximal isotropic subspace from the orthogonal decomposition (2.19).

$$\operatorname{erfc}(s) := \frac{2}{\sqrt{\pi}} \int_s^\infty \mathrm{e}^{-u^2}\, du$$

denotes the complementary error function [1]. The proof is by induction. For $p = 0$ we have

$$\begin{aligned}\sum_{\mathbf{w}\in G_{v_0}(0)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|) dx_{j(\mathbf{w})} &= \frac{1}{4} \operatorname{tr}_{\mathcal{L}_{v_0}}[\mathfrak{S}_{v_0}] \\ &\quad - \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{I}}_{v_0}(0)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{a_{j(\mathbf{w})}}{\sqrt{t}}\right).\end{aligned}$$

Now assume that (4.3) holds for some $p \in \mathbb{N}$ and consider

$$\begin{aligned}&\sum_{\mathbf{w}\in G_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|) dx_{j(\mathbf{w})} \\
&= \sum_{\mathbf{w}\in G_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|) dx_{j(\mathbf{w})} \\
&+ \sum_{\mathbf{w}\in \partial G_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|) dx_{j(\mathbf{w})} \\
&= \frac{1}{4} \operatorname{tr}_{\mathcal{L}_{v_0}}[\mathfrak{S}_{v_0}] - \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{I}}_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right) \\
&+ \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{E}}_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right) \\
&+ \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{I}}_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \left[\operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right) - \operatorname{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right)\right] \\
&= \frac{1}{4} \operatorname{tr}_{\mathcal{L}_{v_0}}[\mathfrak{S}_{v_0}] - \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{I}}_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right) \\
&+ \frac{1}{4} \sum_{\mathbf{w}\in \partial G_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right) \\
&- \frac{1}{4} \sum_{\mathbf{w}\in \partial G^{\mathcal{I}}_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w}) \operatorname{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right).\end{aligned}$$

It remains to prove that the sum of the second and third terms on the r.h.s. is zero. Let $\mathbf{w} \in \partial G_{v_0}(p+1)$ be arbitrary. Write the walk $\mathbf{w}$ as $\mathbf{w} = \{j_{p+1}, v_{p+1}, j_p, \ldots, j_0, v_0, j_0, \ldots, j_p, v_{p+1}, j_{p+1}\}$. Then $\mathbf{w}' := \{j_p, \ldots, j_0, v_0, j_0, \ldots, j_p\} \in \partial G_{v_0}(p)$ with $j_p \in \mathcal{I}$. Hence,

$$W_{\mathcal{M}}(\mathbf{w}) = [\mathfrak{S}_{v_{p+1}}]_{j_p, j_{p+1}} [\mathfrak{S}_{v_{p+1}}]_{j_{p+1}, j_p} W_{\mathcal{M}}(\mathbf{w}')$$

and $|\mathbf{w}| = |\mathbf{w}'| + 2a_{j(\mathbf{w}')}$. Thus,

$$\begin{aligned}
&\sum_{\mathbf{w}\in\partial G_{v_0}(p+1)} W_{\mathcal{M}}(\mathbf{w})\mathrm{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right)\\
&\quad = \sum_{\mathbf{w}'\in\partial G^{\mathcal{I}}_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}')\mathrm{erfc}\left(\frac{|\mathbf{w}'| + 2a_{j(\mathbf{w}')}}{2\sqrt{t}}\right)\\
&\qquad \cdot \sum_{j_{p+1}\in\mathcal{S}(v_{p+1})} [\mathfrak{S}_{v_{p+1}}]_{j_p,j_{p+1}}[\mathfrak{S}_{v_{p+1}}]_{j_{p+1},j_p}.
\end{aligned}$$

By (iii) in Proposition 2.4, we have $\mathfrak{S}^2_{v_{p+1}} = \mathbb{I}$ and, therefore,

$$\sum_{j_{p+1}\in\mathcal{S}(v_{p+1})} [\mathfrak{S}_{v_{p+1}}]_{j_p,j_{p+1}}[\mathfrak{S}_{v_{p+1}}]_{j_{p+1},j_p} = [\mathfrak{S}^2_{v_{p+1}}]_{j_p,j_p} = 1,$$

which completes the proof of (4.3).

