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Direct computation of scattering matrices for general quantum graphs

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Abstract

We present a direct and simple method for the computation of the total scattering matrix of an arbitrary finite noncompact connected quantum graph given its metric structure and local scattering data at each vertex. The method is inspired by the formalism of Reflection–Transmission algebras and quantum field theory on graphs though the results hold independently of this formalism. It yields a simple and direct algebraic derivation of the formula for the total scattering and has a number of advantages compared to existing recursive methods. The case of loops (or tadpoles) is easily incorporated in our method. This provides an extension of recent similar results obtained in a completely different way in the context of abstract graph theory. It also allows us to discuss briefly the inverse scattering problem in the presence of loops using an explicit example to show that the solution is not unique in general. On top of being conceptually very easy, the computational advantage of the method is illustrated on two examples of “three-dimensional” graphs (tetrahedron and cube) for which other methods are rather heavy or even impractical. © 2009 Elsevier B.V. All rights reserved.

1. Introduction

Excitement in the study of systems on quantum graphs has been revived recently as they provide models for the study of transport properties in quantum wires connected through junctions.

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It is largely motivated by the range of different physical applications that can be linked to such models, starting from condensed matter experiments or atomic wires up to chaos and neural networks, for reviews, see *e.g.* [1,2].

A powerful formalism in this respect is that of quantum fields theory on graphs combined with bosonization techniques. One of the central objects in this approach is the total scattering matrix of the graph and the knowledge of its analytic structure. A number of results are already available in [3–6] but essentially for star graphs. Results that apply to more general graphs can be found in [7–12] where spectral properties of the one-dimensional Laplace operator are studied to obtain general information (and/or construction) of the total scattering matrix. A purely algebraic approach (based on RT algebras [13,14]) for general graphs has been presented in [15], but it uses a rather heavy recursive construction, preventing its possible use for the construction of quantum interacting fields on a graph.

The goal of this paper is to provide an efficient and simple technique to compute this matrix for an arbitrary finite noncompact connected quantum graph knowing only its metric structure and local scattering data at each vertex. The point of view taken here is that the complete graph is obtained by assembling star graphs (single vertex graphs with a certain number of edges) which are well-understood. We obtain an explicit formula for the total scattering matrix. It turns out that our results hold beyond the context of quantum field theory on graphs. Not only do they represent an extension of recent results [10] to the case of graphs with loops but our method also provides a direct (as opposed to recursive [15]) and simple derivation, involving not more than basic linear algebra.

The paper is organised as follows. In Section 2 we present our formalism to compute directly the scattering matrix associated to a general quantum graph without loop. Once the notation is settled, the calculation is very simple and effective. In the next section, we show how to extend the techniques to graphs with loops. Then, in Section 4, we illustrate the techniques in computing the scattering matrix for graphs corresponding to Platonic solids, the cases of tetrahedron and cube being treated in great details. Finally, the last section is devoted to a short conclusion on possible applications.

2. General setting and results

We consider a finite noncompact graph with N vertices that we label with $\alpha = 1, \dots, N$ and with internal and external edges. The graph is compact if it has no external edges. At each vertex α are attached possibly several edges. One can endow the graph with a metric structure: the *external edges* are associated to infinite half-lines and are connected to a unique vertex; the *internal edges* are associated to intervals of finite length and connect two vertices, possibly not distinct. In the case where an internal edge connects the same vertex, we call it a loop (also called tadpole in the literature). Two edges are adjacent if they are connected by an internal edge. We consider a connected graph *i.e.* a graph such that for any two vertices α, β there is a sequence $\{\alpha_1 = \alpha, \alpha_2, \dots, \alpha_q = \beta\}$ of adjacent vertices. We define an orientation on the edges, and in the case of internal edges, $(\alpha\beta)$ will define an edge with orientation from vertex α to vertex β . By convention, external edges $(\alpha 0)$ are always oriented from the vertex to infinity. On each of these edges, we attach *modes* (of fields living on the edge)

$$a_j^{\alpha\beta}(p), \quad j = 1, \dots, N_{\alpha\beta}; \quad \beta = 0, 1, \dots, N; \quad \alpha = 1, \dots, N; \quad \alpha \neq \beta,$$

p being an orientation dependent parameter which has the interpretation of a momentum or a rapidity in applications to quantum fields on graphs and with the following conventions:

