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Finite propagation speed and causal free quantum fields on networks

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Abstract

Laplace operators on metric graphs give rise to Klein–Gordon and wave operators. Solutions of the Klein–Gordon equation and the wave equation are studied and finite propagation speed is established. Massive, free quantum fields are then constructed, whose commutator function is just the Klein–Gordon kernel. As a consequence of finite propagation speed, Einstein causality (local commutativity) holds. Comparison is made with an alternative construction of free fields involving RT-algebras.

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1. Introduction

In recent years, the study of quantum systems on networks has received an increasing attention. They are of interest for possible applications in condensed matter physics. The basic idea is to study the behavior of a quantum mechanical particle moving on a given network and where the motion is a free motion away from the nodes of the network. As it turns out, the nodes serve as beam splitters. The quantum mechanical superposition principle then gives rise to interesting interference effects and transport properties can be studied.

In addition, interesting mathematical structures appear giving rise to a host of attractive problems, see, e.g. the articles in [13] and further references given there. In this paper, we study Klein–Gordon and wave equations on any metric graph and for any given Laplace operator thereon. We establish existence, uniqueness and finite propagation speed for given initial data. In addition we construct free quantum fields on arbitrary metric graphs. The construction of such fields was initiated in [3–5]. The results obtained there were applied to a study of spin transport and conductance [4, 5, 42], incorporating additional techniques developed in [4, 6]. The main tool for the construction of these fields was the use of (a simple version of) *RT-algebras* [7, 36–38]. Also the construction there was limited to relatively simple graphs. The construction we present here does not involve RT-algebras and uses only standard and familiar methods of second quantization. However, we will be able to relate our construction to the RT-construction. Spin will not be considered. In order to avoid dealing with infrared problems, we will construct only massive and not massless quantum fields.

We briefly outline our strategy and our results. As a starting point we choose the Hilbert space of square integrable functions on the graph as the one-particle space. Next we make a choice of a self-adjoint Laplacian $-\Delta$ on the graph, which is not necessarily positive. However, $-\Delta$ will always be bounded below. To define $-\Delta$, we follow the discussion in [27] by specifying boundary conditions at the vertices of the graph for the operator given as the second derivative acting on functions on the graph. Given the Laplacian, a mass $m > 0$ and motivated by relativistic quantum theory, we introduce the energy operator $\sqrt{-\Delta + m^2}$, the d'Alembert operator (wave operator) $\Box = \partial_t^2 - \Delta$ and the Klein–Gordon operator $\Box + m^2$.[1] Unique solutions of the classical Klein–Gordon equation for given Cauchy data are then obtained by using

$$\frac{\sin\sqrt{-\Delta + m^2}t}{\sqrt{-\Delta + m^2}}, \tag{1.1}$$

which is the *Klein–Gordon kernel* for $m > 0$ and the *wave kernel* for $m = 0$ and which will be studied in detail. In particular, finite propagation speed will be established. This notion makes sense, since on a metric graph the distance between two points is well defined, so the concepts of two *events*, that is points in spacetime, being space-like separated makes sense.

Finite propagation speed for solutions of the wave equation on smooth manifolds is well studied and understood, see e.g. [8, 12, 44, 45]. So far for spaces with singularities, finite propagation speed has been proved only for the case when the singularities are conical [9]. We recall that finite propagation speed is the earliest time a signal starting at p can arrive at q is just the distance from p to q (in units where $c = 1$). So our result is not too surprising. As it turns out, however, the proof is far from trivial. In fact, we have not been able to prove it for all Laplacians on graphs, which have internal edges. Moreover, for those Laplacians we have been able to consider, at least one of the points p and q has to lie on an external edge. For star graphs, finite propagation speed holds for all Laplacians.

Applying second quantization and a given choice of the Laplacian, we arrive at free fields which satisfy the Klein–Gordon equation. They are Hermitian as soon as the boundary conditions defining the Laplacian are chosen to be real, a notion that will be explained below and which is equivalent to time reversal invariance in quantum mechanics, when the Laplace operator is taken to be a Schrödinger operator. As usual, the non-Hermitian scalar fields carry charge. For their construction, we work with two Laplacians, one for the particle and the other one for the antiparticle. They are such that the boundary conditions defining them are the complex conjugates of each other, again a notion that will be explained in due time. Since the commutator is actually given by the kernel (1.1), Einstein causality (local commutativity) is just another formulation of finite propagation speed. In other words, we show that the commutator vanishes for space-like separated events. Our proof is different from the standard proof of finite propagation speed on smooth manifolds. Our methods, however, do not allow us to prove finite propagation speed and hence Einstein causality in full generality. As a matter of fact, we miss those space-like separated events, whose space components are both points in the interior of the graph. Theorem 33 gives the precise conditions and statements.

The paper is organized as follows. In section 2, we summarize several properties of Laplace operators on metric graphs in a form needed for the next sections. It includes a detailed discussion of their (improper) eigenfunctions. In fact since these eigenfunctions give us the integral kernel of the Klein–Gordon kernel, some of their properties are crucial for

[1] We work in units where $\hbar = c = 1$.

establishing finite propagation speed. In addition to recalling several results from [25, 27, 29, 31], we also establish new and relevant ones. This includes the following. Viewing the Laplacian as the Hamiltonian of a quantum dynamical system, there is an associated scattering theory. As it turns out, the on-shell scattering matrix enters the eigenfunctions [27] and hence also the integral kernel of the Klein–Gordon kernel. The crucial ingredients in proving finite propagation speed are the analytic properties of the S-matrix. In the single vertex case, the information we gain on the S-matrix is so detailed that we are able to establish finite propagation speed even in the case that the Laplacian has bound states.

In section 3, we discuss classical solutions of the Klein–Gordon and the wave equation. There we also formulate the finite propagation speed result, the proof of which is given in appendix B. In section 4 we construct spacetime-dependent relativistic free fields, both Hermitian and non-Hermitian, that satisfy the Klein–Gordon equation and the same boundary conditions as those for the given Laplacian. There we also show that their commutator function equals (minus) the Klein–Gordon kernel (1.1). The proof of the orthonormality of the improper eigenfunctions of the Laplacian is given in appendix A.

2. Laplace operators on metric graphs, their spectral properties and their eigenfunctions

In this section and for the convenience of the reader, we recall the construction of self-adjoint Laplace operators on metric graphs in terms of boundary conditions. We also list several of their properties, in particular their eigenfunctions. They will be needed when we establish finite propagation speed and when we construct free fields and discuss some of their properties. We start with some elementary concepts from graph theory. The material is mainly taken from [25].

2.1. Basic concepts

A finite graph is a 4-tuple $\mathcal{G} = (\mathcal{V}, \mathcal{I}, \mathcal{E}, \partial)$, where $\mathcal{V}$ is a finite set of *vertices*, $\mathcal{I}$ a finite set of *internal edges* and $\mathcal{E}$ a finite set of *external edges*. Elements in $\mathcal{I} \cup \mathcal{E}$ are called *edges*. ∂ is a map, which 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 *final* 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 *compact* if $\mathcal{E} = \varnothing$, 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 and by which every tadpole is counted twice. A vertex is called a *boundary vertex* if it is incident with at least one external edge. The set of all boundary vertices will be denoted by $\partial\mathcal{V}$ such that $|\partial\mathcal{V}| \leqslant |\mathcal{E}|$ holds. The vertices not in $\partial\mathcal{V}$, that is in $\mathcal{V}_{\text{int}} = \mathcal{V}\backslash\partial\mathcal{V}$, are called *internal vertices*.

The compact graph $\mathcal{G}_{\text{int}} = (\mathcal{V}, \mathcal{I}, \varnothing, \partial|_{\mathcal{I}})$ will be called the *interior* of the graph $\mathcal{G} = (\mathcal{V}, \mathcal{I}, \mathcal{E}, \partial)$. It is obtained from $\mathcal{G}$ by eliminating all external edges e. Correspondingly, if $\mathcal{E} \neq \varnothing$, the noncompact graph $\mathcal{G}_{\text{ext}} = (\partial\mathcal{V}, \varnothing, \mathcal{E}, \partial|_{\mathcal{E}})$ is called the *exterior* of $\mathcal{G}$. We will view both $\mathcal{G}_{\text{int}}$ and $\mathcal{G}_{\text{ext}}$ as subgraphs of $\mathcal{G}$ with $\mathcal{G}_{\text{int}} \cap \mathcal{G}_{\text{ext}} = \partial\mathcal{V}$.

Throughout the whole work, we will from now on assume that the graph $\mathcal{G}$ is connected, that is, for any $v, v' \in \mathcal{V}$ there is an ordered sequence $\{v_1 = v, v_2, \ldots, v_{n-1}, v_n = v'\}$ such that any two successive vertices in this sequence are adjacent. In particular, this implies that any vertex of the graph $\mathcal{G}$ has nonzero degree, that is for any vertex there is at least one edge with which it is incident. $\mathcal{G}_{\text{int}}$ is connected if $\mathcal{G}$ is. For connected $\mathcal{G}$, the graph $\mathcal{G}_{\text{ext}}$ is connected if and only if $\partial\mathcal{V}$ consists of one vertex only. By definition a *single vertex graph* is a connected graph which has no internal edges, only one vertex, and at least one external edge. The *star graph* $\mathcal{S}(v) \subseteq \mathcal{E} \cup \mathcal{I}$ associated with the vertex $v \in \mathcal{V}$ consists of the set of the edges adjacent to v and of the vertex v.

We will endow the graph with the following metric structure. Any internal edge $i \in \mathcal{I}$ will be associated with an interval $I_i = [0, a_i]$ with $a_i > 0$ such that the initial vertex of i corresponds to $x = 0$ and the final one to $x = a_i$. The open interval $I_i^o = (0, a_i)$ will be called the interior of the edge i. We call the number a_i the length of the internal edge i. Any external edge $e \in \mathcal{E}$ will be associated with a semi-line $I_e = [0, +\infty)$ whose interior is $I_e^o = (0, +\infty)$. 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* $(\mathcal{G}, \underline{a})$. For the purpose of a compact notation, we set $a_e = \infty$ for $e \in \mathcal{E}$. The metric structure induces a distance function $d(p, q) \geqslant 0$ with the familiar three properties

- $d(p, p) = 0$
- $d(p, q) = d(q, p)$
- $d(p, q) \leqslant d(p, p') + d(p', q)$

for all $p, p', q \in \mathcal{G}$. This defines a topology on $(\mathcal{G}, \underline{a})$, such that $d(p, q)$ is continuous in both variables. For any $e, e' \in \mathcal{E}$ we call $\text{pdist}(e, e') = d(\partial(e), \partial(e'))$ the *passage distance* from the external edge I_e to the external edge $I_{e'}$. Thus, $\text{pdist}(e, e') = 0$ if and only if $\partial(e) = \partial(e')$ and $\text{pdist}(e, e') \geqslant \min_{i\in\mathcal{I}} a_i > 0$, whenever $\partial(e) \neq \partial(e')$. $d(p, q) \geqslant \text{pdist}(e, e')$ holds for any $p \in I_e$ and $q \in I_{e'}$.

On the graph $\mathcal{G}$, there is a natural Lebesgue measure dp. In particular, there is the Hilbert space $L^2(\mathcal{G})$ of square integrable functions on $\mathcal{G}$. We write the scalar product as

$$\langle\psi, \phi\rangle_{\mathcal{G}} = \int_{\mathcal{G}} \overline{\psi(p)}\phi(p)\,\mathrm{d}p \tag{2.1}$$

or simply $\langle\psi, \phi\rangle$, if the context is clear. We write $x \in I_j = [0, a_j]$ for the coordinate of the point $p \in \mathcal{G}$ if p lies on the edge $j \in \mathcal{E} \cup \mathcal{I}$ at the point x and we shall say that the pair (j, x) is the *local coordinate* for p. For short and whenever convenient, we will also view (j, x) as a point in $\mathcal{G}$. A complex valued function on the graph, or more precisely on $\mathcal{G}\backslash\mathcal{V}$, may be considered to be a family $\psi = \{\psi_j\}_{j\in\mathcal{E}\cup\mathcal{I}}$ of complex valued functions ψ_j defined on $(0, a_j)$, so by the convention just made $\psi(j, x) = \psi_j(x)$. With this notation, the scalar product may be written as

$$\langle\psi, \phi\rangle = \sum_{j\in\mathcal{E}\cup\mathcal{I}} \int_0^{a_j} \overline{\psi_j(x)}\phi_j(x)\,\mathrm{d}x.$$

Also we define the derivative $\psi' = \partial_x\psi$ of ψ as

$$(\psi')_j(x) = \frac{\mathrm{d}}{\mathrm{d}x}\psi_j(x).$$

We also introduce the following set of boundary values of ψ and its derivative as

$$\underline{\psi} = \begin{pmatrix} \{\psi_e(0)\}_{e\in\mathcal{E}} \\ \{\psi_i(0)\}_{i\in\mathcal{I}} \\ \{\psi_i(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}, \qquad \underline{\psi}' = \begin{pmatrix} \{\psi_e'(0)\}_{e\in\mathcal{E}} \\ \{\psi_i'(0)\}_{i\in\mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}. \tag{2.2}$$

The ordering of the set $\mathcal{E}$ is arbitrary but fixed as is the ordering in $\mathcal{I}$. Given an ordering, in (2.2) the boundary values on the external edges come first, then the boundary values at the initial vertices and finally the boundary values at the final vertices. Note also that $\underline{\psi}'$ is defined in terms of the inward normal derivative, which is intrinsic, that is independent of the special choice of the orientation on each of the internal edges.

The Laplace operator is defined as

$$(-\Delta_{A,B}\psi)_j(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_j(x), \qquad j \in \mathcal{I}\cup\mathcal{E}$$

with boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0. \tag{2.3}$$

A and B are $(|\mathcal{E}| + 2|\mathcal{I}|) \times (|\mathcal{E}| + 2|\mathcal{I}|)$ matrices. For later reference, we rewrite this condition as

$$(A, B)\begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix} = 0, \tag{2.4}$$

where (A, B) is the $(|\mathcal{E}| + 2|\mathcal{I}|) \times 2(|\mathcal{E}| + 2|\mathcal{I}|)$ matrix obtained by putting the matrices A and B next to each other. So (2.4) is the condition

$$\begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix} \in \mathrm{Ker}(A, B). \tag{2.5}$$

The operator $-\Delta_{A,B}$ is self-adjoint if and only if the matrix (A, B) has maximal rank and the matrix $AB^\dagger$ is Hermitian. Obviously for any invertible C, the pair (CA, CB) gives the same boundary conditions since $\mathrm{Ker}(CA, CB) = \mathrm{Ker}(A, B)$. Moreover, with these conditions, $\mathrm{Ker}(A, B)$ is a maximal isotropic subspace $\mathcal{M}(A, B)$ w.r.t. the canonical Hermitian symplectic form on $\mathcal{C}^{2(|\mathcal{E}|+2|\mathcal{I}|)}$ and all Hermitian subspaces can be written in this form, see [27]. Moreover $\mathcal{M}(A, B) = \mathcal{M}(A', B')$ if and only if $A' = CA$, $B' = CB$ for some invertible C. For a detailed discussion concerning the self-adjointness, see [27, 31]. In addition, if the pair (A, B) satisfies these two conditions, so does the complex conjugate pair $(\bar{A}, \bar{B})$ giving rise to the Laplacian $\Delta_{\bar{A},\bar{B},\underline{a}}$. Let $n_+(AB^\dagger)$ be the number of positive eigenvalues of $AB^\dagger$, counting multiplicities. The identity

$$n_+(AB^\dagger) = n_+(\bar{A}\bar{B}^\dagger) \tag{2.6}$$

is clear. In fact, $AB^\dagger$ and $\bar{A}\bar{B}^\dagger$ actually have the same spectrum.

Proposition 1. *The absolute continuous spectrum of each $-\Delta_{A,B}$ is the interval* $[0, \infty)$. *It has multiplicity equal to the number of external edges, $|\mathcal{E}|$. The number of negative eigenvalues, counting multiplicities, is at most $n_+(AB^\dagger)(\leqslant|\mathcal{E}| + 2|\mathcal{I}|)$. It is equal to $n_+(AB^\dagger)$ if $\mathcal{I} = \varnothing$.*

Below we shall see that the external edges provide a natural labeling for the multiplicities of the absolutely continuous spectrum.

Proof. We claim that all Laplacians $-\Delta_{A,B}$ are finite rank perturbations of each other, that is the difference of two resolvents is always a finite rank operator. To see this, consider the Hilbert space

$$\mathcal{H} = \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_\mathcal{E} \oplus \mathcal{H}_\mathcal{I}, \qquad \mathcal{H}_\mathcal{E} = \oplus_{e\in\mathcal{E}}\mathcal{H}_e, \qquad \mathcal{H}_\mathcal{I} = \oplus_{i\in\mathcal{I}}\mathcal{H}_i, \tag{2.7}$$

where $\mathcal{H}_e = L^2([0,\infty), \mathrm{d}x)$ for all $e \in \mathcal{E}$ and $\mathcal{H}_i = L^2([0,a_i], \mathrm{d}x)$ for all $i \in \mathcal{I}$. Then $L^2(\mathcal{G}) \cong \mathcal{H}$. 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 subset of consisting of elements ψ_j which satisfy

$$\psi_j(0) = \psi'(0) = 0 \qquad \text{when} \quad j \in \mathcal{E}$$
$$\psi_j(0) = \psi'(0) = \psi_j(a_j) = \psi'(a_j) = 0 \qquad \text{when} \quad j \in \mathcal{I}.$$

Let Δ^0 be defined as the second derivative operator, $\Delta^0\psi = \psi''$, with domain

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

Then the deficiency index of $-\Delta^0$ is equal to $(|\mathcal{E}| + 2|\mathcal{I}|, |\mathcal{E}| + 2|\mathcal{I}|)$ and every self-adjoint extension is of the form $-\Delta_{A,B}$ for a suitable boundary condition (A, B). Thus, the claim follows by general results on self-adjoint extensions; see, e.g. appendix A in [1] and the references quoted there. The last statement is just theorem 3.7 in [32]. □

We elaborate on the sufficient criterion $n_+(AB^\dagger) = 0$ for the absence of negative eigenvalues. For given boundary condition (A, B), introduce the meromorphic matrix valued function in k :

$$\mathfrak{S}(\mathsf{k}; A, B) = -(A + \mathrm{i}\mathsf{k}B)^{-1}(A - \mathrm{i}\mathsf{k}B). \tag{2.8}$$

Observe that $\mathfrak{S}(\mathsf{k}; CA, CB) = \mathfrak{S}(\mathsf{k}; A, B)$ holds for all invertible C, so this function depends only on the maximal isotropic subspace defined by (A, B), $\mathfrak{S}(\mathsf{k}; A, B) = \mathfrak{S}(\mathsf{k}; \mathcal{M}(A, B))$.

Lemma 2 ([27], theorem 2.1; [31], theorem 3.12, [32]; theorem 3.7)**.** $\mathfrak{S}(\mathsf{k}; A, B)$ *exists and is unitary for all* $\mathsf{k} > 0$*. Its poles lie on the imaginary axis. There are no poles on the positive imaginary axis if and only if* $AB^\dagger \leqslant 0$ *and then* $-\Delta_{A,B}$ *has no negative eigenvalues.*

The condition $A^\dagger B \leqslant 0$ has the following local formulation, see definition 2.3 in [32], in terms of vertex quantities and which will be used below. By proposition 4.2 in [31] for given boundary conditions (A, B), there is an invertible C such that the two matrices CA and CB have a common block decomposition

$$CA = \bigoplus_{v\in\mathcal{V}} A(v) \qquad CB = \bigoplus_{v\in\mathcal{V}} B(v) \tag{2.9}$$

where the pair $(A(v), B(v))$ gives the boundary conditions at the vertex v. Thus, we obtain

Lemma 3. *The following block decomposition holds for all* k:

$$\mathfrak{S}(\mathsf{k}; A, B) = \bigoplus_{v\in\mathcal{V}} \mathfrak{S}(\mathsf{k}; A(v), B(v)). \tag{2.10}$$

In particular, if the boundary conditions (A, B) *are such that* $AB^\dagger \leqslant 0$*, then* $A(v)B(v)^\dagger \leqslant 0$ *holds for all vertices v and therefore no* $\mathfrak{S}(v; \mathsf{k}) = \mathfrak{S}(\mathsf{k}; A(v), B(v))$ *has poles on the positive imaginary axis.*

With the notation just introduced, there is the following characterization of k-independence.