By the absolute convergence of the series (4.2), from (4.3) it follows that

$$\lim_{p\to\infty} \sum_{\mathbf{w}\in G_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|)dx_{j(\mathbf{w})} = \frac{1}{4}\,\mathrm{tr}_{\mathcal{L}_{v_0}}\mathfrak{S}_{v_0}.$$

Observing that

$$\begin{aligned}
&\sum_{j\in\mathcal{I}\cup\mathcal{E}} \sum_{\mathbf{w}\in\mathcal{W}^A_{j,j}} W_{\mathcal{M}}(\mathbf{w}) \int_{I_j} g_t(2x_j + |\mathbf{w}|)dx_j\\
&\quad = \lim_{p\to\infty} \sum_{v_0\in V} \sum_{\mathbf{w}\in G_{v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|)dx_{j(\mathbf{w})},
\end{aligned}$$

we obtain the claim of the lemma. □

Proof of Lemma 4.4. Any not properly closed walk of type B is obviously of the form

$$\{j_p, v_p, j_{p-1}, \ldots, j_0, v_0, \mathfrak{s}, v_0, j_0, \ldots, j_{p-1}, v_p, j_p\}$$

for some $p \in \mathbb{N}_0$, where $\mathfrak{s}$ stands for the sequence of internal edges and vertices $i'_1, v'_1, \ldots, v'_n, i'_n$ with $i'_1 \neq i'_n$. For an arbitrary $p \in \mathbb{N}_0$ we set

$$\begin{aligned}
\partial F^{\mathcal{I}}_{\mathfrak{s},v_0}(p) := \{&\text{walks of the form } \{j_p, v_p, j_{p-1}, \ldots, j_0, v_0, \mathfrak{s}, v_0, j_0, \ldots, j_{p-1}, v_p, j_p\}\\
&\text{with} \quad j_p \in \mathcal{I}\},\\
\partial F^{\mathcal{E}}_{\mathfrak{s},v_0}(p) := \{&\text{walks of the form } \{j_p, v_p, j_{p-1}, \ldots, j_0, v_0, \mathfrak{s}, v_0, j_0, \ldots, j_{p-1}, v_p, j_p\}\\
&\text{with} \quad j_p \in \mathcal{E}\},
\end{aligned}$$

$$\partial F_{\mathfrak{s},v_0}(p) := \partial F^{\mathcal{I}}_{\mathfrak{s},v_0}(p) \cup \partial F^{\mathcal{E}}_{\mathfrak{s},v_0}(p), \qquad \text{and} \qquad F_{\mathfrak{s},v_0}(p) := \bigcup_{q=0}^{p} \partial F_{\mathfrak{s},v_0}(q).$$

We claim that

$$\begin{aligned}
&\sum_{\mathbf{w}\in F_{\mathfrak{s},v_0}(p)} W_{\mathcal{M}}(\mathbf{w}) \int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})} + |\mathbf{w}|)dx_{j(\mathbf{w})}\\
&\quad = -\frac{1}{4} \sum_{\mathbf{w}\in\partial F^{\mathcal{I}}_{\mathfrak{s},v_0}(p)} W_{\mathcal{M}}(\mathbf{w})\mathrm{erfc}\left(\frac{|\mathbf{w}| + 2a_{j(\mathbf{w})}}{2\sqrt{t}}\right).
\end{aligned} \tag{4.4}$$

The proof is again by induction. For $p=0$ we have

$$\begin{aligned}
&\sum_{\mathbf{w}\in F_{\mathfrak{s},v_0}(0)} W_{\mathcal{M}}(\mathbf{w})\int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})}+|\mathbf{w}|)dx_{j(\mathbf{w})}\\
&= \sum_{\mathbf{w}\in \partial F^{\mathcal{E}}_{\mathfrak{s},v_0}(0)} W_{\mathcal{M}}(\mathbf{w})\int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})}+|\mathbf{w}|)dx_{j(\mathbf{w})}\\
&\quad + \sum_{\mathbf{w}\in \partial F^{\mathcal{I}}_{\mathfrak{s},v_0}(0)} W_{\mathcal{M}}(\mathbf{w})\int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})}+|\mathbf{w}|)dx_{j(\mathbf{w})}.
\end{aligned}\tag{4.5}$$