- $\alpha = 1, 2, \dots, N$ denotes the vertex to which the edge is attached;
- $\beta = 0, 1, 2, \dots, N$ denotes the vertex linked to α by the edge under consideration, with the convention that external edges corresponds to $\beta = 0$;
- $j = 1, \dots, N_{\alpha\beta}$ numbers the different edges between α and β , $N_{\alpha\beta}$ being their total number. We set $N_{\alpha\beta} = 0$ if α is not connected to β .

In this way the ordered triplet (α, β, j) uniquely defines all the oriented edges of the graph. Obviously, (α, β, j) and (β, α, j) define the same edge, but with a different orientation. Hence we have $N_{\alpha\beta} = N_{\beta\alpha}$. We will call internal mode (resp. external mode) a mode living on an internal edge (resp. external edge).

2.1. General case without loops

For the time being, we assume $N_{\alpha\alpha} = 0$ for all $\alpha = 1, \dots, N$ i.e. we do not consider loops. We will see later on that they are easily incorporated in our formalism. The modes are not independent but are related by two types of fundamental relations defining the scattering and propagation on the graph:

- Local scattering at vertex α : Following the RT-algebra formalism (see e.g. [13,14]), this reads

$$\mathbf{a}_j^{\alpha\beta}(p) = \sum_{\gamma=0}^N \sum_{k=1}^{N_{\alpha\gamma}} \mathbf{s}_{\alpha;jk}^{\beta\gamma}(p) \mathbf{a}_k^{\alpha\gamma}(-p) \quad \forall j = 1, \dots, N_{\alpha\beta}; \quad \forall \beta = 0, 1, \dots, N, \quad (2.1)$$

where $\mathbf{s}_{\alpha;jk}^{\beta\gamma}(p)$ are the components of the local scattering matrix $S_\alpha(p)$ which satisfies $S_\alpha(p)S_\alpha(-p) = \mathbb{1}$.

- Propagation on edge $(\alpha\beta j)$: As already mentioned, the edges $(\alpha\beta j)$ and $(\beta\alpha j)$ are identical (up to the orientation), so that the modes $\mathbf{a}_j^{\alpha\beta}(p)$ and $\mathbf{a}_j^{\beta\alpha}(p)$ are related. Denoting by $d_j^{\alpha\beta} = d_j^{\beta\alpha}$ the length of the edge, we have¹

$$\mathbf{a}_j^{\alpha\beta}(p) = \exp(-i d_j^{\alpha\beta} p) \mathbf{a}_j^{\beta\alpha}(-p). \quad (2.2)$$

The aim now is to obtain the scattering relations directly between the external modes i.e. relations of the form

$$\mathbf{a}_j^{\alpha 0}(p) = \sum_{\gamma=1}^N \sum_{k=1}^{N_{\gamma 0}} \mathbf{s}_{tot;jk}^{\alpha\gamma}(p) \mathbf{a}_k^{\gamma 0}(-p) \quad \forall j = 1, \dots, N_{\alpha 0}; \quad \forall \alpha = 1, \dots, N, \quad (2.3)$$

where $\mathbf{s}_{tot;jk}^{\alpha\gamma}(p)$ are the components of the total scattering matrix for the graph, $S_{tot}(p)$. This is most easily achieved by arranging the modes in vectors and using simple linear algebra. Denote $\mathcal{M}_{r \times s}$ the vector space of $r \times s$ matrices over \mathbb{C} . In particular, we identify $\mathcal{M}_{n \times n}$ and $\text{End}(\mathbb{C}^n)$. We denote $E_{i,j}^{r,s}$ the $r \times s$ matrix whose only nonzero entry is 1 at position (i, j) . The set $\{E_{ij}^{rs}\}_{i=1,\dots,r; j=1,\dots,s}$ is a basis of $\mathcal{M}_{r \times s}$. We will drop the superscripts every time this does not cause