Lemma 4. [25] $\mathfrak{S}(\mathsf{k}; A, B)$ *is* k*-independent if and only if* $AB^\dagger = 0$ *and hence if and only if* $A(v)B(v)^\dagger = 0$ *holds for all* $v \in \mathcal{V}$*.*

Alternative characterizations of such boundary conditions are given in [31], remark 3.9, and [25], proposition 2.4. Thus, in the single vertex case, all k-independent S-matrices are of the form

$$S = \mathbb{I} - 2P \tag{2.11}$$

with P being an orthogonal projector and then $S^{-1} = S^{\dagger} = S$ holds. In combination with theorem 3.7 in [32] $-\Delta_{A,B} \geqslant 0$ follows for such boundary conditions, see also lemma 2.

The boundary conditions actually fix the graph. More precisely, given finite intervals I_i $(i \in \mathcal{I})$ and half-lines I_e $(e \in \mathcal{E})$, and functions $\psi = \{\psi_j\}_{j\in\mathcal{I}\cup\mathcal{E}}$ on them, generically the boundary condition (2.3) given by the pair (A, B) uniquely fixes the graph $\mathcal{G}$ with a maximal set of vertices, such that the boundary conditions are *local*, see [27, 31] for details.

For given $l \in \mathcal{E}$, consider the following solution $\psi^l(\mathsf{k})$ of the stationary Schrödinger equation at energy $\mathsf{k}^2 > 0$,

$$-\Delta_{A,B}\psi^l(\,;\mathsf{k}) = \mathsf{k}^2\psi^l(\,;\mathsf{k}) \tag{2.12}$$

and of the form

$$\psi^l_j(x;\mathsf{k}) = \begin{cases} \mathrm{e}^{-\mathrm{i}\mathsf{k}x}\delta_{jl} + S(\mathsf{k})_{jl}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{E} \\ \alpha(\mathsf{k})_{jl}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} + \beta(\mathsf{k})_{jl}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \tag{2.13}$$

So intuitively we are looking at what happens to an incoming plane wave $\mathrm{e}^{-\mathrm{i}\mathsf{k}x}$ in channel l when it moves through the graph. Observe that choosing the Laplacian $-\Delta_{A,B}$ as Schrödinger operator, quantum mechanically this means that we have free motion away from the vertices. The vertices in turn act as *beam splitters* in a way described by the boundary condition (A, B).

The number $S(\mathsf{k})_{jl}$ for $j \neq l$ is the *transmission amplitude* from channel $l \in \mathcal{E}$ to channel $j \in \mathcal{E}$ and $S(\mathsf{k})_{ll}$ is the *reflection amplitude* in channel $l \in \mathcal{E}$. So their absolute value squares may be interpreted as transmission and reflection probabilities, respectively. The elements $S(\mathsf{k})_{jl}$ combine to form the scattering matrix

$$S(\mathsf{k}) = S_{A,B}(\mathsf{k}).$$

The ‘interior’ amplitudes $\alpha(\mathsf{k})_{jl} = \alpha_{A,B}(\mathsf{k})_{jl}$ and $\beta(\mathsf{k})_{jl} = \beta_{A,B}(\mathsf{k})_{jl}$ are also of interest, since they describe how an incoming wave moves through a graph before it is scattered into an outgoing channel.

The condition that $\psi^l(\,;\mathsf{k})$ satisfies the boundary condition leads to the solution

$$\begin{pmatrix} S(\mathsf{k}) \\ \alpha(\mathsf{k}) \\ \beta(\mathsf{k}) \end{pmatrix} = -Z(\mathsf{k})^{-1}(A - \mathrm{i}\mathsf{k}B)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \tag{2.14}$$

with the matrices

$$\begin{aligned} Z(\mathsf{k}) &= Z_{A,B}(\mathsf{k}) = AX(\mathsf{k}) + \mathrm{i}\mathsf{k}BY(\mathsf{k}) \\ X(\mathsf{k}) &= X(\mathsf{k};\underline{a}) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & \mathbb{I} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix} \\ Y(\mathsf{k}) &= Y(\mathsf{k};\underline{a}) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & -\mathbb{I} \\ 0 & -\mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix}. \end{aligned} \tag{2.15}$$

The diagonal $|\mathcal{I}| \times |\mathcal{I}|$ matrices $\mathrm{e}^{\pm\mathrm{i}\mathsf{k}\underline{a}}$ are given by

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

By construction, $Z(\mathsf{k}; A, B, \underline{a})$ is entire in $\mathsf{k} \in \mathbb{C}$. For Neumann boundary conditions the scattering is trivial, $S_{A=0,B=\mathbb{I}}(\mathsf{k}) = \mathbb{I}$.

The $\psi^l(\,;\mathsf{k})$ are not in $L^2(\mathcal{G})$, but rather improper eigenfunctions. Their main properties are collected in

Proposition 5. *For fixed $\mathsf{k} > 0$, the $\psi^l(\,;\mathsf{k})$ are linearly independent. Any function ψ on $\mathcal{G}$ satisfying $-\Delta_{A,B}\psi = \mathsf{k}^2\psi$ is a linear combination of these $\psi^l(\,;\mathsf{k})$, provided k^2 is not a discrete eigenvalue of $-\Delta_{A,B}$.*

The proof will be given in a moment. The next proposition will play an important role in our construction of free quantum fields on the graph $\mathcal{G}$. Set

$$\Sigma^> = \Sigma^>_{A,B} = \{\mathsf{k} > 0 \mid \det Z_{A,B}(\mathsf{k}) = 0\}. \tag{2.16}$$

Proposition 6. *The improper eigenfunctions $\psi^l(\,;\mathsf{k})$ satisfy the the following orthogonality relations*

$$\langle \psi^l(\,;\mathsf{k}), \psi^{l'}(\,;\mathsf{k}')\rangle = 2\pi\delta_{l,l'}\delta(\mathsf{k}-\mathsf{k}') \qquad \mathsf{k},\mathsf{k}' \in \mathbb{R}_+\backslash\Sigma^>. \tag{2.17}$$

For any $\mathsf{k} \in \mathbb{R}_+\backslash\Sigma^>$, they span the space associated with the absolutely continuous spectrum and so the multiplicity of the absolute continuous spectrum equals $|\mathcal{E}|$. In particular, if there are no discrete eigenvalues, then the $\psi^l(\,;\mathsf{k})$ form a complete set of improper eigenfunctions of $-\Delta_{A,B}$ in $L^2(\mathcal{G})$.

That there are no discrete eigenvalues means that (i) $-\Delta_{A,B} \geqslant 0$, (ii) there are no positive eigenvalues and (iii) zero is not an eigenvalue. The proof of (2.17) will be given in appendix A. The remainder follows from the previous proposition. Recalling the notational convention (2.1), (2.17) reads

$$\int_{\mathcal{G}} \overline{\psi^l(p;\mathsf{k})}\,\psi^{l'}(p;\mathsf{k}')\,\mathrm{d}p = 2\pi\delta_{l,l'}\delta(\mathsf{k}-\mathsf{k}'). \tag{2.18}$$

For the proof, we will need a result concerning the existence of positive (=embedded) eigenvalues.

Theorem 7 ([27], theorem 3.1; [32], lemma 3.1)**.** $-\Delta_{A,B}$ *has a positive eigenvalue $E = \mathsf{k}^2$ if and only if $\mathsf{k} \in \Sigma^>$. The multiplicity $n(\mathsf{k})$ is finite. The set $\Sigma^>$ is discrete and has no finite accumulation point in $\mathbb{R}_+$. Any eigenfunction to a positive eigenvalue is identically zero on any external edge.*

For special boundary conditions, one can obtain many positive eigenvalues, just take for example Dirichlet or Neumann boundary conditions. On the other hand, there are also nontrivial boundary conditions, that is ones which do not decouple the external edges from the internal ones, and which give positive eigenvalues, see example 3.2 in [27] and example 4.3 in [30]. Also there are examples with *standard boundary conditions* (cf example 4.5 in [31] for the definition), for which there are positive eigenvalues [24].

Corollary 8. *The quantities $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ depend smoothly on $\mathsf{k} \in \mathbb{R}_+\backslash\Sigma^>$.*

Proof. $Z_{A,B}(\mathsf{k})$ is analytic in $\mathsf{k} \in \mathbb{C}$, so $Z_{A,B}(\mathsf{k})^{-1}$ is smooth in $\mathsf{k} \in \mathbb{R}_+\backslash\Sigma^>$ and the claim follows from the representation (2.14). □

For further reference, we denote by $\psi^{\mathsf{k},\nu}$ for $\mathsf{k} \in \Sigma^{>}$ and $1 \leqslant \nu \leqslant n(\mathsf{k})$ an orthonormal basis of the eigenspace with eigenvalue $E = \mathsf{k}^2 > 0$. By what has just been proved, each such eigenfunction is necessarily of the form

$$\psi_j^{\mathsf{k},\nu}(x) = \begin{cases} 0 & \text{for} \quad j \in \mathcal{E} \\ u_j^{\mathsf{k},\nu} \mathrm{e}^{\mathrm{i}\mathsf{k}x} + v_j^{\mathsf{k},\nu}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \tag{2.19}$$

The orthonormality condition for fixed k is obviously

$$\langle \psi^{\mathsf{k},\nu}, \psi^{\mathsf{k},\nu'} \rangle = \delta_{\nu,\nu'} = \sum_{i\in\mathcal{I}} \left\{ u_i^{\mathsf{k},\nu} \overline{u_i^{\mathsf{k},\nu'}} a_i + v_i^{\mathsf{k},\nu} \overline{v_i^{\mathsf{k},\nu'}} a_i \right.$$
$$\left. + \frac{1}{2\mathrm{i}\mathsf{k}} \left(\overline{v_i^{\mathsf{k},\nu}} u_i^{\mathsf{k},\nu'} (\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i} - 1) - \overline{u_i^{\mathsf{k},\nu}} v_i^{\mathsf{k},\nu'} (\mathrm{e}^{-2\mathrm{i}\mathsf{k}a_i} - 1) \right) \right\}, \tag{2.20}$$

a quadratic form in the u's and v's. Thus, we obtain

Corollary 9. *The degeneracy $n(\mathsf{k})$ of any discrete eigenvalue $E = \mathsf{k}^2 > 0$, that is $\mathsf{k} \in \Sigma^{>}$, satisfies the bound*

$$n(\mathsf{k}) \leqslant 2|\mathcal{I}|. \tag{2.21}$$

In particular, $\Sigma^{>}$ is empty when $\mathcal{G}$ is a single vertex graph.

This result compares with proposition 1. We turn to a proof of proposition 5. Linear independence is clear due to the different occurrence of incoming waves in the different $\psi^l(\,;\mathsf{k})$. Assume now that ψ satisfies $-\Delta_{A,B}\psi = \mathsf{k}^2\psi$ and the boundary conditions (2.3). The components are necessarily of the form $\psi_j(x) = u_j\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} + v_j\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x}$ for all $j \in \mathcal{E} \cup \mathcal{I}$. Set $\phi = \psi - \sum_{k\in\mathcal{E}} v_k \psi^k(\,;\mathsf{k})$ such that ϕ also satisfies $-\Delta_{A,B}\phi = \mathsf{k}^2\phi$ and the boundary conditions. We have to show that $\phi = 0$. Observe that by construction, the components are of the form

$$\phi_j(x) = \begin{cases} \hat{s}_j\,\mathrm{e}^{\mathrm{i}\mathsf{k}x}, & j \in \mathcal{E} \\ \hat{u}_j\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} + \hat{v}_j\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x}, & j \in \mathcal{I} \end{cases}$$

such that ϕ contains no incoming waves. Therefore, the boundary conditions can be written in the form

$$Z(\mathsf{k}) \begin{pmatrix} \underline{s}(\mathsf{k}) \\ \underline{u}(\mathsf{k}) \\ \underline{v}(\mathsf{k}) \end{pmatrix} = 0 \tag{2.22}$$

with

$$\underline{s}(\mathsf{k}) = \{\hat{s}_k\}_{k\in\mathcal{E}}, \qquad \underline{u}(\mathsf{k}) = \{\hat{u}_j\}_{j\in\mathcal{I}}, \qquad \underline{v}(\mathsf{k}) = \{\hat{v}_j\}_{j\in\mathcal{I}}$$

viewed as column vectors. By assumption $\mathsf{k} \notin \Sigma^{>}$, so $\hat{s}_k = \hat{u}_j = \hat{v}_j = 0$ for all $k \in \mathcal{E}$, $j \in \mathcal{I}$, and ϕ indeed vanishes thus concluding the proof of proposition 5.

Theorem 10 ([27] theorem 3.12; [31] corollary 3.16)**.** *The scattering matrix is unitary for all* $\mathsf{k} > 0$,

$$S(k)^\dagger = S(\mathsf{k})^{-1}. \tag{2.23}$$

In addition, the identity

$$S(-\mathsf{k}) = S(\mathsf{k})^{-1} \tag{2.24}$$

between meromorphic matrix valued functions in k *is valid.*

There are analogous relations for $\alpha(\mathsf{k})$, $\beta(\mathsf{k})$ in the form

Lemma 11. *The following identities for meromorphic matrix valued functions in* $\mathsf{k} \in \mathbb{C}$ *hold*

$$\begin{aligned} \alpha(-\mathsf{k}) &= \beta(\mathsf{k})S(-\mathsf{k}) \\ \beta(-\mathsf{k}) &= \alpha(\mathsf{k})S(-\mathsf{k}). \end{aligned} \tag{2.25}$$

Proof. We will simultaneously also give a new proof of (2.24). Arrange the components $\psi_j^l(\,;\mathsf{k})$ as a $(|\mathcal{E}|+|\mathcal{I}|) \times |\mathcal{E}|$ matrix $\psi(\,;\mathsf{k})$, such that the components of $\psi^l(\,;\mathsf{k})$ form the lth column. In view of (2.13), the claims (2.24) and (2.25) combined are equivalent to the relation

$$\psi(\,;-\mathsf{k}) = \psi(\,;\mathsf{k})S(-\mathsf{k}) \tag{2.26}$$

as an identity of meromorphic matrix valued functions. Here, with the meromorphic properties of $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$, we view each $\psi^l(\,;\mathsf{k})$ as meromorphic in k, that is each component $\psi_j^l(x;\mathsf{k})$ is meromorphic in k. So if we *define*

$$\widehat{\psi}(\,;\mathsf{k}) = \psi(\,;-\mathsf{k})S(\mathsf{k}), \tag{2.27}$$

we have to show that

$$\widehat{\psi}(\,;\mathsf{k}) = \psi(\,;\mathsf{k}) \tag{2.28}$$

holds as an identity between meromorphic matrix valued functions. Now $-\Delta_{A,B}\psi^l(\,;\mathsf{k}) = \mathsf{k}^2\psi^l(\,;\mathsf{k})$ holds. Moreover the boundary values $\underline{\psi^l(\,;\mathsf{k})}$ and $\underline{\psi^l(\,;\mathsf{k})}'$ of $\psi^l(\,;\mathsf{k})$, see (2.2), are also meromorphic. Since the boundary conditions are satisfied for all $\mathsf{k} > 0$, they also hold for all k away from the poles by the identity theorem for analytic functions. Therefore, they also hold for all $\psi^l(\,;-\mathsf{k})$ and hence also for all $\widehat{\psi}^l(\,;\mathsf{k})$. Similarly $-\Delta_{A,B}\psi^l(\,;\mathsf{k}) = \mathsf{k}^2\psi^l(\,;\mathsf{k})$ implies $-\Delta_{A,B}\psi^l(\,;-\mathsf{k}) = \mathsf{k}^2\psi^l(\,;-\mathsf{k})$ and therefore also $-\Delta_{A,B}\widehat{\psi}^l(\,;\mathsf{k}) = \mathsf{k}^2\widehat{\psi}^l(\,;\mathsf{k})$. Again by the identity theorem for meromorphic functions, it suffices to prove (2.28) for all $\mathsf{k} \in \mathbb{R}_+\backslash\Sigma^>$. But by proposition 5, each $\widehat{\psi}^l(\,;\mathsf{k})$ is a linear combination of the $\psi^k(\,;\mathsf{k})$. By construction,

$$\widehat{\psi}_j^l(x;\mathsf{k}) = \begin{cases} \mathrm{e}^{-\mathrm{i}\mathsf{k}x}\delta_{jl} + S(\mathsf{k})_{jl}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{E} \\ (\alpha(-\mathsf{k})S(\mathsf{k}))_{jl}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x} + (\beta(-\mathsf{k})S(\mathsf{k}))_{jl}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \tag{2.29}$$

But the eigenfunctions $\psi^l(\,;\mathsf{k})$ and $\widehat{\psi}^l(\,;\mathsf{k})$ satisfy the same defining properties and so by the uniqueness of $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$, we infer (2.28). □

Remark 12. Since $S(\mathsf{k})$ is meromorphic in k, its unitarity for positive k extends to complex k in the form of Hermitian analyticity [11, 40]:

$$S(\mathsf{k})^\dagger = S(\bar{\mathsf{k}})^{-1}. \tag{2.30}$$

Combined with (2.25), this gives

$$S(\mathsf{k})^\dagger = S(-\bar{\mathsf{k}}). \tag{2.31}$$

In particular, $S(\mathsf{k})$ is a Hermitian matrix when k is purely imaginary. Since each $\psi^l(\,;-\mathsf{k})$ satisfies $-\Delta_{A,B}\psi^l(\,;-\mathsf{k}) = \mathsf{k}^2\psi^l(\,;-\mathsf{k})$ and the boundary conditions (A, B), it has to be a linear combination of the $\psi^{l'}(\,;\mathsf{k})$ and so (2.26) just provides the explicit form.

We consider the behavior under complex conjugation. Observe that if (A, B) has maximal rank and $AB^\dagger$ is Hermitian, then the complex conjugate pair $(\bar{A}, \bar{B})$ is also of maximal rank and $\bar{A}\bar{B}^\dagger$ is Hermitian. So $(\bar{A}, \bar{B})$ also gives rise to a Laplacian. The following lemma is trivial.

Lemma 13 [27]**.** *If* ψ *satisfies the boundary condition* (A, B), *then the complex conjugate wavefunction* $\bar{\psi}$ *satisfies the boundary condition* $(\bar{A}, \bar{B})$.

In particular, if ψ is in the domain of $\Delta_{A,B}$, then $\bar{\psi}$ is in the domain of $\Delta_{\bar{A},\bar{B},\underline{a}}$ and

$$\overline{-\Delta_{A,B}\psi} = -\Delta_{\bar{A},\bar{B},\underline{a}}\bar{\psi} \tag{2.32}$$

holds.

This gives the following nice observation, whose proof we omit. Recall relation (2.6) in connection with proposition 1.

Corollary 14. *The spectra of the two Laplacians $\Delta_{A,B}$ and $\Delta_{\bar{A},\bar{B},\underline{a}}$ agree. Moreover, if ψ is an (improper) eigenfunction of $-\Delta_{A,B}$, then $\bar{\psi}$ is an (improper) eigenfunction of $\Delta_{\bar{A},\bar{B},\underline{a}}$ for the same eigenvalue.*

Let ^{T} denote transposition of a matrix.