Obviously, for any $\mathbf{w}\in F_{\mathfrak{s},v_0}(0)$ we have $W_{\mathcal{M}}(\mathbf{w})=[\mathfrak{S}_{v_0}]_{j,i'_1}[\mathfrak{S}_{v_0}]_{i'_n,j}W'_{\mathcal{M}}$, where $W'_{\mathcal{M}}$ is a weight associated with the sequence $\mathfrak{s}$ and $j=j(\mathbf{w})$. Therefore, if $j\in\mathcal{E}$, then

$$W_{\mathcal{M}}(\mathbf{w})\int_{I_j} g_t(2x_j+|\mathbf{w}|)dx_j=\frac{1}{4}[\mathfrak{S}_{v_0}]_{j,i'_1}[\mathfrak{S}_{v_0}]_{i'_n,j}W'_{\mathcal{M}}\operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right),$$

and, if $j\in\mathcal{I}$, then

$$\begin{aligned}
&W_{\mathcal{M}}(\mathbf{w})\int_{I_j} g_t(2x_j+|\mathbf{w}|)dx_j\\
&=\frac{1}{4}[\mathfrak{S}_{v_0}]_{j,i'_1}[\mathfrak{S}_{v_0}]_{i'_n,j}W'_{\mathcal{M}}\left(\operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right)-\operatorname{erfc}\left(\frac{|\mathbf{w}|+2a_j}{2\sqrt{t}}\right)\right).
\end{aligned}$$

Again we use $\mathfrak{S}_{v_0}^2=\mathbb{I}$, which in combination with $i'_1\neq i'_n$ gives

$$\begin{aligned}
&\frac{1}{4}W'_{\mathcal{M}}\operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right)\sum_{j\in\mathcal{S}(v_0)}[\mathfrak{S}_{v_0}]_{j,i'_1}[\mathfrak{S}_{v_0}]_{i'_n,j}\\
&=\frac{1}{4}W'_{\mathcal{M}}\operatorname{erfc}\left(\frac{|\mathbf{w}|}{2\sqrt{t}}\right)\sum_{j\in\mathcal{S}(v_0)}[\mathfrak{S}_{v_0}^2]_{i'_n,i'_1}=0.
\end{aligned}$$

Combining this with (4.5), we get the claim (4.4) for $p=0$. The proof of the induction step follows the same line as in the proof of Lemma 4.3 and will, therefore, be omitted.

By the absolute convergence of the series (4.2), from (4.4) it follows that

$$\lim_{p\to\infty}\sum_{\mathbf{w}\in F_{\mathfrak{s},v_0}(p)} W_{\mathcal{M}}(\mathbf{w})\int_{I_{j(\mathbf{w})}} g_t(2x_{j(\mathbf{w})}+|\mathbf{w}|)dx_{j(\mathbf{w})}=0,$$

which completes the proof of the lemma. □

To complete the proof of Theorem 4.1 it remains to consider the particular case of magnetic perturbations of standard boundary conditions (see Examples 2.6 and 2.8). We assume that the maximal isotropic subspace $\mathcal{M}$ corresponds to the magnetic perturbation of the Laplace operator $-\Delta(\mathcal{M}_{\mathrm{st}},\underline{a})$ with standard boundary conditions, that is,

$$\mathcal{M}=\mathcal{M}_{\mathrm{st}}^U\quad\text{with}\quad U=\bigoplus_{v\in V}U_v,\quad U_v=\operatorname{diag}\left(\{\mathrm{e}^{\mathrm{i}\varphi_j(v)}\}_{j\in\mathcal{S}(v)}\right).$$

First we calculate $\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M})$. Using (2.1), (2.24), and (2.25) we get

$$\begin{aligned}
\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M})&=\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M}_{\mathrm{st}})=\sum_{v\in V}\sum_{j\in\mathcal{S}(v)}[\mathfrak{S}_v(\mathcal{M}_{\mathrm{st}})]_{j,j}\\
&=\sum_{v\in V}(2-\deg(v))=2|V|-|\mathcal{E}|-2|\mathcal{I}|.
\end{aligned}$$