¹ The particular form of this relation comes from the fact that we have in mind applications to quantum fields which are Fourier transforms of the modes considered here, see [15] for instance.

confusion *i.e.* each time the size of the matrix corresponds to the range of the indices. Similarly, we denote $\{e_j^n\}_{j=1,\dots,n}$ the canonical basis of \mathbb{C}^n and we will use a similar convention. Finally, we denote $\mathcal{F}(p)$ the space of all (possibly generalized) functions of $p \in \mathbb{C}$, with the understanding that these functions can be operator-valued in quantum field applications (*cf.* the modes). The following definitions illustrate our notations and conventions. For a given vertex α , we define different vectors:

- We collect the external modes attached to α in

$$A_\alpha(p) = \begin{pmatrix} a_1^{\alpha 0}(p) \\ \vdots \\ a_{N_{\alpha 0}}^{\alpha 0}(p) \end{pmatrix} = \sum_{j=1}^{N_{\alpha 0}} e_j \otimes a_j^{\alpha 0}(p) \in \mathbb{C}^{N_{\alpha 0}} \otimes \mathcal{F}(p). \quad (2.4)$$

- We collect the internal modes attached to α in

$$B_\alpha(p) = \begin{pmatrix} a_1^{\alpha 1}(p) \\ \vdots \\ a_{N_{\alpha 1}}^{\alpha 1}(p) \\ a_1^{\alpha 2}(p) \\ \vdots \\ a_{N_{\alpha 2}}^{\alpha 2}(p) \\ \vdots \\ a_1^{\alpha N}(p) \\ \vdots \\ a_{N_{\alpha N}}^{\alpha N}(p) \end{pmatrix}, \quad (2.5)$$

where only the modes with $N_{\alpha\beta} \neq 0$ appear. For conciseness,² we write this as

$$B_\alpha(p) = \sum_{\beta=1}^N \sum_{j=1}^{N_{\alpha\beta}} e_\beta \otimes e_j \otimes a_j^{\alpha\beta}(p) \in \mathbb{C}^{v_\alpha} \otimes \mathcal{F}(p), \quad (2.6)$$

where $v_\alpha = \sum_{\beta=1}^N N_{\alpha\beta}$ is the number of internal edges attached to α . This makes the following computations a lot more transparent but the reader should remember the actual content and size of each vector.

- Similarly, we collect all the modes attached to α in

$$\mathcal{A}_\alpha(p) = \sum_{\beta=0}^N \sum_{j=1}^{N_{\alpha\beta}} e_{\beta+1} \otimes e_j \otimes a_j^{\alpha\beta}(p) \in \mathbb{C}^{N_\alpha} \otimes \mathcal{F}(p), \quad (2.7)$$

² The explicit, longer formula is

$$B_\alpha(p) = \sum_{p=0}^{q_\alpha} \sum_{\beta=\beta_p+1}^{\beta_{p+1}-1} \sum_{j=1}^{N_{\alpha\beta}} e_{\beta-p}^{N-q_\alpha} \otimes e_j \otimes a_j^{\alpha\beta}(p),$$

where $\{\beta_1, \dots, \beta_{q_\alpha}\}$ are the labels β such that $N_{\alpha\beta} = 0$ and we have set $\beta_0 = 0$ and $\beta_{q_\alpha+1} = N + 1$ for convenience.

where $N_\alpha = N_{\alpha 0} + v_\alpha$ is the total number of edges attached to α . This way, \mathcal{A}_α is the concatenation of A_α and B_α with A_α “sitting on top”.