Lemma 15 ([30] theorem 2.2)**.** *The following identities between meromorphic matrix valued functions hold for arbitrary boundary conditions (A, B):*

$$\begin{aligned} S_{\bar{A},\bar{B}}(\mathsf{k}) &= S_{A,B}(\mathsf{k})^T \\ \alpha_{\bar{A},\bar{B}}(\mathsf{k}) &= \overline{\beta_{A,B}(\bar{\mathsf{k}})}\; S_{A,B}(\mathsf{k})^T \\ \beta_{\bar{A},\bar{B}}(\mathsf{k}) &= \overline{\alpha_{A,B}(\bar{\mathsf{k}})}\; S_{A,B}(\mathsf{k})^T \end{aligned} \tag{2.33}$$

or equivalently

$$\psi_{\bar{A},\bar{B}}(\,;\mathsf{k}) = \overline{\psi_{A,B}(\,;\bar{\mathsf{k}})} S_{A,B}(\mathsf{k})^T. \tag{2.34}$$

Proof. We give an alternative proof along the lines used in the proof of lemma 11. Indeed, with the notation used there, define for complex k

$$\check{\psi}(\,;\mathsf{k}) = \overline{\psi_{A,B}(\,;\bar{\mathsf{k}})}\;\; \overline{S_{A,B}(\bar{\mathsf{k}})^{-1}}, \tag{2.35}$$

where we indicate the dependence on the boundary conditions. The aim is to show

$$\check{\psi}(\,;\mathsf{k}) = \psi_{\bar{A},\bar{B}}(\,;\mathsf{k}), \tag{2.36}$$

from which (2.33) and (2.34) follow. Again by the identity theorem for meromorphic functions, it suffices to prove this relation for $\mathsf{k} > 0$, for which k^2 is not a discrete eigenvalue. For such k by unitarity $\overline{S_{A,B}(\bar{\mathsf{k}})^{-1}} = S_{A,B}(\mathsf{k})^T$ and hence for all $\mathsf{k} \in \mathbb{C}$, again by the identity theorem. By lemma 13 each $\check{\psi}^l(\,;\mathsf{k})$ is an improper eigenfunction of $-\Delta(\bar{A}, \bar{B}, \underline{a})$ with eigenvalue k^2 and hence must be a linear combination of the $\psi^k_{\bar{A},\bar{B}}(\,;\mathsf{k})$. By construction, the components of $\check{\psi}^l(\,;\mathsf{k})$, $\mathsf{k} > 0$ are of the form

$$\begin{aligned} \check{\psi}^l_j(x;\mathsf{k}) &= \begin{cases} \mathrm{e}^{-\mathrm{i}\mathsf{k}x}\delta_{jl} + \overline{S_{A,B}(\mathsf{k})^{-1}}_{jl}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{E} \\ \overline{(\alpha_{A,B}(\mathsf{k})S_{A,B}(\mathsf{k})^{-1})}_{jl}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} + \overline{(\beta_{A,B}(\mathsf{k})S_{A,B}(\mathsf{k})^{-1})}_{jl}\, \mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I} \end{cases} \\ &= \begin{cases} \mathrm{e}^{-\mathrm{i}\mathsf{k}x}\delta_{jl} + S_{A,B}(\mathsf{k})_{lj}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{E} \\ (\overline{\alpha_{A,B}(\mathsf{k})}S_{A,B}(\mathsf{k})^T)_{jl}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} + (\overline{\beta_{A,B}(\mathsf{k})}S_{A,B}(\mathsf{k})^T)_{jl}\, \mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \end{aligned} \tag{2.37}$$

But $\psi^l_{\bar{A},\bar{B}}(\,;\mathsf{k})$ and $\check{\psi}^l(\,;\mathsf{k})$ satisfy the same defining properties and so by the uniqueness of $S_{\bar{A},\bar{B}}(\mathsf{k})$, $\alpha_{\bar{A},\bar{B}}(\mathsf{k})$ and $\beta_{\bar{A},\bar{B}}(\mathsf{k})$, we infer (2.36). □

By corollary 14, we know that $\overline{\psi^l(\,;\mathsf{k})} = \overline{\psi^l_{A,B}(\,;\mathsf{k})}$ are eigenfunctions of $-\Delta_{\bar{A},\bar{B},\underline{a}}$ with eigenvalue k^2. Relation (2.34) shows us that they span the eigenspace of $-\Delta_{\bar{A},\bar{B}}$ for that eigenvalue as does $\psi^l_{\bar{A},B}(\,;\mathsf{k})$. We shall make use of this observation when we construct massive, free charged fields in section 4.3.

By definition the boundary conditions given by the pair (A, B) are *real* if an invertible C exists such that the pair $(A', B') = (CA, CB)$ consists of real matrices A' and B'. An equivalent condition is that there exists an invertible C' with $C'A = \bar{A}$ and $C'B = \bar{B}$, see [30]. As a direct consequence of lemmas 11 and 15, we obtain the following two corollaries

Corollary 16. *For arbitrary boundary conditions* (A, B)*, the relations*

$$\overline{\alpha_{A,B}(\bar{\mathsf{k}})} = \alpha_{\bar{A},\bar{B}}(-\mathsf{k}), \qquad \overline{\beta_{A,B}(\bar{\mathsf{k}})} = \beta_{\bar{A},\bar{B}}(-\mathsf{k}) \tag{2.38}$$

hold as identities between matrix-valued meromorphic functions in $\mathsf{k} \in \mathbb{C}$.

Corollary 17. *If the boundary conditions* (A, B) *are real, then the relations*

$$\overline{S(\bar{\mathsf{k}})} = S(-\mathsf{k}), \qquad \overline{\beta(\bar{\mathsf{k}})} = \alpha(\mathsf{k})S(-\mathsf{k}), \qquad \overline{\alpha(\bar{\mathsf{k}})} = \beta(\mathsf{k})S(-\mathsf{k}) \tag{2.39}$$

and hence

$$\overline{\alpha(\bar{\mathsf{k}})} = \alpha(-\mathsf{k}), \qquad \overline{\beta(\bar{\mathsf{k}})} = \beta(-\mathsf{k}) \tag{2.40}$$

are valid as identities between matrix valued meromorphic functions in $\mathsf{k} \in \mathbb{C}$.

As a consequence of lemma 13, we directly obtain

Corollary 18. *For real boundary conditions* (A, B) $\bar{\psi}$ *is an eigenfunction of* $-\Delta_{A,B}$ *whenever* ψ *is. Therefore, for a given eigenvalue, the associated eigenspace is spanned by real eigenfunctions.*

So if for real boundary conditions we choose the eigenfunctions $\psi^{\mathsf{k},\nu}$ to be real, then in the notation of (2.19) the relations

$$u_j^{\mathsf{k},\nu} = \overline{v_j^{\mathsf{k},\nu}}, \qquad \mathsf{k} \in \Sigma^{>} \tag{2.41}$$

are valid. Similarly, we can rewrite (2.39) as

Corollary 19. *If the boundary conditions are real, then the relation*

$$\overline{\psi(\,;\bar{\mathsf{k}})} = \psi(\,;\mathsf{k})S(-\mathsf{k}) \tag{2.42}$$

is valid.

Also (2.30) and the first relation in (2.39) gives

Lemma 20 (see [27] corollary 3.2; [30] theorem 2.2)**.** *If the boundary conditions* (A, B) *are real, then* $S(\mathsf{k})$ *is a symmetric matrix and so for* k *purely imaginary the matrix* $S(\mathsf{k})$ *is real due to (2.39).*

Remark 21. For arbitrary boundary conditions (A, B), the equivalent exponentiated form of (2.32) is

$$\overline{\mathrm{e}^{\mathrm{i}\Delta_{A,B}t}\,\psi} = \mathrm{e}^{-\mathrm{i}\Delta_{\bar{A},\bar{B},\underline{a}}\,t}\,\overline{\psi}. \tag{2.43}$$

If the boundary conditions (A, B) are real and hence $\Delta_{A,B} = \Delta_{\bar{A},\bar{B},\underline{a}}$ holds, then (2.43) is just the statement that time reversal invariance holds. In the single vertex case, this invariance combined with the hermiticity condition on the field (see below) has been used in [5] to prove that $S(\mathsf{k})$ is then a symmetric matrix.

Combined with (2.11) we obtain

Corollary 22. *For a single vertex graph all* k*-independent S-matrices resulting from real boundary conditions are of the form (2.11) where* P *is a real, symmetric and idempotent matrix,* $P^2 = P$.

2.2. Negative eigenvalues of the Laplace operator and their eigenfunctions

The operator $-\Delta_{A,B}$ may have negative eigenvalues. We introduce the sets

$$\begin{aligned} \Sigma^{\leqslant} &= \Sigma^{<}_{A,B} = \{\mathsf{k} = \mathrm{i}\kappa \mid \kappa \geqslant 0, \mathsf{k}^2 = -\kappa^2 \text{ is an eigenvalue of } -\Delta_{A,B}\} \\ \Sigma^{<} &= \Sigma^{<}_{A,B} = \{\mathsf{k} = \mathrm{i}\kappa \mid \kappa > 0, \mathsf{k}^2 = -\kappa^2 \text{ is an eigenvalue of } -\Delta_{A,B}\} \end{aligned} \tag{2.44}$$

such that trivially $\Sigma^{<} \subseteq \Sigma^{\leqslant}$ and let $\Sigma = \Sigma^{\leqslant} \cup \Sigma^{>}$, the set of all discrete eigenvalues. We will discuss zero as a possible eigenvalue separately in the next subsection 2.3. Since all Laplace operators $-\Delta_{A,B}$ for different (A, B) are finite rank perturbations of each other and since the ones with Dirichlet and/or Neumann boundary conditions are non-negative, $\Sigma^{<}$ is a finite set and the multiplicity of each eigenvalue is finite. If $\mathsf{k}^2 = -\kappa^2 < 0$ is such an eigenvalue with multiplicity $n(\mathsf{k})$, there is a finite, orthonormal basis of eigenfunctions $\psi^{\mathsf{k},\nu}$, $1 \leqslant \nu \leqslant n(\mathsf{k})$. Written in local coordinates, they are all necessarily of the form

$$\psi_j^{\mathsf{k},\nu}(x) = \begin{cases} s_j^{\mathsf{k},\nu}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{E} \\ u_j^{\mathsf{k},\nu}\, \mathrm{e}^{\mathrm{i}\mathsf{k}x} + v_j^{\mathsf{k},\nu}\, \mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for} \quad j \in \mathcal{I}. \end{cases} \tag{2.45}$$

The orthonormality condition for fixed $\mathsf{k} \in \Sigma^{<}$ is easily calculated to be

$$\begin{aligned} \delta_{\nu,\nu'} = \langle \psi^{\mathsf{k},\nu}, \psi^{\mathsf{k},\nu'} \rangle = -\frac{1}{2\mathrm{i}\mathsf{k}} \sum_{e\in\mathcal{E}} \overline{s_j^{\mathsf{k},\nu}} s_j^{\mathsf{k},\nu'} + \sum_{i\in\mathcal{I}} \Bigg\{ u_i^{\mathsf{k},\nu} \overline{u_i^{\mathsf{k},\nu'}} a_i + v_i^{\mathsf{k},\nu} \overline{v_i^{\mathsf{k},\nu'}} a_i \\ + \frac{1}{2\mathrm{i}\mathsf{k}} \Big(\overline{v_i^{\mathsf{k},\nu}} u_i^{\mathsf{k},\nu'} (\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i} - 1) - \overline{u_i^{\mathsf{k},\nu}} v_i^{\mathsf{k},\nu'} (\mathrm{e}^{-2\mathrm{i}\mathsf{k}a_i} - 1) \Big) \Bigg\}. \end{aligned} \tag{2.46}$$

In analogy to corollary 9, we obtain

Corollary 23. *The degeneracy $n(\mathsf{k})$ of any discrete eigenvalue $E = \mathsf{k}^2$ $(\mathsf{k} \in \Sigma^{<})$ satisfies the bound*

$$n(\mathsf{k}) \leqslant |\mathcal{E}| + 2|\mathcal{I}|. \tag{2.47}$$

After a short calculation, the boundary condition can be brought into the form, compare (2.22),

$$Z(\mathsf{k} = \mathrm{i}\kappa) \begin{pmatrix} \underline{s}^{\mathsf{k}=\mathrm{i}\kappa,\nu} \\ \underline{u}^{\mathsf{k}=\mathrm{i}\kappa,\nu} \\ \underline{v}^{\mathsf{k}=\mathrm{i}\kappa,\nu} \end{pmatrix} = 0. \tag{2.48}$$

In case the boundary conditions are real, the $\psi^{\mathsf{k},\nu}$ may be chosen to be real, that is the coefficients $s_e^{\mathsf{k},\nu}$, $u_j^{\mathsf{k},\nu}$ and $v_j^{\mathsf{k},\nu}$ are all real.

Recall that there is a canonical Lebesgue measure dp on $\mathcal{G}$. $\delta(p, q)$ is the Dirac δ-function on $\mathcal{G}$ with the defining property

$$\int_{\mathcal{G}} \delta(p, q) f(q)\, \mathrm{d}q = f(p).$$

Remark 24. The arguments may also be reversed to show that Σ equals the set of zeros of $\det Z(\mathsf{k})$ in the set $\{\mathsf{k} \in \mathbb{C} \mid \mathrm{Re}\,\mathsf{k} = 0, \mathrm{Im}\,\mathsf{k} > 0\} \cup \mathbb{R}_+$ and that the k^2 with $\mathsf{k} \in \Sigma$ form exactly the discrete spectrum. As a result there is a completeness relation written as

$$\frac{1}{2\pi} \sum_l \int_0^\infty \mathrm{d}\mathsf{k}\, \psi^l(p; \mathsf{k}) \overline{\psi^l(q; \mathsf{k})} + \sum_{\mathsf{k}\in\Sigma, 1\leqslant\nu\leqslant n(\mathsf{k})} \psi^{\mathsf{k},\nu}(p) \overline{\psi^{\mathsf{k},\nu}(q)} = \delta(p, q) \qquad p, q \in \mathcal{G}. \tag{2.49}$$

The normalization factor $1/2\pi$ is due to (2.18).

2.2.1. Bound states and poles of the S-matrix in the single vertex case. In the single vertex case, one can actually say much more about bound states. In fact, we will see that they are completely encoded in the S-matrix. Thus, the negative eigenvalues are the poles of the scattering matrix and the corresponding eigenfunctions may be obtained from the residues of the poles. To explain this in detail, let $\mathcal{G}_n$ denote the single vertex graph with $n = |\mathcal{E}|$ half-lines meeting at the single vertex v. We will label these half-lines from 1 to n. The scattering matrix $S(\mathsf{k})$ now simply equals $\mathfrak{S}(\mathsf{k}) = -(A + \mathrm{i}\mathsf{k}B)^{-1}(A - \mathrm{i}\mathsf{k}B)$. As shown in [31], see relation (3.23) there, the $S(\mathsf{k})$ for different k all commute and as a consequence there is a common spectral decomposition [26],

$$S(\mathsf{k}) = \sum_{\kappa\in\mathfrak{I}} S^{\kappa}(\mathsf{k}) = \sum_{\kappa\in\mathfrak{I}} \frac{\mathsf{k}+\mathrm{i}\kappa}{\mathsf{k}-\mathrm{i}\kappa} P^{\kappa} = P^{0} - P^{\infty} + \sum_{\kappa\in\mathfrak{I}_0} \frac{\mathsf{k}+\mathrm{i}\kappa}{\mathsf{k}-\mathrm{i}\kappa} P^{\kappa}. \tag{2.50}$$

$\mathfrak{I} = \mathfrak{I}(A, B)$ is a finite set of different real numbers, including possibly the values $\kappa = 0, \infty$. Also $\mathfrak{I}_0$ is the subset, where these elements have been omitted. The Ps define a decomposition of unity of pairwise orthogonal projectors

$$\sum_{\kappa\in\mathfrak{I}} P^{\kappa} = \mathbb{I}_{n\times n}, \qquad (P^{\kappa})^{\dagger} = P^{\kappa}, \qquad P^{\kappa}P^{\kappa'} = P^{\kappa}\delta_{\kappa\kappa'}. \tag{2.51}$$

Thus P^{κ} is the orthogonal projection onto the eigenspace of $S(\mathsf{k})$ with eigenvalue $(\mathsf{k} + \mathrm{i}\kappa)/(\mathsf{k} - \mathrm{i}\kappa)$ (equal to 1 for $\kappa = 0$ and equal to -1 for $\kappa = \infty$). The multiplicities are $0 \leqslant n_S(\mathrm{i}\kappa) = \mathrm{tr} P^{\kappa}$.

$S(\mathsf{k})$ is k-independent if and only if $\mathfrak{I} = \{0, \infty\}$, that is $\mathfrak{I}_0 = \emptyset$. Then P in (2.11) is just P^{∞} and $P^0 = \mathbb{I} - P^{\infty}$. Moreover $S(\mathsf{k})$ is invertible if and only if $\mathsf{k} \notin \mathrm{i}\mathfrak{I}_0 \cup -\mathrm{i}\mathfrak{I}_0$.

Lemma 25. *If the boundary conditions* (A, B) *are real, then the* P^{κ} *are real, symmetric matrices.*

Proof. Due to the representation

$$P^{\kappa} = \lim_{\tau\to\kappa} \frac{\tau-\kappa}{\tau+\kappa} S(\mathrm{i}\tau), \qquad \kappa \neq 0, \infty,$$

each P^{κ} with $\kappa \in \mathfrak{I}_0$ is real and symmetric by lemma 20. So by the same lemma and with $\tau > \max_{\kappa\in\mathfrak{I}} \kappa$,

$$P^0 - P^{\infty} = S(\mathrm{i}\tau) - \sum_{\kappa\in\mathfrak{I}_0} \frac{\tau+\kappa}{\tau-\kappa} P^{\kappa}$$

$$P^0 + P^{\infty} = \mathbb{I}_{n\times n} - \sum_{\kappa\in\mathfrak{I}_0} P^{\kappa}$$

are real and symmetric and so are both P^0 and P^{∞}. □

Our next aim is to determine the eigenfunctions $\psi^{\mathsf{k},\nu}$ out of these data. We will conform to our previous notation and show $\Sigma = \Sigma^{<} = \{\mathrm{i}\kappa \mid 0 < \kappa \in \mathfrak{I}_0\}$, such that the negative eigenvalues of $-\Delta_{A,B}$ are of the form $-\kappa^2$. Given κ, there are orthonormal unit vectors $\underline{s}^{\mathrm{i}\kappa,\nu}$ $(1 \leqslant \nu \leqslant n(\mathrm{i}\kappa))$ in $\mathbb{C}^n$ which span the eigenspace of P^{κ} for the eigenvalue 1 (= Ran P^{κ}),

$$P^{\kappa'}\underline{s}^{\mathrm{i}\kappa,\nu} = \delta_{\kappa',\kappa}\underline{s}^{\mathrm{i}\kappa,\nu} \tag{2.52}$$

and hence

$$S(\mathsf{k})\underline{s}^{\mathrm{i}\kappa,\nu} = \frac{\mathsf{k}+\mathrm{i}\kappa}{\mathsf{k}-\mathrm{i}\kappa}\underline{s}^{\mathrm{i}\kappa,\nu}. \tag{2.53}$$

Observe that the entire set of the $\underline{s}^{\mathrm{i}\kappa,\nu}$ is automatically orthonormal by (2.51) and (2.52)

$$\sum_{j=1}^{n} \overline{s_j^{\mathrm{i}\kappa,\nu}}\, s_j^{\mathrm{i}\kappa',\nu'} = \delta_{\kappa,\kappa'}\delta_{\nu,\nu'}. \tag{2.54}$$

When the boundary conditions and hence also the projectors are real by the previous lemma, these eigenvectors may then be chosen to be real. We define the family of functions $\psi^{\mathrm{i}\kappa,\nu}$ in $L^2(\mathcal{G}_n)$ in terms of its components as

$$\psi_j^{\mathrm{i}\kappa,\nu}(x) = s_j^{\mathrm{i}\kappa,\nu}\sqrt{2\kappa}\,\mathrm{e}^{-\kappa x} \qquad 1 \leqslant j \leqslant n, \qquad 1 \leqslant \nu \leqslant n(\mathrm{i}\kappa). \tag{2.55}$$

The orthonormality of this set follows from the orthonormality (2.54) of the $\underline{s}^{\mathrm{i}\kappa,\nu}$. The next result shows how the bound states are encoded in the scattering matrix.

Proposition 26. *Let $\mathcal{G}$ be a single vertex graph. For $0 < \kappa < \infty$ appearing in the spectral decomposition (2.50) the $\psi^{\mathrm{i}\kappa,\nu}$ as defined by (2.55) are normalized eigenfunctions of $-\Delta_{A,B}$ with eigenvalue $-\kappa^2$ satisfying the boundary conditions. Conversely, if $-\kappa^2$ with $0 < \kappa < \infty$ is an eigenvalue, then $S(\mathsf{k})$ has a pole at $\mathsf{k} = \mathrm{i}\kappa$. In particular, the multiplicity of each such eigenvalue is $n_S(\mathrm{i}\kappa)$ and the number n_b of bound states (counting multiplicities) equals*

$$n_b = \sum_{0<\kappa\in\mathfrak{I}_0} n_S(\mathrm{i}\kappa).$$

By this lemma, there are at most $n = |\mathcal{E}|$ bound states when $\mathcal{G}$ is a single vertex graph. It is easy to construct examples where this upper bound actually is also obtained.