Let $H_1(\mathcal{G},\mathbb{Z})$ be the first homology group of the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$. There is a canonical map $\Gamma:\mathfrak{C}\to H_1(\mathcal{G},\mathbb{Z})$, which satisfies

$$\Gamma(\mathfrak{c}_{rev})=-\Gamma(\mathfrak{c}),\qquad \Gamma(p\mathfrak{c})=p\Gamma(\mathfrak{c}),\qquad p\in\mathbb{N}.$$

In particular, $\Gamma(\mathfrak{c})=0$ when $\mathfrak{c}=\mathfrak{c}_{\mathrm{rev}}$. Therefore, the map Γ is not injective. In general it is also not surjective. For any cycle $\mathfrak{c}\in\mathfrak{C}$ we set

$$\Phi(\mathfrak{c}):=\widetilde{\Phi}(\Gamma(\mathfrak{c})),$$

where $\widetilde{\Phi}(\Gamma(\mathfrak{c}))$ is the magnetic flux through the homological cycle $\Gamma(\mathfrak{c})$ as defined in [27]. If

$$\mathbf{w}=\{j_0,v_0,j_1,\ldots,j_n,v_n,j_0\}$$

is an arbitrary walk in the equivalence class $\mathfrak{c}$, then by explicit calculations the magnetic flux through the cycle $\mathfrak{c}$ (see [27]) is given by

$$\Phi(\mathfrak{c})=\sum_{k=0}^{n-1}\big(\varphi_{j_k}(v_k)-\varphi_{j_{k+1}}(v_k)\big)+\left(\varphi_{j_n}(v_n)-\varphi_{j_0}(v_n)\right). \tag{4.6}$$

Obviously,

$$W_{\mathcal{M}}(\mathfrak{c})=W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c})\mathrm{e}^{\mathrm{i}\Phi(\mathfrak{c})}$$

and

$$\Phi(\mathfrak{c}_{\mathrm{rev}})=-\Phi(\mathfrak{c}). \tag{4.7}$$

By Proposition 2.4, we have $W_{\mathcal{M}}(\mathfrak{c}_{\mathrm{rev}})=\overline{W_{\mathcal{M}}(\mathfrak{c})}$. In particular, if $\mathfrak{c}_{\mathrm{rev}}=\mathfrak{c}$, then $W_{\mathcal{M}}(\mathfrak{c})$ is real. Since $\Phi(\mathfrak{c}_{\mathrm{rev}})=-\Phi(\mathfrak{c})$ and $W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c}_{\mathrm{rev}})=W_{\mathcal{M}_{\mathrm{st}}}(\mathfrak{c})$, the factor $\mathrm{e}^{\mathrm{i}p\Phi(\mathfrak{c})}$ in (4.1) can be replaced by $\cos(p\Phi(\mathfrak{c}))$. This completes the proof of Theorem 4.1.

5. Applications to Inverse Problems

In this section we present an application of the trace formula in Theorem 4.1 to inverse spectral and scattering problems. Throughout the whole section we will assume that the maximal isotropic subspace $\mathcal{M}$ satisfies any of the equivalent assumption of Proposition 2.4.

For the noncompact graph $\mathcal{G}$ let $S(\lambda;\mathcal{M},\underline{a}):\mathcal{K}_{\mathcal{E}}\to\mathcal{K}_{\mathcal{E}}$, $\lambda>0$, be the scattering matrix for the triple $(-\Delta(\mathcal{M};\underline{a}),\ -\Delta_+,\mathcal{J})$ defined in [26] according to the scattering theory in two Hilbert spaces [51, Chapter 2]. Here $\mathcal{J}$ is the identification operator defined in Section 4. The scattering matrix is continuous with respect to the spectral parameter $\lambda>0$ (see [24] or [29, Theorem 3.12]).