With the same conventions, we introduce

$$S_\alpha(p) = \sum_{\beta, \gamma=0}^N \sum_{j=1}^{N_{\alpha\beta}} \sum_{k=1}^{N_{\alpha\gamma}} E_{\beta+1, \gamma+1} \otimes E_{jk} \otimes \mathfrak{s}_{\alpha; jk}^{\beta\gamma}(p) \in \text{End}(\mathbb{C}^{N_\alpha}) \otimes \mathcal{F}(p), \quad (2.8)$$

so the relations (2.1) read

$$\mathcal{A}_\alpha(p) = S_\alpha(p) \mathcal{A}_\alpha(-p), \quad \forall \alpha = 1, \dots, N. \quad (2.9)$$

The set of relations (2.9) can be gathered into a single one:

$$\mathcal{A}(p) = S(p) \mathcal{A}(-p) \quad \text{with} \quad \mathcal{A}(p) = \sum_{\alpha=1}^N e_\alpha \otimes \mathcal{A}_\alpha(p) \quad \text{and} \quad S(p) = \sum_{\alpha=1}^N E_{\alpha\alpha} \otimes S_\alpha(p). \quad (2.10)$$

Remark that $\mathcal{A}(p) \in \mathbb{C}^{N_e + 2N_i} \otimes \mathcal{F}(p)$ where $N_e = \sum_{\alpha=1}^N N_{\alpha 0}$ is the total number of external edges and $N_i = \sum_{1 \leq \alpha \leq \beta \leq N} N_{\alpha\beta}$ is the total number of internal edges. Then, we introduce

$$B(p) = \sum_{\alpha=1}^N e_\alpha \otimes B_\alpha(p) \in \mathbb{C}^{2N_i} \otimes \mathcal{F}(p), \quad (2.11)$$

and

$$E(p) = \sum_{\alpha, \beta=1}^N \sum_{j=1}^{N_{\alpha\beta}} E_{\alpha, \beta} \otimes E_{\beta, \alpha} \otimes E_{jj} \otimes \exp(-i d_j^{\alpha\beta} p) \in \text{End}(\mathbb{C}^{2N_i}) \otimes \mathcal{F}(p), \quad (2.12)$$

so the relations (2.2) read

$$B(p) = E(p) B(-p). \quad (2.13)$$

It is easy to see that

$$E(p) E(-p) = \sum_{\alpha, \beta=1}^N \sum_{j=1}^{N_{\alpha\beta}} E_{\alpha, \alpha} \otimes E_{\beta, \beta} \otimes \mathbb{I}_{N_{\alpha\beta}}$$

that acts as the identity matrix $\mathbb{1}_{2N_i}$. The final step is to decompose the matrix $S(p)$ into four submatrices related to external or internal edges:

$$S^{(11)}(p) = \sum_{\alpha=1}^N \sum_{j, k=1}^{N_{\alpha 0}} E_{\alpha\alpha} \otimes E_{jk} \otimes \mathfrak{s}_{\alpha; jk}^{00}(p) \in \text{End}(\mathbb{C}^{N_e}) \otimes \mathcal{F}(p), \quad (2.14)$$

$$S^{(12)}(p) = \sum_{\alpha, \gamma=1}^N \sum_{j=1}^{N_{\alpha 0}} \sum_{k=1}^{N_{\alpha\gamma}} E_{\alpha\alpha} \otimes E_{1, \gamma} \otimes E_{jk} \otimes \mathfrak{s}_{\alpha; jk}^{0\gamma}(p) \in \mathcal{M}_{N_e \times 2N_i} \otimes \mathcal{F}(p), \quad (2.15)$$

$$S^{(21)}(p) = \sum_{\alpha, \beta=1}^N \sum_{j=1}^{N_{\alpha\beta}} \sum_{k=1}^{N_{\alpha 0}} E_{\alpha\alpha} \otimes E_{\beta, 1} \otimes E_{jk} \otimes \mathfrak{s}_{\alpha; jk}^{\beta 0}(p) \in \mathcal{M}_{2N_i \times N_e} \otimes \mathcal{F}(p), \quad (2.16)$$

$$S^{(22)}(p) = \sum_{\alpha, \beta, \gamma=1}^N \sum_{j=1}^{N_{\alpha\beta}} \sum_{k=1}^{N_{\alpha\gamma}} E_{\alpha\alpha} \otimes E_{\beta, \gamma} \otimes E_{jk} \otimes \mathfrak{s}_{\alpha; jk}^{\beta\gamma}(p) \in \text{End}(\mathbb{C}^{2N_i}) \otimes \mathcal{F}(p). \quad (2.17)$$