Proof. As for the boundary values of $\psi^{\mathrm{i}\kappa,\nu}$ and its derivative we have

$$\underline{\psi}^{\mathrm{i}\kappa,\nu} = \sqrt{2\kappa}\,\underline{s}^{\mathrm{i}\kappa,\nu}, \qquad \underline{\psi}^{\mathrm{i}\kappa,\nu\,\prime} = -\kappa\sqrt{2\kappa}\,\underline{s}^{\mathrm{i}\kappa,\nu} = -\kappa\,\underline{\psi}^{\mathrm{i}\kappa,\nu}$$

and we have to show that

$$A\underline{\psi}^{\mathrm{i}\kappa,\nu} + B\underline{\psi}^{\mathrm{i}\kappa,\nu\prime} = \sqrt{2\kappa}(A-\kappa B)\underline{s}^{\mathrm{i}\kappa,\nu} = 0.$$

As established in [29], see also [31] proposition 3.7, we may instead of (A, B) equivalently use the pair $(A(\mathsf{k}), B(\mathsf{k}))$, where

$$A(\mathsf{k}) = -\frac{1}{2}(S(\mathsf{k}) - \mathbb{I}_{n\times n}), \qquad B(\mathsf{k}) = \frac{1}{2\mathrm{i}\mathsf{k}}(S(\mathsf{k}) + \mathbb{I}_{n\times n})$$

and where $\mathsf{k} > 0$ is arbitrary. Actually by the proof given there, k may be chosen arbitrary in the domain of analyticity of $S(\mathsf{k})$ and for which $S(\mathsf{k})$ is invertible. By

$$\det S(\mathsf{k}) = (-1)^{n_S(\mathrm{i}\infty)} \prod_{\kappa\in\mathfrak{I}_0} \left(\frac{\mathsf{k}+\mathrm{i}\kappa}{\mathsf{k}-\mathrm{i}\kappa}\right)^{n_S(\mathrm{i}\kappa)}, \tag{2.56}$$

this is the case if k is chosen outside the set $\mathrm{i}\mathfrak{I}_0 \cup -\mathrm{i}\mathfrak{I}_0$. In a moment we shall have the opportunity to make use of this observation. A trivial calculation using (2.53) gives

$$\begin{aligned}(A(\mathsf{k}) - \kappa B(\mathsf{k}))\underline{s}^{\kappa,\nu} &= \frac{1}{2}\left(\left(-1-\frac{\kappa}{\mathrm{i}\mathsf{k}}\right)S(\mathsf{k}) + \left(1-\frac{\kappa}{\mathrm{i}\mathsf{k}}\right)\mathbb{I}_{n\times n}\right)\underline{s}^{\kappa,\nu}\\ &= \frac{1}{2}\left(\left(-1-\frac{\kappa}{\mathrm{i}\mathsf{k}}\right)\frac{\mathsf{k}+\mathrm{i}\kappa}{\mathsf{k}-\mathrm{i}\kappa} + \left(1-\frac{\kappa}{\mathrm{i}\mathsf{k}}\right)\right)\underline{s}^{\kappa,\nu} = 0.\end{aligned}$$

As for the converse let $\psi \neq 0$ be an eigenfunction of $-\Delta_{A,B}\psi$ with eigenvalue $-\kappa_0^2$ with $\kappa_0 > 0$, $-\Delta_{A,B}\psi = -\kappa_0^2\psi$. Then, ψ is necessarily of the form $\psi_j(x) = c_j \exp -\kappa_0 x$. Let $0 \neq \underline{c} \in \mathbb{C}^n$ denote the column vector with components c_j. Since ψ satisfies the boundary conditions, the relation

$$(A - \kappa_0 B)\underline{c} = 0 \tag{2.57}$$

holds or equivalently by the above remarks

$$(A(\mathsf{k}) - \kappa_0 B(\mathsf{k}))\underline{c} = 0, \qquad \mathsf{k} \notin \mathrm{i}\mathfrak{I} \cup -\mathrm{i}\mathfrak{I},$$

which when written out gives

$$S(\mathsf{k})\underline{c} = \frac{\mathsf{k} + \mathrm{i}\kappa_0}{\mathsf{k} - \mathrm{i}\kappa_0}\underline{c}. \tag{2.58}$$

Thus, $S(\mathsf{k})$ has a pole at $\mathsf{k} = \mathrm{i}\kappa_0 \in \mathrm{i}\mathfrak{I}$ and $P^{\kappa_0}\underline{c} = \underline{c}$. For a single vertex graph, $Z(\mathsf{k})$ as defined by (2.15) equals $A + \mathrm{i}\mathsf{k}B$. Observe that we used only (2.57) to establish (2.58). Therefore, the condition $\det(A + \mathrm{i}\mathsf{k}_0 B) = 0$ for $\mathsf{k}_0 \neq 0$, cf remark 24, is equivalent to k_0 being a pole for $S(\mathsf{k})$. Moreover, the discrete spectrum with its multiplicities is given in terms of the scattering matrix as

$$\Sigma = \{\mathrm{i}\kappa \mid 0 < \kappa \in \mathfrak{I}_0\}, \qquad n(\mathrm{i}\kappa) = n_S(\mathrm{i}\kappa), \qquad 0 < \kappa \in \mathfrak{I}_0. \tag{2.59}$$

□

As a further, related consequence of this proposition, the relation

$$P^{\kappa}_{jl} = \sum_{1 \leqslant \nu \leqslant n(\mathrm{i}\kappa)} s_j^{\mathrm{i}\kappa,\nu}\overline{s_l^{\mathrm{i}\kappa,\nu}} \tag{2.60}$$

holds for the matrix elements of P^{κ}.

As for the role of P^0 and P^{∞}, we have

Lemma 27. *The relations*

$$\ker A = \operatorname{Ran} P^0, \qquad \ker B = \operatorname{Ran} P^{\infty} \tag{2.61}$$

hold, so in particular $AP^0 = 0$, $BP^{\infty} = 0$.

Proof. By our previous discussion $\ker A = \ker A(\mathsf{k}) = \ker(S(\mathsf{k}) - \mathbb{I})$ and $\ker B = \ker B(\mathsf{k}) = \ker(S(\mathsf{k}) + \mathbb{I})$ for $\mathsf{k} \notin \mathrm{i}\mathfrak{I} \cup -\mathrm{i}\mathfrak{I}$. □

The known relation $\ker A \perp \ker B = 0$, see lemma 3.4 in [31], is of course compatible with this result. Consider any piecewise constant function ψ, that is a function which is constant on each edge. Then ψ is completely determined by its boundary values $\underline{\psi}$. Moreover, if $\underline{\psi} \in \ker A$, then ψ satisfies the boundary condition (2.3).

2.3. Zero as an eigenvalue

In this subsection, we establish necessary and sufficient conditions for $-\Delta_{A,B}$ to have 0 as an eigenvalue. Let $\psi \neq 0$ be such a square integrable eigenfunction, $-\Delta_{A,B}\psi = 0$. Then necessarily $\psi_e(x) = 0$ for all $e \in \mathcal{E}$ while $\psi_i(x) = \gamma_i + \delta_i x$ for $i \in \mathcal{I}$ and some $\gamma_i, \delta_i \in \mathbb{C}$, not all vanishing. So with $\underline{\gamma} = \{\gamma_i\}_{i\in\mathcal{I}}$, $\underline{\delta} = \{\gamma_i\}_{i\in\mathcal{I}} \in \mathbb{C}^{|\mathcal{I}|}$, viewed as column vectors and with the notation (2.2):

$$\underline{\psi} = \begin{pmatrix} \underline{0} \\ \underline{\gamma} \\ \underline{\gamma} + T_{\underline{a}}\underline{\delta} \end{pmatrix} = U_{\underline{a}} \begin{pmatrix} \underline{\gamma} \\ \underline{\delta} \end{pmatrix}, \qquad \underline{\psi}' = \begin{pmatrix} \underline{0} \\ \underline{\delta} \\ -\underline{\delta} \end{pmatrix} = V \begin{pmatrix} \underline{\gamma} \\ \underline{\delta} \end{pmatrix}$$

with the diagonal matrix $T_{\underline{a}} = \operatorname{diag}\{a_i\}_{i\in\mathcal{I}}$ and

$$U_{\underline{a}} = \begin{pmatrix} 0 & 0 \\ \mathbb{I} & 0 \\ \mathbb{I} & T_{\underline{a}} \end{pmatrix}, \qquad V = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \\ 0 & -\mathbb{I} \end{pmatrix}.$$

So the boundary condition (2.4) takes the form

$$(A, B)\begin{pmatrix}\underline{\psi}\\ \underline{\psi}'\end{pmatrix} = (AU_{\underline{a}}, BV)\begin{pmatrix}\underline{\gamma}\\ \underline{\delta}\end{pmatrix} = 0. \tag{2.62}$$

Using the condition (2.5) and viewing

$$\begin{pmatrix}U_{\underline{a}}\\ V\end{pmatrix}$$

as a $2(|\mathcal{E}| + 2|\mathcal{I}|) \times 2|\mathcal{I}|$ matrix, we arrive at

Proposition 28. *The following relation is valid:*

$$\dim \operatorname{Ker} \Delta_{A,B} = \dim\left(\operatorname{Ker}(A, B) \cap \operatorname{Ran}\begin{pmatrix}U_{\underline{a}}\\ V\end{pmatrix}\right) = \dim \operatorname{Ker}(AU_{\underline{a}}, BV). \tag{2.63}$$

Observe that $\dim \operatorname{Ker}(A, B) = |\mathcal{E}| + 2|\mathcal{I}|$ while $\dim \operatorname{Ran}\left(\begin{smallmatrix}U_{\underline{a}}\\ V\end{smallmatrix}\right) = 2|\mathcal{I}|$ since $\operatorname{Ker}\left(\begin{smallmatrix}U_{\underline{a}}\\ V\end{smallmatrix}\right) = 0$. Generically subspaces of these dimensions have trivial intersection in a space of dimension equal to $2(|\mathcal{E}| + 2|\mathcal{I}|)$, that is they are transversal. This property remains valid even if one space, namely $\operatorname{Ker}(A, B)$, is required to be maximal isotropic. As a consequence, for generic boundary conditions (A, B), we conclude that $-\Delta_{A,B}$ does not have zero as an eigenvalue.

Example 29. Consider the interval $[0, a]$ with Robin boundary conditions at both ends

$$\cos\tau_0\psi(0) + \sin\tau_0\psi'(0) = 0, \qquad \cos\tau_1\psi(a) - \sin\tau_1\psi'(a) = 0. \tag{2.64}$$

Then,

$$(AU_{\underline{a}}, BV) = \begin{pmatrix}\cos\tau_0 & \sin\tau_0\\ \cos\tau_1 & a\cos\tau_1 - \sin\tau_1\end{pmatrix}$$

has non-trivial kernel if and only if $a - \tan\tau_0 - \tan\tau_1 = 0$ or $\cos\tau_0 = \cos\tau_1 = 0$ (Neumann boundary conditions).

2.4. *Walk representation of the amplitudes $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$*

In this section, we will provide an expansion of the amplitudes $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ in terms of walks on the graph. We will use this result to give the proof of theorem 33 in appendix B. For the scattering matrix $S(\mathsf{k})$, such an expansion was already established in [31]. The extension to $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ is similar and goes as follows. For the convenience of the reader we recall those parts of the notion of a walk as introduced in [31] and extended in [32] and which are relevant for our purpose. 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

$$\{j, v_0, j_1, v_1, \ldots, j_n, v_n, j'\} \tag{2.65}$$

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.

When $j, j' \in \mathcal{E}$, this definition is equivalent to that given in [31].

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 (2.65) enters the final edge j through the final vertex $v_0 = v_0(\mathbf{w})$ and leaves the initial edge j' through the initial vertex $v_n = v_n(\mathbf{w})$. A trivial walk $\{j, v, j'\}$ enters j and leaves j' through the same vertex v. Assume that the edges $j, j' \in \mathcal{E} \cup \mathcal{I}$ are not tadpoles. The following distance relation holds for a point p in $\mathcal{G}$ with local coordinate (j, x) and the final and initial vertices of a walk of the form (2.65)

$$d(p, v_0(\mathbf{w})) := \begin{cases} x & \text{if} \quad p \cong (j, x), \qquad v_0(\mathbf{w}) = \partial^-(j), \\ a_j - x & \text{if} \quad p \cong (j, x), \qquad v_0(\mathbf{w}) = \partial^+(j), \end{cases} \tag{2.66}$$

and similarly

$$d(q, v_n(\mathbf{w})) := \begin{cases} x' & \text{if} \quad q \cong (j', x'), \qquad v_n(\mathbf{w}) = \partial^-(j'), \\ a_{j'} - x' & \text{if} \quad q \cong (j', x'), \qquad v_n(\mathbf{w}) = \partial^+(j'). \end{cases} \tag{2.67}$$

The *score* $\underline{n}(\mathbf{w})$ of a walk $\mathbf{w}$ is the set $\{n_i(\mathbf{w})\}_{i\in\mathcal{I}}$ with $n_i(\mathbf{w}) \geqslant 0$ being the number of times the walk $\mathbf{w}$ traverses the internal edge $i \in \mathcal{I}$ such that

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

holds. 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. Obviously we have the

Lemma 30. *If $p \cong (j, x)$ and $q \cong (j', x')$ and if the edges j, j' are not tadpoles, then the distance between p and q satisfies*

$$d(p, q) \leqslant \inf_{\mathbf{w}\in\mathcal{W}_{j,j'}} (d(p, v_0(\mathbf{w})) + |\mathbf{w}| + d(q, v_n(\mathbf{w}))) \tag{2.68}$$

with equality if $j \neq j'$.

Observe that with this notation $d(p, v_0(\mathbf{w})) \leqslant a_j$ and $d(q, v_n(\mathbf{w})) \leqslant a_{j'}$.

Using relation (3.33) in [31], relation (2.14) may be rewritten as

$$\begin{pmatrix} S(\mathsf{k}) \\ \alpha(\mathsf{k}) \\ \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}}\beta(\mathsf{k}) \end{pmatrix} = (\mathbb{I} - \mathfrak{S}(\mathsf{k})T(\mathsf{k}))^{-1}\mathfrak{S}(\mathsf{k}) \begin{pmatrix} \mathbb{I}_{n\times n} \\ 0_{m\times n} \\ 0_{m\times n} \end{pmatrix}. \tag{2.69}$$

For the sake of clarity, we have indicated the type of matrices with $n = |\mathcal{E}|$, $m = |\mathcal{I}|$. Also $\mathfrak{S}(\mathsf{k}) = \mathfrak{S}(\mathsf{k}; A, B)$, see (2.8), and

$$T(\mathsf{k}) = T(\mathsf{k}, \underline{a}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & 0 \end{pmatrix}.$$

So $S(\mathsf{k})$ alone is obtained as

$$S(\mathsf{k}) = (\mathbb{I}_{n\times n} \quad 0_{n\times m} \quad 0_{n\times m})(\mathbb{I} - \mathfrak{S}(\mathsf{k})T(\mathsf{k}))^{-1}\mathfrak{S}(\mathsf{k}) \begin{pmatrix} \mathbb{I}_{n\times n} \\ 0_{m\times n} \\ 0_{m\times n} \end{pmatrix}. \tag{2.70}$$

Alternative ways of obtaining $S(\mathsf{k})$ out of the single vertex scattering matrices $\mathfrak{S}(\mathsf{k})$ and the metric structure of $\mathcal{G}$ are given in [17, 22, 23, 30, 42]. Analogous relations for the amplitudes $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ are

$$\begin{aligned}\alpha(\mathsf{k}) &= (0_{m\times n}\quad 1_{m\times m}\quad 0_{m\times m})(\mathbb{I}-\mathfrak{S}(\mathsf{k})T(\mathsf{k}))^{-1}\mathfrak{S}(\mathsf{k})\begin{pmatrix}\mathbb{I}_{n\times n}\\ 0_{m\times n}\\ 0_{m\times n}\end{pmatrix}\\ \beta(\mathsf{k}) &= (0_{m\times n}\quad 0_{m\times m}\quad \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}})(\mathbb{I}-\mathfrak{S}(\mathsf{k})T(\mathsf{k}))^{-1}\mathfrak{S}(\mathsf{k})\begin{pmatrix}\mathbb{I}_{n\times n}\\ 0_{m\times n}\\ 0_{m\times n}\end{pmatrix}.\end{aligned} \tag{2.71}$$

As a consequence of relation (2.70), the expansion

$$S(\mathsf{k})_{ee'} = \sum_{\mathbf{w}\in\mathcal{W}_{ee'}} S(\mathbf{w};\mathsf{k})_{ee'}\,\mathrm{e}^{\mathrm{i}\mathsf{k}|\mathbf{w}|} \tag{2.72}$$

with

$$S(\mathbf{w};\mathsf{k})_{ee'} = \prod_{l=1}^{k} S(v_l;\mathsf{k})_{i_l i_{l-1}} \tag{2.73}$$

is valid. $S(v;\mathsf{k})$ is the single vertex scattering matrix obtained from the boundary conditions at the vertex v. Also this matrix is indexed by those edges having v in their boundary, that is by the edges in the star graph $\mathcal{S}(v)$. For this we have to assume that there are no *tadpoles*, that is edges whose endpoints are the same vertex. For the details on the expansion (2.72), see [31]. But then by the same arguments, we also obtain similar expansions for the amplitudes $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$. Indeed, for $i\in\mathcal{I}$ and $e\in\mathcal{E}$, let $\mathcal{W}_{ie}^{\pm}$ be the set of walks in $\mathcal{W}_{ie}$ such that $v_0(\mathbf{w})=\partial^{\pm}(i)$. $\mathcal{W}_{ie}^{-}$ and $\mathcal{W}_{ie}^{+}$ are disjoint and $\mathcal{W}_{ie}=\mathcal{W}_{ie}^{-}\cup\mathcal{W}_{ie}^{+}$. Then (2.71) implies

$$\begin{aligned}\alpha(\mathsf{k})_{ie} &= \sum_{\mathbf{w}\in\mathcal{W}_{ie}^{-}} S(\mathbf{w};\mathsf{k})_{ie}\,\mathrm{e}^{\mathrm{i}\mathsf{k}|\mathbf{w}|}\\ \beta(\mathsf{k})_{ie} &= \sum_{\mathbf{w}\in\mathcal{W}_{ie}^{+}} S(\mathbf{w};\mathsf{k})_{ie}\,\mathrm{e}^{\mathrm{i}\mathsf{k}(a_i+|\mathbf{w}|)}\end{aligned} \tag{2.74}$$

with otherwise the same notation as in (2.73).

3. Classical solutions of the Klein–Gordon and the wave equation

3.1. Existence and uniqueness of solutions

Fix boundary conditions (A,B) and introduce the D'Alembert wave operator

$$\Box_{A,B} = \frac{\partial^2}{\partial t^2} - \Delta_{A,B}.$$

For the given mass $m>0$, by definition the Klein–Gordon operator is $\Box_{A,B}+m^2$, which we will discuss first.

3.1.1. The Klein–Gordon equation. Our first discussion for the construction of solutions is close to the familiar one in the relativistic case. Namely, assume $m>0$ to be such that $-\Delta_{A,B}+m^2>0$. Then actually there is $c>0$ such that $-\Delta_{A,B}+m^2>c^2\mathbb{I}$ holds. Indeed, with $\varepsilon_{A,B}=\inf\operatorname{spec}-\Delta_{A,B}\leqslant 0$, the relation $\varepsilon_{A,B}+m^2>0$ is valid and so the choice $c=1/2(\varepsilon_{A,B}+m^2)$ is used. We introduce the self-adjoint energy operator

$$h = h_{A,B,m^2} = \sqrt{-\Delta_{A,B}+m^2}. \tag{3.1}$$

By what has just been said $h > c\mathbb{I}$, so h has a bounded inverse, $0 < h^{-1} < c^{-1}\mathbb{I}$. For any $f \in L^2(\mathcal{G})$ define

$$f^{(\pm)}(p,t) = (\mathrm{e}^{\mp \mathrm{i} h t} f)(p) \tag{3.2}$$

which satisfy

$$\pm \mathrm{i}\frac{\partial}{\partial t} f^{(\pm)}(p,t) = h f^{(\pm)}(p,t) \tag{3.3}$$

provided $f \in \mathcal{D}(h)$. Moreover both $f^{(\pm)}(p,t)$ satisfy the Klein–Gordon equation

$$(\Box_{A,B} + m^2) f^{(\pm)}(p,t) = 0 \tag{3.4}$$

provided the stronger initial condition $f \in \mathcal{D}(-\Delta_{A,B})$ is valid. Indeed, since $\mathcal{D}(-\Delta_{A,B})$ is left invariant under $\exp(\mp \mathrm{i} t h)$ (h and $-\Delta_{A,B}$ trivially commute), the functions $f^{(\pm)}(p,t)$ are in $\mathcal{D}(-\Delta_{A,B})$ for all times. Due to the choice of the sign in (3.2), $f^{(+)}(p,t)$ is called a positive energy solution and $f^{(-)}(p,t)$ a negative energy solution of the Klein–Gordon equation with initial condition $f^{(\pm)}(p,t=0) = f(p)$.