Let $\xi(\lambda;\mathcal{M},\underline{a})$ be the spectral shift function associated with the triple $(-\Delta(\mathcal{M};\underline{a}),$ $-\Delta_+,\mathcal{J})$ (see [51, Section 8.11]). It satisfies the trace formula

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}}\left[\mathrm{e}^{t\Delta(\mathcal{M};\underline{a})}-\mathcal{J}\mathrm{e}^{t\Delta_+}\mathcal{J}^\dagger\right]&+\mathrm{tr}_{\mathcal{H}_{\mathcal{E}}}\left[(\mathcal{J}^\dagger\mathcal{J}-I_{\mathcal{H}_{\mathcal{E}}})\mathrm{e}^{t\Delta_+}\right]\\ &=-t\int_0^\infty\xi(\lambda;\mathcal{M},\underline{a})\mathrm{e}^{-t\lambda}d\lambda,\quad t>0,\end{aligned} \tag{5.1}$$

and is fixed uniquely by the condition $\xi(-1;\mathcal{M},\underline{a})=0$. From the definition of the operator $\mathcal{J}$ it follows that the second term on the r.h.s. of (5.1) vanishes. Thus,

$$\mathrm{tr}_{\mathcal{H}}\left(\mathrm{e}^{t\Delta(\mathcal{M},\underline{a})}-\mathcal{J}\mathrm{e}^{t\Delta_+}\mathcal{J}^\dagger\right)=-t\int_0^\infty\mathrm{e}^{-\lambda t}\xi(\lambda;\mathcal{M})d\lambda,\quad t>0.$$

By the Birman-Krein theorem the spectral shift function is related to the scattering matrix,

$$\det{}_{\mathcal{K}_{\mathcal{E}}}S(\lambda;\mathcal{M},\underline{a})=\exp\{-2\pi i\xi(\lambda;\mathcal{M},\underline{a})\}\qquad \text{a.e.}\quad \lambda\in\mathbb{R}_+. \tag{5.2}$$

By the continuity of the scattering matrix and due to (5.2) one can choose the branch of the logarithm such that

$$s(\lambda;\mathcal{M},\underline{a}) := \frac{1}{2\mathrm{i}}\log\det\nolimits_{\mathcal{K}_{\mathcal{E}}} S(\lambda;\mathcal{M},\underline{a}) \tag{5.3}$$

is continuous with respect to $\lambda\in(0,\infty)$ and satisfies

$$s(0+;\mathcal{M},\underline{a}) = -\pi\left(\xi(0+;\mathcal{M},\underline{a}) + N(0+;\mathcal{M},\underline{a})\right),$$

where $N(\lambda;\mathcal{M},\underline{a})$ is the counting function for the eigenvalues of the operator $-\Delta(\mathcal{M},\underline{a})$. The function (5.3) is called the *scattering phase*. The scattering phase and the eigenvalue counting function uniquely determine the spectral shift function,

$$\xi(\lambda;\mathcal{M},\underline{a}) = -\frac{1}{\pi}s(\lambda;\mathcal{M},\underline{a}) - N(\lambda;\mathcal{M},\underline{a}),\quad \lambda\in\mathbb{R}_+.$$

For compact graphs the spectral shift function is determined by the eigenvalue counting function alone, $\xi(\lambda;\mathcal{M},\underline{a}) = -N(\lambda;\mathcal{M},\underline{a})$, $\lambda\in\mathbb{R}_+$.

Proposition 5.1. *Assume that the graph $\mathcal{G}$ (compact or noncompact) has no tadpoles. Let the maximal isotropic subspace $\mathcal{M}$ satisfy any of the equivalent conditions of Proposition 2.4 and define local boundary conditions. Then the spectral shift function $\mathbb{R}_+\ni\lambda\mapsto\xi(\lambda)$ uniquely determines the set*

$$\Big\{\ell>0\,\Big|\,\sum_{\substack{\mathfrak{c}\in\mathfrak{C}\\ |\mathfrak{c}|=\ell}} W_{\mathcal{M}}(\mathfrak{c})\neq 0\Big\}. \tag{5.4}$$

In [35] the set (5.4) is called the “reduced length spectrum”.