Therefore, the set of all the relations we have becomes

$$A(p) = S^{(11)}(p)A(-p) + S^{(12)}(p)B(-p), \quad (2.18)$$

$$B(p) = S^{(21)}(p)A(-p) + S^{(22)}(p)B(-p), \quad (2.19)$$

$$B(p) = E(p)B(-p). \quad (2.20)$$

Assuming that $E(p) - S^{(22)}(p)$ is invertible this yields the desired relations in the form

$$A(p) = S_{tot}(p)A(-p), \quad (2.21)$$

with

$$S_{tot}(p) = S^{(11)}(p) + S^{(12)}(p)[E(p) - S^{(22)}(p)]^{-1}S^{(21)}(p). \quad (2.22)$$

The internal modes can be expressed in terms of the external ones:

$$B(p) = [E(-p) - S^{(22)}(-p)]^{-1}S^{(21)}(-p)A(p). \quad (2.23)$$

These two formulas are the central result of this work. We note that in the course of our investigation, we discovered that the analog of the result (2.22) has been found in [10] in the setting of abstract graph theory and using the formalism of Grassmann variables. However, the proof is based on the notion of generalized star product [8] and requires a rather involved proof by induction on the size of the graph. Here, it is obtained directly by simple linear algebra and ready to use for computations (either analytical or numerical).

2.2. Discussion

We have checked that our formula reproduces known results obtained by other methods for simple graphs (star-triangle, etc.) [7,8,15]. In the following, we present in detail the computation for new graphs, especially in 3D, for which the previous methods are impractical analytically. Our method presents several advantages compared to previous ones. First, as just mentioned, it is computationally easier and one does not have to worry about the sequence of steps used in iterative methods where one has to make sure that fusing two given vertices and then a third gives the same results a fusing the first and third and then the second (*cf.* [15]). The only task involved is the inversion of a matrix and there are well-known efficient methods both analytically and numerically. Then, we have an explicit formula which shows the location of the poles of S_{tot} (on top of the possible ones from the local matrices which are given data in our approach). They are solutions of

$$\det(E(p) - S^{(22)}(p)) = 0. \quad (2.24)$$

This is important as these poles play a fundamental role in the computation of physical quantities like the conductance in quantum systems defined on graphs (see [5,15]). Finally, for quantum systems on compact graphs, *i.e.* without external edges, the same equation provides the allowed modes on the graph. In this respect, (2.24) is the generalization to an arbitrary compact quantum graph of the quantization equation

$$e^{2ikL} = 1, \quad (2.25)$$

for a particle in a box of length L . The matrix $S^{(22)}(p)$ accounts here for the one particle scattering occurring at the vertices. In the theory of integrable systems, this type of equations is sometimes called Bethe ansatz equations. However, here we emphasize that it is not related to such an ansatz. In condensed matter physics, the information given by this equation together with the dispersion relation of the model provides the basis of band structure analysis.

Scattering matrix of a graph and RT algebras

We would like to comment on the fact that we call S_{tot} the scattering matrix of the graph. This comes from the terminology one encounters when one takes a graph such as those described in this paper to model quantum wires for instance. In this context, our method gives the matrix which is known to be the scattering matrix in those models. Also, in the context of quantum field theory on graphs, the total scattering matrix that we obtain is precisely the matrix whose elements are the transition amplitudes between asymptotic states. Indeed, using the formalism of quantum field theory, the modes $a_j^{\alpha\beta}(p)$, which are used as labels in the previous general setting, acquire the status of Fourier modes of the quantum fields living on the edges of the graph. Together with another set of modes, denoted $a_j^{\dagger\alpha\beta}(p)$, they are creation and annihilation operators acting in a Fock space and obeying the RT-algebra relations. This situation has been described and used in detail in [3,4] for star graphs and in [16] for a simple line of edges. Following the latter, we know that relations (2.1) and (2.2) (together with their hermitian conjugates), in the case where the local scattering matrices derive from the self-adjoint extensions of the one-dimensional Laplace operator, ensure that the complex scalar field