For any $g \in L^2(\mathcal{G})$, let $g^{(\pm)}(p,t)$ be defined similarly to $f^{(\pm)}(p,t)$. If in addition $g \in \mathcal{D}(-\Delta_{A,B})$, an easy calculation shows that

$$\pm \mathrm{i}(f^{(\pm)}(\cdot,t), \overleftrightarrow{\partial_t}\, g^{(\pm)}(\cdot,t))_{\mathcal{G}} = \langle f, g\rangle_{\mathcal{G}} \tag{3.5}$$

$$(f^{(\pm)}(\cdot,t), \overleftrightarrow{\partial_t}\, g_{\mp}(\cdot,t))_{\mathcal{G}} = 0 \tag{3.6}$$

holds for all t. In the standard context for the Klein–Gordon equation in Minkowski space, this result is well known; see e.g. [43], section 3b. In particular, the last relation is read as an orthogonality relation between positive and negative energy solutions.

We can use these observations to solve the initial problem for the hyperbolic differential equation defined by the operator $\Box_{A,B} + m^2$ within the L^2 context. Indeed, for given $f, \dot f$ with $f \in \mathcal{D}(-\Delta_{A,B}) = \mathcal{D}(h^2)$ and $\dot f \in \mathcal{D}(h)$, we will provide a solution $f(p,t)$ to the Klein–Gordon equation satisfying the initial conditions

$$f(p,t=0) = f(p), \qquad \partial_t f(p,t=0) = \dot f(p). \tag{3.7}$$

Following standard notation, we call the pair $(f, \dot f)$ *Cauchy data* for the Klein–Gordon equation. In fact with the choice

$$f^{(\pm)} = \tfrac{1}{2}(f \pm \mathrm{i} h^{-1} \dot f) \in \mathcal{D}(-\Delta_{A,B}),$$

the function

$$f(p,t) = (\mathrm{e}^{-\mathrm{i}ht} f^{(+)})(p) + (\mathrm{e}^{\mathrm{i}ht} f^{(-)})(p) \tag{3.8}$$

solves the initial condition (3.7) and satisfies the Klein–Gordon equation. We make the convention to say that $f(p,t)$ is a solution for all times if for all t $f(\,,t) \in \mathcal{D}(-\Delta_{A,B})$ holds, $f(\,,t)$ is twice differentiable w.r.t. t in the strong topology in $L^2(\mathcal{G})$ and $\partial_t f(\,,t) \in \mathcal{D}(h)$ and finally if $f(p,t)$ satisfies the Klein–Gordon equation. Similarly we suggest a solution for small times if these properties only hold when $|t| < \varepsilon$ for some $\varepsilon > 0$. Obviously $f(p,t)$, as given by (3.8), is a solution for all times.

In standard contexts there is the well-known uniqueness of solutions of hyperbolic differential equations for given Cauchy data. The standard proof uses energy conservation, see e.g. [12, 44, 45]. In the present context we have

Proposition 31. *For given boundary conditions (A, B) let $m > 0$ be such that $-\Delta_{A,B} + m^2 > 0$. Set $h = \sqrt{-\Delta_{A,B} + m^2}$ and let Cauchy data $(f, \dot f)$ be given with $f \in \mathcal{D}(-\Delta_{A,B})$ and*

$\dot{f} \in \mathcal{D}(h)$. *Then the solution for small times exists, is unique, therefore extendable to all times and of the form (3.8).*

Proof. For any solution $g(p, t)$ (for small times), we introduce the energy form

$$0 \leqslant E(g(\,,t)) = \langle \partial_t g(\,,t), \partial_t g(\,,t)\rangle_{\mathcal{G}} + \langle hg(\,,t), hg(\,,t)\rangle_{\mathcal{G}}. \tag{3.9}$$

Since the scalar product $\langle\,,\,\rangle_{\mathcal{G}}$ on $L^2(\mathcal{G})$ is positive definite and since $h > c\mathbb{I} > 0$, for given t $E(g(\,,t)) = 0$ holds if and only if $g(\,,t) = \partial_t g(\,,t) = 0$. Also $E(g(\,,t))$ is conserved

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E(g(,t)) &= \left\langle \partial_t^2 g(,t), \partial_t g(,t)\right\rangle_{\mathcal{G}} + \left\langle \partial_t g(,t), \partial_t^2 g(,t)\right\rangle_{\mathcal{G}}\\ &\quad + \langle h\partial_t g(,t), hg(,t)\rangle_{\mathcal{G}} + \langle hg(,t), h\partial_t g(,t)\rangle_{\mathcal{G}}\\ &= -\langle(-\Delta_{A,B}+m^2)g(,t), \partial_t g(,t)\rangle_{\mathcal{G}} - \langle \partial_t g(,t), (-\Delta_{A,B}+m^2)g(,t)\rangle_{\mathcal{G}}\\ &\quad + \langle \partial_t g(,t), (-\Delta_{A,B}+m^2)g(,t)\rangle_{\mathcal{G}} + \langle(-\Delta_{A,B}+m^2)g(,t), \partial_t g(,t)\rangle_{\mathcal{G}}\\ &= 0. \end{aligned}\tag{3.10}$$

We use this as follows. Let $f_1(p,t)$ and $f_2(p,t)$ be two solutions for small times for the same Cauchy data $(f, \dot{f})$ and set $g = f_1 - f_2$. By assumption and linearity, $g(p, t)$ is also a solution for small times. Moreover g has vanishing Cauchy data, $g(\,,t=0) = \partial_t g(\,,t=0) = 0$, which implies $E(g(\,,t=0)) = 0$. But this in turn implies $E(g(\,,t)) = 0$ for all small t by (3.10) and therefore $g(\,,t) = \partial_t g(\,,t) = 0$ for all small t. □

Concerning the existence of solutions for given initial data, the positivity condition $-\Delta_{A,B} + m^2 > 0$ may actually be dropped at the price of stronger domain conditions. To see this, we use operator calculus in combination with the spectral theorem to rewrite the solution (3.8) to the Klein–Gordon equation as

$$f(\cdot,t) = \cos ht\; f + \frac{\sin ht}{h}\,\dot{f}, \tag{3.11}$$

where both $\cos ht$ and $\sin ht/h$ are bounded self-adjoint operators for all real t. The solutions at different times s and t are then related by

$$f(\cdot,t) = \frac{\sin h(t-s)}{h}\,\overset{\leftrightarrow}{\partial_s}\, f(\cdot,s) \tag{3.12}$$

and we observe that this last relation indeed makes sense without the positivity condition $-\Delta_{A,B} + m^2 > 0$. More precisely, for any boundary condition (A, B) and mass $m > 0$, introduce the Klein–Gordon kernel

$$G_{A,B,m^2}(t) = \frac{\sin\sqrt{-\Delta_{A,B}+m^2}\,t}{\sqrt{-\Delta_{A,B}+m^2}} \tag{3.13}$$

which is well defined by the operator calculus. In fact, for fixed t and $m \geqslant 0$, the functions

$$z \quad\mapsto\quad \frac{\sin\sqrt{z+m^2}\,t}{\sqrt{z+m^2}}, \qquad z \quad\mapsto\quad \cos\sqrt{z+m^2}\,t \tag{3.14}$$

are entire in $z \in \mathbb{C}$ and bounded and real on the real axis. So both $G_{A,B,m^2}(t)$ and $\partial_t G_{A,B,m^2}(t)$ are bounded self-adjoint operators for all t and all $m \geqslant 0$. In order to avoid extra superfluous discussion for the case $m = 0$, we also make the convention

$$\left.\frac{\sin\sqrt{\mathsf{k}^2+m^2}\,t}{\sqrt{\mathsf{k}^2+m^2}}\right|_{m=0} = \frac{\sin \mathsf{k}t}{\mathsf{k}}. \tag{3.15}$$

To sum up,

$$f(\cdot,t) = \partial_t G_{A,B,m^2}(t)\; f + G_{A,B,m^2}(t)\dot{f} \tag{3.16}$$

is well defined for all t. It satisfies the Klein–Gordon equation and solves the initial problem if both f and $\dot{f}$ are in $\mathcal{D}(-\Delta_{A,B})$. Also (3.16) extends to

$$f(\cdot,t) = G_{A,B,m^2}(t-s)\overset{\leftrightarrow}{\partial_s} f(s), \tag{3.17}$$

valid for all t and s. It generalizes (3.12). So far, we have not been able to prove uniqueness of the solution in this general case, namely when $-\Delta_{A,B}+m^2$ is not necessarily a positive operator.

3.1.2. The wave equation. We turn to a discussion of the wave operator $\Box_{A,B}$. Consider any boundary condition (A, B). By the discussion in the previous subsection,

$$f(\cdot,t) = \partial_t G_{A,B,m^2=0}(t)\ f + G_{A,B,m^2=0}(t)\dot{f} \tag{3.18}$$

is a solution of the wave equation $\Box_{A,B}\, f(p,t) = 0$ for given Cauchy data $f, \dot{f} \in \mathcal{D}(-\Delta_{A,B})$. Concerning uniqueness, there is a result analogous to the one for the Klein–Gordon equation, see proposition 31, given as

Proposition 32. *Let the boundary conditions (A, B) be such that $-\Delta_{A,B}$ is non-negative and has no zero eigenvalue. Then the solution (3.18) is the unique solution to the wave equation.*

In terms of the boundary conditions (A, B) proposition 1 gives a sufficient condition for the absence of negative eigenvalues, that is $n_+(AB^\dagger) = 0$, while proposition (28) provides necessary and sufficient conditions for the absence of zero as an eigenvalue.

Proof. Again we use the energy function (3.10), now with the choice $h = \sqrt{-\Delta_{A,B}} \geqslant 0$. By assumption $hg = 0$ implies $g = 0$. So again for given t $E(g(\,,t)) = 0$ holds if and only if $g(\,,t) = \partial_t g(\,,t) = 0$. The proof now proceeds as the one for proposition 31. □

3.2. Finite propagation speed

In this subsection, we will assume the boundary conditions (A, B) to be such that $\Sigma^{>}_{A,B}$ is empty and that zero is not an eigenvalue of $-\Delta_{A,B}$. The aim is to analyze support properties of the integral kernel of the operator $G_{A,B,m^2}(t)$. When $m > 0$, we set $\omega(\mathsf{k}) = \sqrt{\mathsf{k}^2+m^2}$. The completeness relation (2.49) gives

$$\begin{aligned} G_{A,B,m^2}(t)(p,q) &= \frac{1}{4\pi}\sum_l \int_{-\infty}^{\infty} \mathrm{d}\mathsf{k}\ \psi^l(p;\mathsf{k})\overline{\psi^l(q;\mathsf{k})}\frac{\sin\omega(\mathsf{k})t}{\omega(\mathsf{k})} \\ &\quad + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} \psi^{\mathsf{k},\nu}(p)\overline{\psi^{\mathsf{k},\nu}(q)}\frac{\sin\omega(\mathsf{k})t}{\omega(\mathsf{k})}. \end{aligned} \tag{3.19}$$

By our convention (3.15), when $m = 0$ this simplifies to

$$\begin{aligned} G_{A,B,m^2=0}(t)(p,q) &= \frac{1}{4\pi}\sum_l \int_{-\infty}^{\infty} \mathrm{d}\mathsf{k}\ \psi^l(p;\mathsf{k})\overline{\psi^l(q;\mathsf{k})}\frac{\sin\mathsf{k}t}{\mathsf{k}} \\ &\quad + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} \psi^{\mathsf{k},\nu}(p)\overline{\psi^{\mathsf{k},\nu}(q)}\frac{\sin\mathsf{k}t}{\mathsf{k}}. \end{aligned} \tag{3.20}$$

Observe that due to the self-adjointness of $-\Delta_{A,B}$ and as is obvious from (3.19) and (3.20), the relation

$$\overline{G_{A,B,m^2}(t)(p,q)} = G_{A,B,m^2}(t)(q,p) \tag{3.21}$$

holds for all $m \geqslant 0$. In addition, due to (2.32) the relation

$$\overline{G_{A,B,m^2}(t)(p,q)} = G_{\bar{A},\bar{B},m^2}(t)(q,p) \tag{3.22}$$

is valid. As a consequence, for real boundary conditions $G_{A,B,m^2}(t)(q,p)$ is real.

We define the space of events to be $\mathbb{R} \times \mathcal{G}$ and write an event as (t,p). By definition, two events (t,p) and (s,q) are *space-like separated* if $d(p,q) > |t-s|$.

Theorem 33. *Assume one of the following two conditions is satisfied.*

- *$\mathcal{G}$ is a single vertex graph ($\mathcal{I} = \varnothing$),*
- *$\mathcal{G}$ is arbitrary and $-\Delta_{A,B}$ has no discrete eigenvalues.*

Then for any $m \geqslant 0$, the integral kernel $G_{A,B,m^2}(t-s)(p,q)$ vanishes whenever (t,p) and (s,q) are space-like separated and if in addition at least one of the two points p and q is in $\mathcal{G}_{\mathrm{ext}}$.

So far we have not been able to remove the restriction that p or q must lie in $\mathcal{G}_{\mathrm{ext}}$. As a particular case, we obtain

Corollary 34. *$G_{A,B,m^2}(t)(p,q)$ vanishes for all $p \in I_e \subset \mathcal{G}_{\mathrm{ext}}$ and all $q \in I_{e'} \subset \mathcal{G}_{\mathrm{ext}}$ whenever $t > 0$ is smaller than the passage distance, $t < \mathrm{pdist}(e,e')$.*

So a signal entering the external edge e cannot arrive at the external edge e' before a time larger than the passage distance $\mathrm{pdist}(e,e')$. This result is of course only nontrivial when the endpoints of the edges are different, $\partial(e) \neq \partial(e')$, since otherwise $\mathrm{pdist}(e,e') = 0$.

For the free fields to be constructed in the next section this implies local commutativity (with the above restriction). We reformulate finite propagation speed in a more familiar form. For any closed subset $\mathcal{O}$ of $\mathcal{G}$ and any $0 < d$ define

$$\mathcal{O}^d = \{p \in \mathcal{G} | \min_{q \in \mathcal{O}} d(p,q) \leqslant d\},$$

the closed set of points in $\mathcal{G}$ with distance less or equal to d from $\mathcal{O}$.

Corollary 35. *Under the conditions of the theorem, the following holds for the solution of the Klein–Gordon equation (or the wave equation) for given Cauchy data $(f, \dot{f})$.*

- *If f and $\dot{f}$ both have support in $\mathcal{O} \subset \mathcal{G}_{\mathrm{ext}}$, then $f(\cdot,t)$ has support in $\mathcal{O}^{|t|}$ for all t.*
- *If f and $\dot{f}$ both have support in $\mathcal{O}$, then $\mathrm{supp} f(\cdot,t) \cap \mathcal{G}_{\mathrm{ext}} \subset \mathcal{O}^{|t|}$ for all t.*

In particular, if both f and $\dot{f}$ have support on the external edge I_e, then $f(\cdot,t)$ vanishes on any external edge $I_{e'}$ $(e' \neq e)$ as long as $|t| < \mathrm{pdist}(e,e')$.

4. Free quantum fields on metric graphs

In this section, we will construct free fields on the graph $\mathcal{G}$. The reader is supposed to be familiar with the basic concepts of *second quantization*; see, e.g., [19, 20, 43, 47]. Also from now on, we will assume that the boundary conditions (A,B) are chosen in such a way that there are no positive (or zero) eigenvalues of $-\Delta_{A,B}$, that is $\Sigma^{>} = \varnothing$ and $\Sigma = \Sigma^{<}$, so bound states are still allowed. As a trivial consequence of this assumption, the graph has to have at least one external edge, $\mathcal{E} \neq \varnothing$, since otherwise the entire spectrum is discrete and there are positive eigenvalues. Finally we will assume that $m > 0$ is chosen such that $-\Delta_{A,B} + m^2 > 0$.

4.1. Creation and annihilation operators and the RT-algebra

We introduce the creation and annihilation operators [2]

$$\begin{aligned} & a^l(\mathsf{k}),\ a^l(\mathsf{k})^\star, && \mathsf{k} > 0 \\ & a^{\mathsf{k},\nu},\ a^{\mathsf{k},\nu\star}, && \mathsf{k}\in\Sigma,\quad 1\leqslant\nu\leqslant n(\mathsf{k}) \end{aligned} \tag{4.1}$$

satisfying the commutation relations

$$[a^l(\mathsf{k}), a^{l'}(\mathsf{k}')^\star] = 2\pi\delta_{ll'}\delta(\mathsf{k}-\mathsf{k}'), \qquad [a^{\mathsf{k},\nu}, a^{\mathsf{k}',\nu'\star}] = \delta_{\mathsf{k},\mathsf{k}'}\delta_{\nu,\nu'}, \tag{4.2}$$

while all other commutators vanish. These operators act in the bosonic Fock space $\mathfrak{F}(\mathcal{H}_1)$ with $\mathcal{H}_1 = L^2(\mathcal{G})$ as the choice of the one-particle space, that is

$$\mathfrak{F}(\mathcal{H}_1) = \mathbb{C}\oplus\mathcal{H}_1\oplus\cdots\oplus\mathcal{H}_n\oplus\cdots \tag{4.3}$$

$$\mathcal{H}_n = \underbrace{\mathcal{H}_1 \underset{s}{\otimes} \mathcal{H}_1 \underset{s}{\otimes} \mathcal{H}_1 \underset{s}{\otimes} \mathcal{H}_1}_{n}, \tag{4.4}$$

such that $\mathcal{H}_n$ is the n-particle space. $\otimes_s$ denotes the symmetric tensor product. $a^l(\mathsf{k})^\star$ has the interpretation of a creation of a particle with wavefunction $\psi^l(\,;\mathsf{k})$, while $a^{\mathsf{k},\nu\star}$ is the creation operator of a particle with (bound state) wavefunction $\psi^{\mathsf{k},\nu}$. The normalization in (4.2) is chosen in accordance with (2.17), (2.19) and (2.46). For reasons which will become clear in a moment, we elaborate on this. By the completeness relation (2.49) any wavefunction $f\in L^2(\mathcal{G})$ has a *Fourier type* expansion of the form

$$f(p) = \sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{d}\mathsf{k}\,\widetilde{f}_l(\mathsf{k})\psi^l(p;\mathsf{k}) + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} \widetilde{f}^\nu(\mathsf{k})\psi^{\mathsf{k},\nu}(p) \tag{4.5}$$

with expansion coefficients given as

$$\widetilde{f}_l(\mathsf{k}) = \frac{1}{\sqrt{2\pi}}\int_{p\in\mathcal{G}} \overline{\psi^l(p;\mathsf{k})}f(p)\,\mathrm{d}p, \qquad \widetilde{f}^\nu(\mathsf{k}) = \int_{p\in\mathcal{G}}\overline{\psi^{\mathsf{k},\nu}(p)}f(p)\,\mathrm{d}p \tag{4.6}$$

such that the *Parseval equality* holds in the form

$$\langle f, f\rangle_{\mathcal{G}} = \sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{d}\mathsf{k}|\widetilde{f}_l(\mathsf{k})|^2 + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} |\widetilde{f}^\nu(\mathsf{k})|^2, \tag{4.7}$$

thus establishing an isometry of Hilbert spaces

$$L^2(\mathcal{G}) \cong L^2([0,\infty), d\mathsf{k}) \oplus \mathbb{C}^{N_\Sigma}$$

where

$$N_\Sigma = \sum_{\mathsf{k}\in\Sigma=\Sigma^<} n(\mathsf{k}) \leqslant |\mathcal{E}| + 2|\mathcal{I}|$$

is the total number of bound states, counting multiplicities. With this notation, the creation operator for a particle with an arbitrary wavefunction f is of the form

$$a^\star(f) = \sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{d}\mathsf{k}\,\widetilde{f}_l(\mathsf{k})a^l(\mathsf{k})^\star + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} \widetilde{f}^\nu(\mathsf{k})a^{\mathsf{k},\nu\star} \tag{4.8}$$

and correspondingly its adjoint $a(f)$ is the annihilation operator for the wavefunction f.