Proof. Using standard formulas for the inverse Laplace transform and, in particular, the fact that $t^{-3/2}\mathrm{e}^{-a/t}$, $a>0$, is the Laplace transform of $(\pi a)^{-1/2}\sin(2\sqrt{a\lambda})$, from Theorem 4.1 we get

$$\begin{aligned}-\xi(\lambda;\mathcal{M},\underline{a}) &= \frac{L}{\pi}\sqrt{\lambda} + \frac{1}{4}\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M}) - \frac{|\mathcal{E}|}{4}\\ &\quad+\frac{1}{\pi}\sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}}\sum_{p\in\mathbb{N}}\frac{1}{p}W_{\mathcal{M}}(\mathfrak{c})^p\sin\left(p|\mathfrak{c}|\sqrt{\lambda}\right),\quad \lambda>0,\end{aligned} \tag{5.5}$$

where the series converges in the sense of distributions on $\mathbb{R}_+$. For $\mathsf{k}\in\mathbb{R}$ define the function $u(\mathsf{k})$ via

$$u(\mathsf{k}) := \begin{cases}-\xi(\mathsf{k}^2;\mathcal{M},\underline{a}) & \text{if}\quad \mathsf{k}>0,\\ \ \ \xi(\mathsf{k}^2;\mathcal{M},\underline{a}) & \text{if}\quad \mathsf{k}<0.\end{cases}$$

Using (5.5) we can calculate the distributional derivative of u,

$$\begin{aligned}u'(\mathsf{k}) &= \frac{L}{\pi} + \left(\frac{1}{2}\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M}) - \frac{|\mathcal{E}|}{2}\right)\delta(\mathsf{k})\\ &\quad+\frac{1}{\pi}\sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}}\sum_{p\in\mathbb{N}}W_{\mathcal{M}}(\mathfrak{c})^p|\mathfrak{c}|\cos\left(p|\mathfrak{c}|\mathsf{k}\right),\quad \mathsf{k}\in\mathbb{R},\end{aligned}$$

where δ stands for the Dirac δ-distribution. Its Fourier transform with respect to k yields

$$\begin{aligned}\int_{\mathbb{R}}\mathrm{e}^{\mathrm{i}\omega\mathsf{k}}u'(\mathsf{k})d\mathsf{k} &= 2L\delta(\omega) + \frac{1}{2}\operatorname{tr}_{\mathcal{K}}\mathfrak{S}(\mathcal{M}) - \frac{|\mathcal{E}|}{2}\\ &\quad+\sum_{\mathfrak{c}\in\mathfrak{C}_{\mathrm{prim}}}\sum_{p\in\mathbb{N}}W_{\mathcal{M}}(\mathfrak{c})^p|\mathfrak{c}|\left[\delta(\omega-p|\mathfrak{c}|)+\delta(\omega+p|\mathfrak{c}|)\right],\end{aligned}$$

which implies the claim. □

Theorem 5.2. *Assume that the graph $\mathcal{G}$ (compact or noncompact) has no tadpoles. Let the maximal isotropic subspace $\mathcal{M}$ satisfy any of the equivalent conditions of Proposition 2.4 and define local boundary conditions on the graph $\mathcal{G}$. Assume, in addition, that*

(i) *the lengths a_i $(i \in \mathcal{I})$ of the internal edges of the graph $\mathcal{G}$ are rationally independent, that is, the equation*

$$\sum_{i\in\mathcal{I}} n_i\, a_i = 0$$

with integer $n_i \in \mathbb{Z}$ *has no non-trivial solution;*

(ii) *for any vertex $v \in V$, none of the matrix elements $[\mathfrak{S}_v]_{j,j'}$, $j, j' \in \mathcal{S}(v)$, vanishes.*

Then the spectral shift function $\mathbb{R}_+ \ni \lambda \mapsto \xi(\lambda)$ uniquely determines the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$.

Proof. All arguments of Section 4 in [35] remain valid for boundary conditions satisfying assumption (ii) of the theorem. Thus, the set (5.4) uniquely determines the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$. Combining this with Proposition 5.1 we obtain the claim. □

Note that assumption (ii) of Theorem 5.2 implies that if $\mathcal{M}_v$ corresponds to the standard boundary conditions at the vertex v or its magnetic perturbation, then necessarily $\deg(v) \neq 2$.

Remark 5.3. *As in* [42] *the assumption on the rational independence of the edge lengths can be slightly relaxed.*

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