$$\phi_j^{\alpha\beta}(x, t) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} a_j^{\alpha\beta}(p) e^{ipx - ip^2 t} \quad (2.26)$$

living on the edge (α, β, j) with $x \in [0, d_j^{\alpha\beta}]$ satisfies the Schrödinger equation³

$$(i\partial_t + \partial_x^2)\phi_j^{\alpha\beta}(x, t) = 0, \quad (2.27)$$

together with the boundary conditions

$$\sum_{\gamma=0}^N \sum_{k=1}^{N_{\alpha\gamma}} (C_{\alpha;jk}^{\beta\gamma} \phi_k^{\alpha\gamma}(0, t) + D_{\alpha;jk}^{\beta\gamma} \partial_x \phi_k^{\alpha\gamma}(0, t)) = 0, \quad (2.28)$$

where the matrices C_α and D_α form the local scattering matrix $S_\alpha(p)$ as explained in [7]. In this setting, an incoming asymptotic state on the j -th external edge attached to the vertex α is given by $a_j^{\dagger\alpha 0}(p)$ with $p < 0$ while an outgoing state corresponds to $p > 0$. Hence the scattering amplitude between an incoming and an outgoing state is

$$\langle 0 | a_j^{\beta 0}(-q) a_k^{\dagger\alpha 0}(p) | 0 \rangle, \quad p, q > 0, \quad (2.29)$$

where $|0\rangle$ is the vacuum state annihilated by the a 's (see [13] for more details). The RT algebra formalism then enables to compute this scattering amplitude using the following exchange relations between the external (and independent) generators

³ This is just an example of governing equation one might want to use on the edges. For a relativistic model, one simply changes the dispersion relation and the measure appropriately in (2.26).

$$\mathfrak{a}_j^{\alpha 0}(p) \mathfrak{a}_k^{\beta 0}(q) - \mathfrak{a}_k^{\beta 0}(q) \mathfrak{a}_j^{\alpha 0}(p) = 0, \quad (2.30)$$

$$\mathfrak{a}_j^{\dagger \alpha 0}(p) \mathfrak{a}_k^{\dagger \beta 0}(q) - \mathfrak{a}_k^{\dagger \beta 0}(q) \mathfrak{a}_j^{\dagger \alpha 0}(p) = 0, \quad (2.31)$$

$$\mathfrak{a}_j^{\alpha 0}(p) \mathfrak{a}_k^{\dagger \beta 0}(q) - \mathfrak{a}_k^{\dagger \beta 0}(q) \mathfrak{a}_j^{\alpha 0}(p) = 2\pi \delta_{jk} \delta_{\alpha\beta} \delta(p-q) + 2\pi \mathfrak{s}_{tot;jk}^{\alpha\beta}(p) \delta(p+q), \quad (2.32)$$

where $\mathfrak{s}_{tot;jk}^{\alpha\beta}(p)$ are the elements of the total scattering matrix $S_{tot}(p)$ obtained in (2.22) from (2.1) and (2.2). Then one gets

$$\langle 0 | \mathfrak{a}_j^{\beta 0}(-q) \mathfrak{a}_k^{\dagger \alpha 0}(p) | 0 \rangle = 2\pi \mathfrak{s}_{tot;jk}^{\alpha\beta}(-q) \delta(p-q), \quad p, q > 0. \quad (2.33)$$

This also shows that, given the metric and local scattering data of the graph, the total scattering matrix is unique.