[2] We stick to the standard notational convention in QFT and use $\star$ to denote the adjoint (only) in this case.

The (self-adjoint) number operator, the second quantization of the identity operator on the one-particle space, is

$$\mathbf{N} = \frac{1}{2\pi}\sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{dk}\, a^l(\mathsf{k})^\star a^l(\mathsf{k}) + \sum_{\mathsf{k}\in\Sigma, 1\leqslant\nu\leqslant n(\mathsf{k})} a^{\mathsf{k},\nu\,\star} a^{\mathsf{k},\nu}. \tag{4.9}$$

We define $h = \sqrt{-\Delta_{A,B} + m^2}$, see the discussion in section 3.1, to be the one-particle Hamilton operator, so its second quantization is the self-adjoint operator

$$\mathbf{H} = \frac{1}{2\pi}\sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{dk}\, \omega(\mathsf{k})\, a^l(\mathsf{k})^\star a^l(\mathsf{k}) + \sum_{\mathsf{k}\in\Sigma, 1\leqslant\nu\leqslant n(\mathsf{k})} \omega(\mathsf{k}) a^{\mathsf{k},\nu\,\star} a^{\mathsf{k},\nu} \tag{4.10}$$

and we observe that $\omega(\mathsf{k})$ is positive for all $\mathsf{k} \in \Sigma^< = \Sigma$ by the choice of $m > 0$.

The operator

$$\mathbf{P} = \frac{1}{2\pi}\sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{dk}\, \mathsf{k}\, a^l(\mathsf{k})^\star a^l(\mathsf{k}) \tag{4.11}$$

can be given the interpretation of the sum of the absolute value of the momenta of all particles in a state of the Fock space which does not contain particles with bound state wavefunctions. Stated more abstractly, let P_{ac} be the orthogonal projector onto the subspace of $L^2(\mathcal{G})$ corresponding to the absolutely continuous spectrum of $-\Delta_{A,B}$. Then $\mathbf{P}$ is the second quantization of the one-particle operator $\sqrt{-\Delta_{A,B} P_{ac}}$. That there is no proper momentum operator in the familiar sense has of course to do with the fact that the configuration space is a graph. So the notion of translations in space and with the momentum operator as infinitesimal generator does not make sense. But what remains is some kind of absolute value of momentum reminiscent of the conservation of the absolute value of the momentum of a (classical) particle under elastic scattering. Both $\mathbf{N}$ and $\mathbf{P}$ commute with H_0 and are therefore conserved under time evolution.

With these preparatory remarks, we are now in the position to provide an explicit construction of *RT (reflection–transmission)-algebras* [7, 36, 37]. The main observation is that k in $a^l(\mathsf{k})$ and $a^l(\mathsf{k})^\star$ is positive. So we are *free to define* creation and annihilation operators also for negative k. Indeed, we may set

$$\begin{aligned} a^l(-\mathsf{k}) &= \sum_{l'\in\mathcal{E}} S(\mathsf{k})_{l\,l'} a^{l'}(\mathsf{k}) \\ a^l(-\mathsf{k})^\star &= \sum_{l'\in\mathcal{E}} S(-\mathsf{k})_{l'\,l} a^{l'}(\mathsf{k})^\star, \qquad \mathsf{k} > 0, \end{aligned} \tag{4.12}$$

where we recall the general relation $S(-\mathsf{k}) = S(\mathsf{k})^{-1} = S(\mathsf{k})^\dagger$ valid for all real $\mathsf{k} \neq 0$. With this definition, the relations (4.12) remain valid for $\mathsf{k} < 0$ and then $a^l(\mathsf{k})^\star$ is again the adjoint of $a^l(\mathsf{k})$. Since for $\mathsf{k} > 0$ the operator $a^{l'}(\mathsf{k})^\star$ creates a particle with wavefunction $\psi^l(\,;\mathsf{k})$, by linearity the operator $a^l(-\mathsf{k})^\star$ as defined by (4.12) creates a particle with wavefunction

$$\sum_{l'\in\mathcal{E}} S(-\mathsf{k})_{l'l}\psi^{l'}(p;\mathsf{k}),$$

which by (2.26) equals $\psi^l(\,;-\mathsf{k})$. This gives the first part of the next lemma, while the second part follows by an easy calculation.

Lemma 36. *For any $\mathsf{k} > 0$ the operator $a^l(-\mathsf{k})^\star$ as defined by (4.12) creates a particle with wavefunction $\psi^l(\,;-\mathsf{k})$. The extended family of operators*

$$\{a^l(\mathsf{k}), a^l(\mathsf{k})^\star\}_{l\in\mathcal{E},-\infty<\mathsf{k}<\infty}$$

satisfies the commutation relations

$$[a^l(\mathsf{k}), a^{l'}(\mathsf{k}')^\star] = \delta_{l\,l'}\delta(\mathsf{k}-\mathsf{k}') + S(\mathsf{k})_{ll'}\delta(\mathsf{k}+\mathsf{k}'), \qquad -\infty < \mathsf{k},\mathsf{k}' < \infty, \quad l,l' \in \mathcal{E}, \tag{4.13}$$

again with all other commutators vanishing.

Remark 37. This realization of a RT-algebra agrees with the one used in [4, 42]. The construction (4.12) of the $a^l(-\mathsf{k})$ and $a^l(-\mathsf{k})^\star$ out of the $a^{l'}(\mathsf{k})$ and $a^{l'}(\mathsf{k})^\star$ is reminiscent of the action of the Weyl group in the root space of a Lie algebra, by which any root is obtained from the set of positive roots [14]. A different context, where a (scalar) scattering matrix appears in commutation relations, is provided in [15].

4.2. *The free Hermitian quantum field*

For reasons to become clear in a moment, in this subsection the boundary conditions (A, B) will be taken to be real. The field operator, again of dimension zero, is defined to be

$$\begin{aligned}\Phi(t,p) &= \mathrm{e}^{\mathrm{i}\mathbf{H}t}\Phi(p)\,\mathrm{e}^{-\mathrm{i}\mathbf{H}t}\\ &= \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}(\overline{\psi^l(p;\mathsf{k})}\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}a^l(\mathsf{k})^\star + \text{h.c.})\\ &\quad + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})}\frac{1}{\sqrt{2\omega(\mathsf{k})}}(\overline{\psi^{\mathsf{k},\nu}(p)}\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}a^{\mathsf{k},\nu\star} + \text{h.c.}).\end{aligned} \tag{4.14}$$

where h.c. denotes Hermitian conjugate. By construction, this field is Hermitian and $\Phi(t+s,p) = \mathrm{e}^{\mathrm{i}\mathbf{H}t}\Phi(s,p)\,\mathrm{e}^{-\mathrm{i}\mathbf{H}t}$ holds. Again we use a similar notational convention as the one used for a local description of functions on $\mathcal{G}$. Thus for its restriction to an edge j and with the local coordinate $(j,x)\, x \in [0,a_j]$ for a point p, there the field is given as

$$\Phi_j(t,x) = \begin{cases} \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}((\mathrm{e}^{\mathrm{i}\mathsf{k}x}\delta_{jl} + \overline{S(\mathsf{k})_{jl}}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x})\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\,a^l(\mathsf{k})^\star + \text{h.c.}) \\ \quad + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})}\frac{1}{\sqrt{2\omega(\mathsf{k})}}\big(\overline{s_j^{\mathsf{k},\nu}}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x}\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\,a^{\mathsf{k},\nu\star} + \text{h.c.}\big), & j\in\mathcal{E}\\ \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}((\overline{\alpha(\mathsf{k})_{jl}}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x} + \overline{\beta(\mathsf{k})_{jl}}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x})\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\,a^l(\mathsf{k})^\star + \text{h.c.}) \\ \quad + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})}\frac{1}{\sqrt{2\omega(\mathsf{k})}}\big(\big(\overline{u_j^{\mathsf{k},\nu}}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} + \overline{v_j^{\mathsf{k},\nu}}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x}\big)\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\,a^{\mathsf{k},\nu\star} + \text{h.c.}\big), & j\in\mathcal{I}.\end{cases} \tag{4.15}$$

Observe that the $\psi^{\mathsf{k},\nu}(p)$ need not be chosen real. However, the reality of the boundary conditions comes as follows into play. By corollary 18, the $\overline{\psi^l(p;\mathsf{k})}$ and the $\overline{\psi^{\mathsf{k},\nu}(p)}$ are also eigenfunctions of $-\Delta_{A,B}$. Since the boundary conditions are real, we can use lemma 20 and (4.12) to simplify the first terms in (4.15) using the RT-algebra notation and $\omega(-\mathsf{k}) = \omega(\mathsf{k})$

$$\begin{aligned}&\sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}((\mathrm{e}^{\mathrm{i}\mathsf{k}x}\delta_{jl} + \overline{S(\mathsf{k})_{jl}}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x})\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}a^l(\mathsf{k})^\star + \text{h.c.})\\ &\qquad = \int_{-\infty}^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}(\mathrm{e}^{\mathrm{i}(\mathsf{k}x+\omega(\mathsf{k})t)}a^j(\mathsf{k})^\star + \text{h.c.}), \qquad j\in\mathcal{E}\\ &\sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}((\overline{\alpha(\mathsf{k})_{jl}}\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x} + \overline{\beta(\mathsf{k})_{jl}}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x})\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}a^l(\mathsf{k})^\star + \text{h.c.})\\ &\qquad = \sum_{l\in\mathcal{E}}\int_{-\infty}^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}(\beta(-\mathsf{k})_{jl}\,\mathrm{e}^{\mathrm{i}(\mathsf{k}x+\omega(\mathsf{k})t)}a^l(\mathsf{k})^\star + \text{h.c.}), \qquad j\in\mathcal{I}.\end{aligned} \tag{4.16}$$

Let Ω denote the vacuum.

Proposition 38. *The Hermitian field Φ satisfies the Klein–Gordon equation*

$$(\Box_{A,B} + m^2)\Phi(p,t) = 0.$$

For all times t the boundary conditions

$$A\underline{\Phi}(t) + B\underline{\Phi}'(t) = 0$$

are valid in the sense of expectation values in states which are linear combinations of states of the form

$$\prod_i a(f_i)^\star\Omega$$

with $f_i \in \mathcal{D}(-\Delta_{A,B} + m^2)$.

Proof. For general boundary conditions (A, B), we recall that if ψ satisfies the boundary condition (2.3), then $\bar{\psi}$ satisfies the boundary condition $(\bar{A}, \bar{B})$. As a consequence, if the boundary conditions (A, B) are real, then both $\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\psi^l(\,;\mathsf{k})$ and $\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t}\overline{\psi^l(\,;\mathsf{k})}$ satisfy the boundary condition (2.3) for all $l \in \mathcal{E}$ and all $\mathsf{k} \in \mathbb{R}_+$ and the claim follows from the construction of Φ and the choice of the states. We omit details. □

We also introduce the conjugate field

$$\Pi(p,t) = \dot{\Phi}(p,t) = \frac{\partial}{\partial t}\Phi(p,t). \tag{4.17}$$

Using the completeness relation for the eigenfunctions of $-\Delta_{A,B}$ in the form (2.49), we derive the

Theorem 39. *For the boundary conditions (A, B), the equal time commutation relation*

$$[\Phi(p,t), \Pi(q,t)] = i\delta(p,q), \qquad p, q \in \mathcal{G} \tag{4.18}$$

is valid.

Observe that this relation fixes the normalization of the field.

4.3. The free complex quantum field

We now construct a complex field Ψ, which has the advantage of being able to carry (electric) charge. Associated is a particle with that charge and an antiparticle with the opposite charge. Accordingly the one-particle space $\mathcal{H}_1$ is chosen to be $L^2(\mathcal{G}) \oplus L^2(\mathcal{G})$, the first for a particle and the second for the corresponding antiparticle.

The one-particle Hamiltonian h on that space is chosen to be

$$h = \sqrt{-\Delta_{A,B} + m^2} \oplus 0 \, + \, 0 \oplus \sqrt{-\Delta_{\bar{A},\bar{B}} + m^2}. \tag{4.19}$$

The boundary conditions (A, B) themselves may be chosen arbitrarily. To simplify the exposition, we assume that $-\Delta_{A,B}$ and hence also $-\Delta_{\bar{A},\bar{B}}$ has no discrete spectrum, cf corollary 14. So in particular $-\Delta_{A,B} \geqslant 0$, $-\Delta_{\bar{A},\bar{B}} \geqslant 0$. Since the boundary conditions (A, B) are not necessarily real, relation (2.42) need not hold. However, $\overline{\psi(\,;\mathsf{k})}$ satisfies the boundary conditions $(\bar{A}, \bar{B})$ by lemma 13. The creation and annihilation operators for the particles are as before, see (4.2). As for the antiparticles, for $l \in \mathcal{E}$ and $\mathsf{k} > 0$, introduce operators $b^l(\mathsf{k})$ and their adjoints $b^l(\mathsf{k})^\star$ satisfying commutation relations of the same form and commuting with all $a^{l'}(\mathsf{k}')$ and $a^{l'}(\mathsf{k}')^\star$. They are the annihilation and creation operators for the antiparticle with wavefunction $\overline{\psi^l(\,;\mathsf{k})} = \overline{\psi^l_{A,B}(\,;\mathsf{k})}$, which we recall differs from $\psi^l_{\bar{A},\bar{B},\underline{a}}(\,;\mathsf{k})$. Correspondingly we set

$$b^l(-\mathsf{k}) = \sum_{l'\in\mathcal{E}} S(-\mathsf{k})_{l'l} b^{l'}(\mathsf{k}) = \sum_{l'\in\mathcal{E}} \overline{S(\mathsf{k})}_{ll'} b^{l'}(\mathsf{k})$$
$$b^l(-\mathsf{k})^\star = \sum_{l'\in\mathcal{E}} \overline{S(-\mathsf{k})}_{l'l} b^{l'}(\mathsf{k})^\star = \sum_{l'\in\mathcal{E}} S(\mathsf{k})_{ll'} b^{l'}(\mathsf{k})^\star \qquad \mathsf{k} > 0,$$

with $S(\mathsf{k}) = S_{A,B}(\mathsf{k})$. By (2.26), the interpretation is that $b^l(-\mathsf{k})^\star$ creates a particle with wavefunction $\overline{\psi^l(\,;-\mathsf{k})}$. $\mathbf{H}$, the second quantization of h as given by (4.19), is

$$\mathbf{H} = \frac{1}{2\pi}\sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{d}\mathsf{k}\;\omega(\mathsf{k}) a^l(\mathsf{k})^\star a^l(\mathsf{k}) + \frac{1}{2\pi}\sum_{l\in\mathcal{E}}\int_0^\infty \mathrm{d}\mathsf{k}\;\omega(\mathsf{k}) b^l(\mathsf{k})^\star b^l(\mathsf{k}).$$

The field Ψ and its adjoint is now given as

$$\Psi(t,p) = \mathrm{e}^{\mathrm{i}\mathbf{H}t}\Psi(p)\,\mathrm{e}^{-\mathrm{i}\mathbf{H}t} = \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}\psi^l(p;\mathsf{k})(\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t} b^l(\mathsf{k})^\star + \mathrm{e}^{-\mathrm{i}\omega(\mathsf{k})t} a^l(\mathsf{k}))$$
$$\Psi^\dagger(t,p) = \mathrm{e}^{\mathrm{i}\mathbf{H}t}\Psi^\dagger(p)\,\mathrm{e}^{-\mathrm{i}\mathbf{H}t} = \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}\overline{\psi^l(p;\mathsf{k})}(\mathrm{e}^{-\mathrm{i}\omega(\mathsf{k})t} b^l(\mathsf{k}) + \mathrm{e}^{\mathrm{i}\omega(\mathsf{k})t} a^l(\mathsf{k})^\star). \tag{4.20}$$

In local coordinates and in terms of the RT-algebra, we can write the field Ψ (and similarly its adjoint) as

$$\Psi_j(t,x) = \begin{cases} \int_{-\infty}^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}(\mathrm{e}^{\mathrm{i}(\omega(\mathsf{k})t-\mathsf{k}x)}\,b^j(\mathsf{k})^\star + \mathrm{e}^{-\mathrm{i}(\omega(\mathsf{k})t+\mathsf{k}x)}a^j(\mathsf{k})), & j\in\mathcal{E} \\ \sum_{l\in\mathcal{E}}\int_{-\infty}^\infty \frac{\mathrm{d}\mathsf{k}}{\sqrt{2\pi}}\frac{1}{\sqrt{2\omega(\mathsf{k})}}\beta_{jl}(\mathsf{k})(\mathrm{e}^{\mathrm{i}(\omega(\mathsf{k})t-\mathsf{k}x)}\,b^l(\mathsf{k})^\star + \mathrm{e}^{-\mathrm{i}(\omega(\mathsf{k})t+\mathsf{k}x)}a^l(\mathsf{k})), & j\in\mathcal{I}. \end{cases} \tag{4.21}$$

Use has been made of (2.25). The motivation for this definition of the one-particle Hilbert space for the antiparticle, the corresponding one-particle Hamiltonian and finally the field Ψ stems from

Proposition 40. *The field $\Psi(p,t)$ and its adjoint $\Psi^\dagger(p,t)$ satisfy the Klein–Gordon equation*

$$(\Box + m^2)\Psi(p,t) = 0, \qquad (\Box + m^2)\Psi^\dagger(p,t) = 0$$

and the boundary conditions

$$A\underline{\Psi}(t) + B\underline{\Psi}'(t) = 0 = \bar{A}\underline{\Psi}^\dagger(t) + \bar{B}\underline{\Psi}^{\dagger\prime}(t)$$

for all times.

As in proposition 38, the last relation holds in the sense of an expectation value in suitable states.

Let $\mathcal{C}$ denote charge conjugation, the operation which interchanges particles and antiparticles. In addition, introduce the antilinear and antiunitary time reversal map $\mathcal{T}$, cf remark 21. Then there is $\mathcal{C}\mathcal{T}$ invariance, that is

$$\mathcal{C}\mathcal{T}\Psi(p,t)(\mathcal{C}\mathcal{T})^{-1} = \Psi(p,-t) \tag{4.22}$$

holds.

4.4. The commutator function

In this subsection, we calculate the commutator of the fields. For the Hermitian field, we obtain

$$[\Phi(t,p),\Phi(s,q)] = \sum_{l\in\mathcal{E}}\int_0^\infty \frac{\mathsf{dk}}{2\pi}\frac{1}{2\omega(\mathsf{k})}(\overline{\psi^l(p;\mathsf{k})}\psi^l(q;\mathsf{k})\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})(t-s)} - \psi^l(p;\mathsf{k})\overline{\psi^l(q;\mathsf{k})}\,\mathrm{e}^{-\mathrm{i}\omega(\mathsf{k})(t-s)}) + \sum_{\mathsf{k}\in\Sigma,1\leqslant\nu\leqslant n(\mathsf{k})} \times\frac{1}{2\omega(\mathsf{k})}(\overline{\psi^{\mathsf{k},\nu}(p)}\psi^{\mathsf{k},\nu}(q)\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})(t-s)} - \psi^{\mathsf{k},\nu}(p)\overline{\psi^{\mathsf{k},\nu}(q)}\,\mathrm{e}^{-\mathrm{i}\omega(\mathsf{k})(t-s)}). \tag{4.23}$$

Since the boundary conditions are real, the reality properties

$$\sum_{l\in\mathcal{E}}\overline{\psi^l(p;\mathsf{k})}\psi^l(q;\mathsf{k}) = \sum_{l\in\mathcal{E}}\psi^l(p;\mathsf{k})\overline{\psi^l(q;\mathsf{k})}; \qquad \sum_{1\leqslant\nu\leqslant n(\mathsf{k})}\psi^{\mathsf{k},\nu}(p)\overline{\psi^{\mathsf{k},\nu}(q)} = \sum_{1\leqslant\nu\leqslant n(\mathsf{k})}\overline{\psi^{\mathsf{k},\nu}(p)}\psi^{\mathsf{k},\nu}(q) \tag{4.24}$$

hold. Indeed, the first relation is easily derived from (2.42). To prove the second one, observe that for given $\mathsf{k}\in\Sigma=\Sigma^<$, both sides give the unique integral kernel for the orthogonal projector in $L^2(\mathcal{G})$ onto the eigenspace of $-\Delta_{A,B}$ with eigenvalue $\mathsf{k}^2<0$. In fact, since the $\psi^{\mathsf{k},\nu}$ form an orthonormal basis in that space, so do their complex conjugates. Inserting the relations (4.24) into (4.23) gives the first part of the next theorem. The proof of the second part is even easier and will therefore be omitted.

Theorem 41. *The commutator for the free Hermitian field with real boundary conditions* (A,B) *is given as*

$$[\Phi(t,p),\Phi(s,q)] = -\mathrm{i}G_{A,B,m^2}(t)(p,q). \tag{4.25}$$

Similarly for the complex field and arbitrary boundary conditions (A,B), *the commutators are*

$$[\Psi(t,p),\Psi(s,q)^\dagger] = -\mathrm{i}G_{A,B,m^2}(t)(p,q), \qquad [\Psi(t,p),\Psi(s,q)] = 0. \tag{4.26}$$

The last relation of course also implies $[\Psi(t,p)^\dagger,\Psi(s,q)^\dagger]=0$. In the Minkowski space context, it is well known that (up to a sign) the Klein–Gordon kernel equals the commutator function; see e.g. [43] section 7c and (4.28) below. So in analogy to the Minkowski space context and as a consequence of finite propagation speed, we have local commutativity in the form

Corollary 42. *For space-like separated events* (t,p) *and* (s,q), *the commutators (4.30) and (4.31) vanish provided as least one of the points* p *and* q *lies in* $\mathcal{G}_{\mathrm{ext}}$.

4.5. Examples

We illustrate our discussion in the context of single vertex graphs with two simple examples. First we make the following notational convention. If p has local coordinate (i,x) and q the local coordinate (j,y) and for given (A,B) and m we set

$$G_{ij}(t,x;s,y) = G_{A,B,m^2}(t-s)(p,q). \tag{4.27}$$

Also we will need the following quantities. Let $\Delta(t, x; m)$ be the usual relativistic commutator function of mass m in 1 + 1 spacetime dimensions:

$$\Delta(t, x; m) = \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\omega(\mathrm{k})} \, \mathrm{e}^{\mathrm{ik}x} (\mathrm{e}^{-\mathrm{i}\omega(\mathrm{k})t} - \mathrm{e}^{\mathrm{i}\omega(\mathrm{k})t}) = \Delta^{(+)}(t, x; m) + \Delta^{(-)}(t, x; m) \tag{4.28}$$

$$= -\int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} \, \mathrm{e}^{\mathrm{ik}x} \frac{\sin \omega(\mathrm{k})t}{\omega(\mathrm{k})}. \tag{4.29}$$

More explicitly

$$\Delta(t, x; m) = \begin{cases} 0 & t^2 - x^2 < 0 \\ -\operatorname{sign} t \, N_0(m\sqrt{t^2 - x^2}) & t^2 - x^2 > 0. \end{cases} \tag{4.30}$$

N_0 is the zeroth Neumann function (a Bessel function of the second kind). For large argument, it satisfies

$$N_0(z) \simeq \sqrt{\frac{2}{\pi z}} \sin(z - \pi/4) \qquad \text{for} \quad 1 \ll z. \tag{4.31}$$

For a more detailed discussion of the commutator function in local coordinates and which will be needed in the proof of theorem 33 in appendix B, introduce the distribution in $0 < x, -\infty < t < \infty$

$$\begin{aligned} \mathfrak{D}(t, x; m, \kappa) &= \frac{1}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\omega(\mathrm{k})} \, \mathrm{e}^{\mathrm{ik}x} (\mathrm{e}^{-\mathrm{i}\omega(\mathrm{k})t} - \mathrm{e}^{\mathrm{i}\omega(\mathrm{k})t}) \frac{\mathrm{k} + \mathrm{i}\kappa}{\mathrm{k} - \mathrm{i}\kappa} \\ &= \mathfrak{D}^{(+)}(t, x; m, \kappa) + \mathfrak{D}^{(-)}(t, x; m, \kappa) \\ &= -\int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} \, \mathrm{e}^{\mathrm{ik}x} \frac{\sin \omega(\mathrm{k})t}{\omega(\mathrm{k})} \frac{\mathrm{k} + \mathrm{i}\kappa}{\mathrm{k} - \mathrm{i}\kappa} \end{aligned} \tag{4.32}$$

with $m > 0$ and κ real, the values $\kappa = 0, \infty$ being allowed, that is

$$\mathfrak{D}(t, x; m, \kappa = 0) = \Delta(t, x; m), \qquad \mathfrak{D}(t, x; m, \kappa = \infty) = -\Delta(t, x; m). \tag{4.33}$$

By construction $\mathfrak{D}(t, x; m, \kappa)$ is odd in t. For $\kappa \neq \infty$, write

$$\begin{aligned} \mathfrak{D}(t, x; m, \kappa) &= \Delta(t, x; m) + \mathfrak{d}(t, x; m, \kappa) \\ &= \mathfrak{D}^{(+)}(t, x; m, \kappa) + \mathfrak{D}^{(-)}(t, x; m, \kappa) \\ \mathfrak{D}^{(\pm)}(t, x; m, \kappa) &= \Delta^{(\pm)}(t, x; m) + \mathfrak{d}^{(\pm)}(t, x; m, \kappa) \end{aligned} \tag{4.34}$$

with the *bona fide* function

$$\begin{aligned} \mathfrak{d}(t, x; m, \kappa) &= \frac{2\mathrm{i}\kappa}{2\pi \mathrm{i}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\omega(\mathrm{k})} \, \mathrm{e}^{\mathrm{ik}x} (\mathrm{e}^{-\mathrm{i}\omega(\mathrm{k})t} - \mathrm{e}^{\mathrm{i}\omega(\mathrm{k})t}) \frac{1}{\mathrm{k} - \mathrm{i}\kappa} \\ &= \mathfrak{d}^{(+)}(t, x; m, \kappa) + \mathfrak{d}^{(-)}(t, x; m, \kappa) \\ &= -2\mathrm{i}\kappa \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} \, \mathrm{e}^{\mathrm{ik}x} \frac{\sin \omega(\mathrm{k})t}{\omega(\mathrm{k})} \frac{1}{\mathrm{k} - \mathrm{i}\kappa}, \end{aligned} \tag{4.35}$$

such that $\mathfrak{d}^{(-)}(t, x; m, \kappa) = -\mathfrak{d}^{(+)}(-t, x; m, \kappa) = \overline{\mathfrak{d}^{(+)}(t, x; m, \kappa)}$. It is easy to show that for given m and κ, $\mathfrak{d}^{(\pm)}$ are uniformly bounded functions of x and t and Hölder continuous in both x and t of Hölder index <1. $\mathfrak{D}^{(+)}, \mathfrak{d}^{(+)}$ and $\mathfrak{D}^{(-)}, \mathfrak{d}^{(-)}$ are positive and negative energy solutions of the usual Klein–Gordon equation, respectively:

$$\left(\partial_t^2 - \partial_x^2 + m^2\right)\mathfrak{D}^{(\pm)}(x, t; m, \kappa) = \left(\partial_t^2 - \partial_x^2 + m^2\right)\mathfrak{d}^{(\pm)}(x, t; m, \kappa) = 0.$$

Moreover, the differential equation

$$\left(\frac{\partial}{\partial x} + \kappa\right) \mathfrak{d}^{(\pm)}(x, t; m, \kappa) = -2\kappa \Delta^{(\pm)}(x, t : m) \tag{4.36}$$

holds. $\mathfrak{d}^{(\pm)}(t, x; m, \kappa)$ decays at least like $|t|^{-1/2}$ for large t and fixed x. This is well known from the theory of Haag–Ruelle scattering theory, see e.g. [16, 20]. Sufficient conditions for stronger decay are also well known but do not apply here. When $0 < x < |t|$, the *stationary phase approximation* gives

$$\mathfrak{d}^{(\pm)}(t, x; m, \kappa) \cong (1 - v^2)^{-1/4} \frac{\kappa}{\pm\frac{mv}{\sqrt{1-v^2}} - \mathrm{i}\kappa} \, \mathrm{e}^{\mp(\phi(x,t)+\mathrm{i}\frac{\pi}{4}\operatorname{sign} t)} \frac{1}{\sqrt{2\pi m|t|}}, \tag{4.37}$$

with $v = x/t$ and $\phi(x, t) = m\sqrt{1 - v^2}\, t$. As a function of t and for fixed x, the $t^{-1/2}$ decay as well as the oscillations are visible in numerical computations of $\mathfrak{d}^{(\pm)}$.

Example 43. (The half-line with Robin boundary conditions at the origin). View the positive real axis $\mathbb{R}_+$ as a single vertex graph with one external edge, $|\mathcal{E}| = 1$. All possible boundary conditions at the origin giving rise to self-adjoint copulations are the Robin boundary conditions and which are real

$$\cos\tau\,\psi(0) + \sin\tau\,\psi'(0) = 0, \qquad 0 \leqslant \tau < \pi. \tag{4.38}$$

They interpolate between Dirichlet ($\sin\tau = 0$) and Normans ($\cos\tau = 0$) boundary conditions.

Denote the resulting Laplace operator by $-\Delta_\tau$. The scattering matrix is now just a function

$$S_\tau(\mathsf{k}) = -\frac{\cos\tau - \mathrm{i}\mathsf{k}\sin\tau}{\cos\tau + \mathrm{i}\mathsf{k}\sin\tau} \tag{4.39}$$

satisfying $S_\tau(-\mathsf{k}) = S_\tau(\mathsf{k})^{-1}$ for $\mathsf{k} \in \mathbb{C}$ and being of modulus 1 for $\mathsf{k} \in \mathbb{R}\backslash\{0\}$, as it should. There is a pole of $S_\tau(\mathsf{k})$ at $\mathsf{k} = \mathrm{i}\cot\tau$. So for $\cot\tau < 0$, this pole lies in the lower k-half-plane *(the second physical sheet)*. Then there is no bound state and $-\Delta_\tau \geqslant 0$. Conversely $\cot\tau > 0$ gives rise to a pole of $S(\mathsf{k})$ in the upper half-plane at $\mathsf{k} = \mathrm{i}\cot\tau$ and correspondingly there is one bound state with (normalized and real) bound state wavefunction

$$\psi_{b,\tau}(x) = \sqrt{2\cot\tau}\,\mathrm{e}^{-\cot\tau\, x} \tag{4.40}$$

and with bound state energy

$$\varepsilon_\tau = -\cot^2\tau < 0. \tag{4.41}$$

As a consequence $-\Delta_\tau \geqslant \varepsilon_b$. Observe that $S_\tau(\mathsf{k})$ is real on the imaginary axis, as should be by remark 12. Note also the agreement with lemma 2 and proposition 1. In fact, in the present case, $AB^\dagger = \cos\tau\sin\tau = \cot\tau\sin^2\tau$.

By our general discussion, the improper eigenfunctions in this example are given as

$$\psi_\tau(x; \mathsf{k}) = \mathrm{e}^{-\mathrm{i}\mathsf{k}x} + S_\tau(\mathsf{k})\,\mathrm{e}^{\mathrm{i}\mathsf{k}x}, \qquad \mathsf{k} > 0. \tag{4.42}$$

This set is complete if $\cot\tau < 0$ while for $\cot\tau > 0$ this set combined with the bound state wavefunction (4.40) forms a complete set. For finite $\cot\tau \neq 0$ and with the condition $m > \max(0, \cot\tau)$, such that $\omega(\mathrm{i}\cot\tau) > 0$ for the mass, we obtain $(0 < x, y)$

$$\begin{aligned} G(t, x; s, y) = {} & -\Delta(t - s, x - y; m) - \Delta(t - s, x + y; m) - \mathfrak{d}(t - s, x + y; m, \cot\tau) \\ & + \Theta(\cot\tau)2\cot\tau\frac{\sin(\omega(\mathrm{i}\cot\tau)\cdot(t - s))}{\omega(\mathrm{i}\cot\tau)}\,\mathrm{e}^{-\cot\tau(x+y)}. \end{aligned} \tag{4.43}$$

Θ is the Heaviside step function.

This example also provides a nice illustration to a long standing problem, namely to what extent the scattering matrix is determined by the cross section [10, 18, 33, 34, 35, 39]. Define the scattering amplitude $T_\tau(\mathsf{k})$ by $S_\tau(\mathsf{k}) = 1 + 2\mathrm{i}\,T_\tau(\mathsf{k})$, that is

$$T_\tau(\mathsf{k}) = -\mathrm{i}\frac{\cos\tau}{\cos\tau + \mathrm{i}\mathsf{k}\sin\tau}. \tag{4.44}$$

The knowledge of $|T_\tau(\mathsf{k})|^2$ for all $\mathsf{k} > 0$ only fixes $\sin^2\tau$. An additional information, namely whether there is a bound state or not, is needed to fix τ itself. A way to overcome this dilemma and to solve this inverse problem in the present context of quantum graphs has been proposed in [28].

The next example is the single vertex graph with two external lines which may also be viewed as the real line with the origin as a distinguished point. As boundary conditions we take the the one describing the δ-potential of strength λ at the origin. This is a very popular model for describing a pointlike impurity.

Example 44. (The single vertex graph with two external edges ($n = |\mathcal{E}| = 2$) and with a boundary condition describing the δ-potential on the line)

The graph is obtained by considering two copies of $\mathbb{R}_+$ with their origins identified. The real boundary conditions are given as

$$A = \begin{pmatrix} 1 & -1 \\ 0 & \lambda \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}.$$

The choices $\lambda < 0$ and $\lambda > 0$ describe an attractive and a repulsive δ-potential on $\mathbb{R}$, respectively.

The resulting on-shell scattering matrix is a symmetric 2×2 matrix

$$S_\lambda(\mathsf{k}) = \frac{1}{2\mathsf{k} + \mathrm{i}\lambda}\begin{pmatrix} -\mathrm{i}\lambda & 2\mathsf{k} \\ 2\mathsf{k} & -\mathrm{i}\lambda \end{pmatrix} = \frac{2\mathsf{k} - \mathrm{i}\lambda}{2\mathsf{k} + \mathrm{i}\lambda}\,\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \tag{4.45}$$

The second expression gives the spectral decomposition (2.50) of the scattering matrix for this example, that is $P^0 = 0$ and

$$P^{-\lambda/2} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \qquad P^\infty = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}. \tag{4.46}$$

It has the additional symmetry

$$S_\lambda(\mathsf{k}) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} S_\lambda(\mathsf{k}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.47}$$

describing invariance of the boundary conditions under the interchange of the two edges. Using local coordinates, we arrange the components $\psi_j^l(x; \mathsf{k})$ $(j, l = 1, 2; x > 0)$ of the two improper eigenfunctions $\psi^l(\,;\mathsf{k})$ as a 2×2 matrix

$$\begin{pmatrix} \mathrm{e}^{-\mathrm{i}\mathsf{k}x} - \frac{\mathrm{i}\lambda}{2\mathsf{k}+\mathrm{i}\lambda}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} & \frac{2\mathsf{k}}{2\mathsf{k}+\mathrm{i}\lambda}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} \\ \frac{2\mathsf{k}}{2\mathsf{k}+\mathrm{i}\lambda}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} & \mathrm{e}^{-\mathrm{i}\mathsf{k}x} - \frac{\mathrm{i}\lambda}{2\mathsf{k}+\mathrm{i}\lambda}\,\mathrm{e}^{\mathrm{i}\mathsf{k}x} \end{pmatrix}.$$

Like the S-matrix, this matrix is symmetric, reflecting the parity invariance of the δ-potential. Also ordinary plane waves appear when $\lambda = 0$, as they should. The relation (2.26) is easily verified. In the attractive case $\lambda < 0$, there is a bound state with bound state energy $\epsilon_\lambda = -\lambda^2/4$. The two local components of the bound state wavefunction are both of the form

$$\psi_j(x) = \sqrt{-\frac{\lambda}{2}}\,\mathrm{e}^{\frac{\lambda x}{2}} \qquad j = 1, 2. \tag{4.48}$$

Observe that

$$AB^\dagger = \begin{pmatrix} 0 & 0 \\ 0 & \lambda \end{pmatrix}$$

and recall again lemma 2 and proposition 1 concerning the number of bound states.

With the notational convention (4.27), G_{A,B,m^2} in local coordinates can be written as a 2×2 matrix in the form, see (B.2),

$$\begin{aligned} G(t,x;s,y) = &-\Delta(t-s,x-y;m)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} - \Delta(t-s,x+y;m)\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\\ &-\mathfrak{d}(t-s,x+y;m,-\lambda/2)\,\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}\\ &+\Theta(-\lambda)(-\lambda)\frac{\sin(\omega(-\mathrm{i}\lambda/2)(t-s))}{\omega(-\mathrm{i}\lambda/2)}\,\mathrm{e}^{\frac{\lambda(x+y)}{2}}\,\frac{1}{2}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix}. \end{aligned} \tag{4.49}$$

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Appendix A. Proof of relation (2.17)

The general idea of proof follows a familiar route; see, e.g. [46]. However, the boundary conditions defining the Laplacian enter in a simple but crucial way, which warrant a more detailed discussion. In addition, the regularity of the scattering matrix $S(\mathsf{k})$ for $\mathsf{k} > 0$ away from $\Sigma^{>}$ will be used. For given $R > 0$, let $\mathcal{G}_R$ be the set obtained from $\mathcal{G}$ by deleting from any external edge e all points with distance larger than R from its initial vertex v_e. On each edge e we introduce an extra vertex at distance R from v_e denoted by $v_{e,R}$. Obviously $\mathcal{G}_R$ is a compact graph and a closed subset of $\mathcal{G}$. In particular $\mathcal{G}_R$ has no external edges and hence is compact. The set of vertices of $\mathcal{G}_R$ is given as

$$\mathcal{V}_{\mathcal{G}_R} = \mathcal{V} \cup \{v_{e,R}\}_{e\in\mathcal{E}}.$$

In other words, $\mathcal{G}_R$ is obtained from $\mathcal{G}$ by removing the external edges $e \in \mathcal{E}$, each isomorphic to the half-line $[0,\infty)$ and replacing each of them by a closed interval of the form $[0, R]$, where the vertex $v_e = \partial(e)$ corresponds to $0 \in [0, R]$ and the new vertex $v_{e,R}$ to $R \in [0, R]$. Correspondingly there is a Hilbert space $L^2(\mathcal{G}_R)$ with the scalar product denoted by $\langle\, ,\, \rangle_R$. By restriction, any function f on $\mathcal{G}$ defines a function on $\mathcal{G}_R$ also denoted by f. In this way, any element in $L^2(\mathcal{G})$ defines an element in $L^2(\mathcal{G}_R)$ and

$$\lim_{R\to\infty}\langle f, g\rangle_R = \langle f, g\rangle$$

clearly holds for any $f, g \in L^2(\mathcal{G})$. As for the claim (2.17), the functions $\psi^l(\,;\mathsf{k})$ are elements in each $L^2(\mathcal{G}_R)$ but not of $L^2(\mathcal{G})$, as already mentioned. Now we write

$$\langle\psi^l(;\mathsf{k}),\psi^{l'}(;\mathsf{k}')\rangle_R = -\frac{1}{\mathsf{k}^2-\mathsf{k}'^2}(\langle\Delta_{A,B}\psi^l(;\mathsf{k}),\psi^{l'}(;\mathsf{k}')\rangle_R - \langle\psi^l(;\mathsf{k}),\Delta_{A,B}\psi^{l'}(;\mathsf{k}')\rangle_R)$$

and perform a partial integration. Since the functions $\psi^l(\,;\mathsf{k})$ satisfy the boundary conditions, what remains are only contributions from $\psi^l(\,;\mathsf{k})$ and its first derivative at the vertices $v_{e,R}$. We now observe

$$\begin{aligned} \psi^l(v_{e,R};\mathsf{k}) &= \psi^l_e(x=R;\mathsf{k}) = \mathrm{e}^{-\mathrm{i}R\mathsf{k}}\delta_{le} + S(\mathsf{k})_{el}\,\mathrm{e}^{\mathrm{i}R\mathsf{k}}\\ \frac{\mathrm{d}}{\mathrm{d}x}\psi^l(v_{e,R};\mathsf{k}) &= \frac{\mathrm{d}}{\mathrm{d}x}\psi^l_e(x=R;\mathsf{k}) = -\mathrm{i}\mathsf{k}\,\mathrm{e}^{-\mathrm{i}R\mathsf{k}}\delta_{le} + \mathrm{i}\mathsf{k}S(\mathsf{k})_{el}\,\mathrm{e}^{\mathrm{i}R\mathsf{k}} \end{aligned}$$

and obtain

$$\begin{aligned}\langle\psi^{l}(;\mathsf{k}),\psi^{l'}(;\mathsf{k}')\rangle_R &= -\frac{1}{\mathsf{k}^2-\mathsf{k}'^2}\sum_{e\in\mathcal{E}}((\mathrm{i}\mathsf{k}\,\mathrm{e}^{\mathrm{i}R\mathsf{k}}\delta_{le}-\mathrm{i}\mathsf{k}\overline{S(\mathsf{k})_{el}}\,\mathrm{e}^{-\mathrm{i}R\mathsf{k}})(\mathrm{e}^{-\mathrm{i}R\mathsf{k}'}\delta_{l'e}+S(\mathsf{k}')_{el'}\,\mathrm{e}^{\mathrm{i}R\mathsf{k}'})\\ &\quad-(\mathrm{e}^{\mathrm{i}R\mathsf{k}}\delta_{le}+\overline{S(\mathsf{k})_{el}}\,\mathrm{e}^{-\mathrm{i}R\mathsf{k}})(-\mathrm{i}\mathsf{k}'\,\mathrm{e}^{-\mathrm{i}R\mathsf{k}'}\delta_{l'e}+\mathrm{i}\mathsf{k}'S(\mathsf{k}')_{el'}\,\mathrm{e}^{\mathrm{i}R\mathsf{k}'}))\\ &= -\frac{\mathrm{i}}{\mathsf{k}-\mathsf{k}'}\left(\mathrm{e}^{\mathrm{i}R(\mathsf{k}-\mathsf{k}')}\delta_{ll'}-\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}S(\mathsf{k}')_{el'}\mathrm{e}^{-\mathrm{i}R(\mathsf{k}-\mathsf{k}')}\right)\\ &\quad+\frac{\mathrm{i}}{\mathsf{k}+\mathsf{k}'}(\overline{S(\mathsf{k})_{l'l}}\,\mathrm{e}^{-\mathrm{i}R(\mathsf{k}+\mathsf{k}')}+S(\mathsf{k}')_{ll'}\,\mathrm{e}^{\mathrm{i}R(\mathsf{k}+\mathsf{k}')}).\end{aligned}$$

Since $\mathsf{k}+\mathsf{k}'>0$, the second term on the r.h.s. vanishes for $R\to\infty$ in the sense of distributions by the Riemann–Lebesgue lemma. As for the first term, write

$$\begin{aligned}&-\frac{\mathrm{i}}{\mathsf{k}-\mathsf{k}'}\left(\mathrm{e}^{\mathrm{i}R(\mathsf{k}-\mathsf{k}')}\delta_{ll'}-\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}S(\mathsf{k}')_{el'}\,\mathrm{e}^{-\mathrm{i}R(\mathsf{k}-\mathsf{k}')}\right)\\ &\qquad=2\frac{\sin R(\mathsf{k}-\mathsf{k}')}{\mathsf{k}-\mathsf{k}'}\delta_{ll'}-\frac{\mathrm{i}}{\mathsf{k}-\mathsf{k}'}\left(\delta_{ll'}-\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}S(\mathsf{k}')_{el'}\right)\mathrm{e}^{-\mathrm{i}R(\mathsf{k}-\mathsf{k}')}.\end{aligned}\tag{A.1}$$

Here the first term converges in the sense of distributions to $2\pi\delta(\mathsf{k}-\mathsf{k}')\delta_{ll'}$ as $R\to\infty$. As for the second term, we use the unitarity of $S(\mathsf{k})$ to write

$$\delta_{ll'}-\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}S(\mathsf{k}')_{el'}=\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}(S(\mathsf{k})_{el'}-S(\mathsf{k}')_{el'}).$$

By corollary 8, all matrix elements of $S(\mathsf{k})$ are differentiable functions of $\mathsf{k}\in\mathbb{R}_+\backslash\Sigma^>$. Since all matrix elements also are bounded by 1 due to unitarity, we have the estimate

$$|S(\mathsf{k})_{ll'}-S(\mathsf{k}')_{ll'}|\leqslant\text{const}\cdot|\mathsf{k}-\mathsf{k}'|,\qquad \mathsf{k},\mathsf{k}'\in\mathbb{R}_+\backslash\Sigma^>,\qquad l,l'\in\mathcal{E},$$

whenever $|\mathsf{k}-\mathsf{k}'|$ is small. Observe that $\mathbb{R}_+\backslash\Sigma^>$ is a union of open, pairwise disjoint intervals. This gives the estimate

$$\frac{|\delta_{ll'}-\sum_{e\in\mathcal{E}}\overline{S(\mathsf{k})_{el}}S(\mathsf{k}')_{el'}|}{|\mathsf{k}-\mathsf{k}'|}\leqslant\text{const},\qquad \mathsf{k},\mathsf{k}'\in\mathbb{R}_+\backslash\Sigma^>,\qquad l,l'\in\mathcal{E},$$

again whenever $|\mathsf{k}-\mathsf{k}'|$ is small. Therefore and again by the Riemann–Lebesgue lemma the second term in (A.1) tends to zero as $R\to\infty$.

Appendix B. Proof of theorem 33

B.1. Proof of theorem 33 in the single vertex case

In the single vertex case, besides a proof of the theorem, in this appendix we will provide a detailed analysis of the Klein–Gordon kernel when written in local coordinates, see the convention (4.27). We obtain

$$\begin{aligned}G_{ij}(t,x;s,y)&=-\Delta(t-s,x-y;m)\delta_{ij}+\int_{-\infty}^{\infty}\frac{\mathrm{d}\mathsf{k}}{2\pi}S(\mathsf{k})_{ij}\,\mathrm{e}^{\mathrm{i}\mathsf{k}(x+y)}\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}\\ &\quad+\sum_{0<\kappa\in\mathfrak{I}_0}2\kappa P_{ij}^{\kappa}\,\mathrm{e}^{-\kappa(x+y)}\frac{\sin(\omega(\mathrm{i}\kappa)(t-s))}{\omega(\mathrm{i}\kappa)},\end{aligned}\tag{B.1}$$

where we used corollary 17 and relations (2.55), (2.59) and (2.60). Recall also the convention (3.15) for the case $m=0$. We can rewrite this as

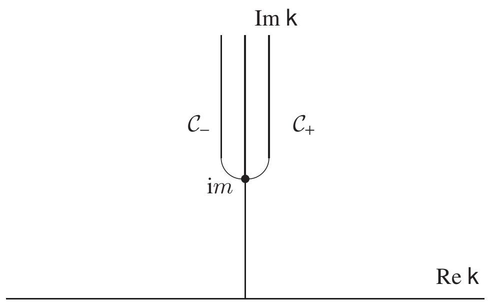

Figure B1. The upper k-half-plane with a cut from im to i∞ for the function $\omega(\mathsf{k})$. $\mathcal{C}_\pm$ form the lips of the cut.

$$\begin{aligned} G_{ij}(t,x;s,y) &= -\Delta(t-s,x-y;m)\delta_{ij} - \Delta(t-s,x+y;m)\big(\delta_{ij} - 2P^{\infty}_{ij}\big) \\ &\quad - \sum_{\infty\neq\kappa\in\mathfrak{I}} \mathfrak{d}(t-s,x+y;m,\kappa)P^{\kappa}_{jl} \\ &\quad + \sum_{0<\kappa\in\mathfrak{I}_0} 2\kappa P^{\kappa}_{jl}\,\mathrm{e}^{-\kappa(x+y)}\frac{\sin(\omega(\mathrm{i}\kappa)(t-s))}{\omega(\mathrm{i}\kappa)}. \end{aligned} \tag{B.2}$$

Note that P^{∞} may be the zero matrix. We shall use the representation (B.1) to prove the theorem.

For the single vertex graph, the distance between two points p and q with local coordinates (i,x) and (j,y) is

$$d(p,q) = d((i,x),(j,y)) = \begin{cases} |x-y| & i=j \\ x+y & i\neq j. \end{cases} \tag{B.3}$$

As a consequence, the first term on the r.h.s. of (B.1) vanishes for space-like separations, a well-known property of the relativistic commutator function. As for the integral in (B.1), insert the relation (2.50). We observe that $d((i,x),(j,y)) \leqslant x+y$ is always valid, so for space-like separations $x+y>|t-s|$ holds and thus we can deform the integral from $-\infty$ to $+\infty$ to the integral from $-\infty+\mathrm{i}\rho$ to $+\infty+\mathrm{i}\rho$ for arbitrary $\rho>0$. Indeed, by the analyticity of the first function in (3.14) we can apply Cauchy's theorem. During this deformation, we pick up a residue at each of the poles $\mathsf{k}=\mathrm{i}\kappa$ with $0<\kappa<\rho$. Each such term, however, is compensated by the corresponding term in the sum in (B.1). When we let $\rho\to+\infty$, we claim that the integral from $-\infty+\mathrm{i}\rho$ to $+\infty+\mathrm{i}\rho$ vanishes. To see this,view the function $\mathsf{k}\mapsto\omega(\mathsf{k})$ as analytic in the cut (open) upper k-half-plane with a cut from im to i∞, see figure B1. In this cut upper k-half-plane, the estimate $\operatorname{Im}\omega(\mathsf{k})\leqslant\operatorname{Im}\mathsf{k}$ holds.

Moreover both functions

$$\frac{1}{2\mathrm{i}\omega(\mathsf{k})}\,\mathrm{e}^{\mathrm{i}\omega(\mathsf{k})(t-s)}, \qquad -\frac{1}{2\mathrm{i}\omega(\mathsf{k})}\,\mathrm{e}^{-\mathrm{i}\omega(\mathsf{k})(t-s)} \tag{B.4}$$

are also analytic there and their sum equals

$$\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}$$

there. Furthermore, this sum has no discontinuity across the cut, as it should since it is entirely analytic. Indeed, replace k by the variable $m\leqslant\lambda<\infty$ via $\mathsf{k}=\mathrm{i}\lambda-\epsilon$ on the left lip $\mathcal{C}_-$ and $\mathsf{k}=\mathrm{i}\lambda+\epsilon$ on the right lip $\mathcal{C}_+$ with $\epsilon>0$. But on the left lip,

$$\lim_{\epsilon\downarrow 0}\omega(\mathrm{i}\lambda-\epsilon) = \sqrt{\lambda^2-m^2}$$

while on the right lip

$$\lim_{\epsilon\downarrow 0}\omega(\mathrm{i}\lambda+\epsilon)=-\sqrt{\lambda^2-m^2}.$$

Using $\mathrm{Im}\,\omega(\mathsf{k})\leqslant \mathrm{Im}\,\mathsf{k}$ for k in the upper half-plane, we can therefore estimate

$$\left|\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}\right|\leqslant\frac{\mathrm{e}^{\mathrm{Im}\mathsf{k}|t-s|}}{|\omega(\mathsf{k})|}. \tag{B.5}$$

in the upper half-plane and which combined with

$$|\mathrm{e}^{\mathrm{i}\mathsf{k}(x+y)}|=\mathrm{e}^{-\mathrm{Im}\mathsf{k}(x+y)}$$

proves the claim. This concludes the proof of theorem 33 when the graph is a single vertex graph. Observe that we have actually proved

$$G_{ij}(t,x;s,y)=-\Delta(t-s,x-y;m)\delta_{ij}\qquad\text{when}\quad x+y>|t-s|. \tag{B.6}$$

(B.2) compares with (B.6), valid when $x+y>|t-s|$. If at least one of the points p and q is far away from the vertex, that is $x\gg 1$ or $y\gg 1$, then the last term on the r.h.s. of (B.2) becomes exponentially small, uniformly for all times t and s. To sum up, as far as commutators are concerned and by comparison with (4.30), the contribution from $\mathfrak{d}$ in (B.2) compares with the two preceding terms there.

Remark 45. We observe from the proof that in the single vertex case, the bound state contributions in the definition of the fields are necessary in order to obtain locality. A somewhat similar observation was made in the context of integrable models in quantum field theory [21]. There it was observed that bound state contributions in the form factors of the sine–Gordon model were crucial for determining the wavefunction renormalization constant. Moreover, in the articles [2, 41], local commutation relations for certain integrable models were established, see in particular relation (54) in [2], for which also contributions from bound states are relevant.

B.2. Proof of theorem 3 for an arbitrary graph when $\Sigma=\varnothing$

We turn to the case of an arbitrary graph with the spectral assumption $\Sigma=\varnothing$ for the Laplacian $-\Delta_{A,B}$, that is with the assumption that there are no bound states. In local coordinates

$$G_{ij}(t,x;s,y)$$
$$=\begin{cases}-\Delta(t-s,x-y;m)\delta_{ij}+\displaystyle\int_{-\infty}^{\infty}\frac{\mathrm{dk}}{2\pi}S(\mathsf{k})_{ij}\,\mathrm{e}^{\mathrm{i}\mathsf{k}(x+y)}\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})} & \text{for}\quad i,j\in\mathcal{E}\\ \displaystyle\int_{-\infty}^{\infty}\frac{\mathrm{dk}}{2\pi}(\alpha(\mathsf{k})_{ij}\,\mathrm{e}^{\mathrm{i}\mathsf{k}(x+y)}+\beta(\mathsf{k})_{ij}\,\mathrm{e}^{\mathrm{i}\mathsf{k}(-x+y)})\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})} & \text{for}\quad i\in\mathcal{I},j\in\mathcal{E}\\ \displaystyle\int_{-\infty}^{\infty}\frac{\mathrm{dk}}{2\pi}((\alpha_{A,B}(\mathsf{k})\,\mathrm{e}^{\mathrm{i}\mathsf{k}x}+\beta_{A,B}(\mathsf{k})\,\mathrm{e}^{-\mathrm{i}\mathsf{k}x})\beta_{\bar{A},\bar{B}}(-\mathsf{k})^T)_{ij}\,\mathrm{e}^{\mathrm{i}\mathsf{k}y}\frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})} & \\ \quad\text{for}\quad i,j\in\mathcal{I}.\end{cases} \tag{B.7}$$

Relation (2.23) has been used for the case $i,j\in\mathcal{E}$, corollary 11 for the case $i\in\mathcal{I}$, $j\in\mathcal{E}$. Lemma 11 and corollary 16 have been used for the case $i,j\in\mathcal{I}$. Consider first the case $j,l\in\mathcal{E}$. The first term, the relativistic commutator function, has already been dealt with and vanishes for space-like separations. As for the integral we insert the path space expansion (2.72) for the scattering matrix to obtain the representation

$$\sum_{\mathbf{w}\in\mathcal{W}_{ij}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} S(\mathbf{w};\mathsf{k})_{ij}\, \mathrm{e}^{\mathrm{ik}(x+y+|\mathbf{w}|)} \frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}. \tag{B.8}$$

Here and in what follows, we will freely interchange summation and integration. This is permitted as can be shown with help of proposition 5.6 in [31] and where one allows the lengths a_i of the internal edges become complex with a positive imaginary part. We omit details.

For events, which are space-like separated, $x + y + |\mathbf{w}| \geqslant d((i, x), (j, y)) > |t - s|$ is valid for any $\mathbf{w} \in \mathcal{W}_{ij}$ whenever $i, j \in \mathcal{E}$. Also by lemma 2, the assumption $\Sigma = \varnothing$ implies $AB^\dagger \leqslant 0$ which in turn implies that $A(v)B(v)^\dagger \leqslant 0$ holds for all vertices v by lemma 3. This in turn implies that each $S(v;\mathsf{k})$, which is of the form $-(A(v) + \mathrm{i}\mathsf{k}B(v))^{-1}(A(v) - \mathrm{i}\mathsf{k}B(v))$, has no poles and and hence is analytic in the upper half-plane and polynomially bounded there, again by lemma 2. As a consequence each $S(\mathbf{w};\mathsf{k})_{jl}$ is analytic in the upper half-plane and polynomially bounded. These considerations again allow us to make a deformation of the integration over k in (B.8) from the real axis $(-\infty, +\infty)$ to the parallel line $(-\infty+\mathrm{i}\rho, +\infty+\mathrm{i}\rho)$. Combining the estimate (B.5) with

$$|\mathrm{e}^{\mathrm{ik}(x+y+|\mathbf{w}|)}| = \mathrm{e}^{-\mathrm{Im}\mathsf{k}((x+y+|\mathbf{w}|)}$$

and the polynomial bound of each $S(\mathbf{w};\mathsf{k})_{jl}$ in the limit $\rho \to +\infty$, we obtain a vanishing contribution. In other words, each summand in (B.8) vanishes. This concludes our discussion of the case $i, j \in \mathcal{E}$.

We turn to the case $i \in \mathcal{I}$ and $j \in \mathcal{E}$ and discuss the integral involving the $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ amplitudes separately. By the walk expansion (2.74),

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} \alpha(\mathsf{k})_{ij}\, \mathrm{e}^{\mathrm{ik}(x+y)} \frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})} \\ = \sum_{\mathbf{w}\in\mathcal{W}^-_{ij}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} S(\mathbf{w};\mathsf{k})_{ij}\, \mathrm{e}^{\mathrm{ik}(x+|\mathbf{w}|+y)} \frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}\end{aligned} \tag{B.9}$$

and we observe that $d((j, x), (l, y)) \leqslant x + |\mathbf{w}| + y$, holds for all $\mathbf{w} \in \mathcal{W}^-_{jl}$, see (2.66). Hence for space-like separation and for each summand we can again deform the integration contour to $(-\infty + \mathrm{i}\rho, +\infty + \mathrm{i}\rho)$ and thus this expression then vanishes when $\rho \to \infty$. As for the term containing the amplitude $\beta(\mathsf{k})$, again the walk expansion gives

$$\begin{aligned}\int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} \beta(\mathsf{k})_{ij}\, \mathrm{e}^{\mathrm{ik}(-x+y)} \frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})} \\ = \sum_{\mathbf{w}\in\mathcal{W}^+_{ij}} \int_{-\infty}^{\infty} \frac{\mathrm{dk}}{2\pi} S(\mathbf{w};\mathsf{k})_{ij}\, \mathrm{e}^{\mathrm{ik}(a_i-x+|\mathbf{w}|+y)} \frac{\sin(\omega(\mathsf{k})(t-s))}{\omega(\mathsf{k})}.\end{aligned} \tag{B.10}$$

Now $d((j, x), (l, y)) \leqslant a_i - x + |\mathbf{w}| + y$ holds for all $\mathbf{w} \in \mathcal{W}^+_{ij}$, cf again (2.66), and the previous arguments can again be applied.

In the case $j, l \in \mathcal{I}$, the arguments just used do not work. This is the reason why we have been unable to establish finite propagation speed inside the graph, that is in $\mathcal{G}_{\mathrm{int}}$. Indeed, now the contour deformation into the upper k-half-plane cannot be carried out, since $\beta_{\tilde{A},\tilde{B}}(-\mathsf{k})$ will have poles in the upper half-plane. Also the walk representation of $\beta_{\tilde{A},\tilde{B}}(-\mathsf{k})$ for $\mathsf{k} > 0$ does not have the form needed to invoke the arguments we have used so far.

Remark 46. The reason we had to impose the condition $\Sigma = \varnothing$ for a general graph is that in the presence of bound states we do not (yet) have sufficient control over the matrix valued functions $S(\mathsf{k})$, $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ at the poles. Recall that in the single vertex case, we had proposition 26 at our disposal. However, we expect Einstein causality still to be valid without this condition.

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