2.3. Properties

To be consistent, our general formula should not depend on the numbering of the internal edges or vertices (internal permutation) and should transform appropriately under a permutation of the external modes (external permutation). Let Π be an external permutation acting on $A(p)$ and P an internal permutation acting on $B(p)$. It is easy to see that this induces the transformations

$$S^{(11)}(p) \rightarrow \Pi S^{(11)}(p) \Pi^{-1}, \quad (2.34)$$

$$S^{(12)}(p) \rightarrow \Pi S^{(12)}(p) P^{-1}, \quad (2.35)$$

$$S^{(21)}(p) \rightarrow P S^{(21)}(p) \Pi^{-1}, \quad (2.36)$$

$$S^{(22)}(p) \rightarrow P S^{(22)}(p) P^{-1}, \quad (2.37)$$

$$E(p) \rightarrow P E(p) P^{-1}, \quad (2.38)$$

producing $S_{tot} \rightarrow \Pi S_{tot} \Pi^{-1}$ as it should. Therefore, in examples or applications, one can always fix a convenient numbering of edges and vertices and work up to an external permutation.

In view of physical application, we must also be concerned with the properties of S_{tot} . We have seen already that $S_\alpha(p) S_\alpha(-p) = \mathbb{1}_{N_\alpha}$. This implies

$$S_{tot}(p) S_{tot}(-p) = \mathbb{1}_{N_e}. \quad (2.39)$$

To see this, note that the block matrix made of (2.14)–(2.17) is related to $S(p)$ given in (2.10) by

$$\mathcal{S}(p) \equiv \left(\begin{array}{c|c} S^{(11)}(p) & S^{(12)}(p) \\ \hline S^{(21)}(p) & S^{(22)}(p) \end{array} \right) = P S(p) P^{-1}, \quad (2.40)$$

where P is the permutation matrix defined by

$$P \mathcal{A}(p) = \begin{pmatrix} A(p) \\ B(p) \end{pmatrix}. \quad (2.41)$$

Then by direct calculation and upon using $\mathcal{S}(p) \mathcal{S}(-p) = \mathbb{1}_{N_e+2N_i}$ and $E(p) E(-p) = \mathbb{1}_{2N_i}$ we get

$$\begin{aligned} S_{tot}(p) S_{tot}(-p) &= \mathbb{1}_{N_e} + S^{(12)}(p) (E(p) - S^{(22)}(p))^{-1} \\ &\quad \times M(E(-p) - S^{(22)}(-p))^{-1} S^{(21)}(-p), \end{aligned} \quad (2.42)$$

where

$$\begin{aligned} M &= \mathbb{1}_{2N_i} - (E(p) - S^{(22)}(p))(E(-p) - S^{(22)}(-p)) - (E(p) - S^{(22)}(p))S^{(22)}(-p) \\ &\quad - S^{(22)}(p)(E(-p) - S^{(22)}(-p)) - S^{(22)}(p)S^{(22)}(-p) \\ &= 0. \end{aligned} \quad (2.43)$$

Now the local scattering matrices can be required to have additional properties, like unitarity. This is the case in particular if they arise from non-dissipative local boundary conditions emerging from self-adjoint extensions of the free one-dimensional Hamiltonian (see e.g. [7]). One then has unitarity

$$S_\alpha^\dagger(p) = S_\alpha^{-1}(p). \quad (2.44)$$

Following the same type of argument as above, one finds that S_{tot} is also unitary.

We finish this section by providing a few properties of $E(p)$. It is symmetric and we have already seen that $E(p)E(-p) = \mathbb{1}_{2N_i}$. In particular $E(0)^2 = \mathbb{1}_{2N_i}$ so its eigenvalues are ± 1 and are equally degenerate. Also, $E(0)$ is a permutation matrix and $E(p)$ is a generalized permutation matrix (with coefficients of the type $e^{-ipd_j^{\alpha\beta}}$) which can be written as a product of a permutation matrix and a diagonal matrix

$$E(p) = D(p)E(0) = E(0)D(p), \quad (2.45)$$

where

$$D(p) = \sum_{\alpha, \beta=1}^N \sum_{j=1}^{N_{\alpha\beta}} E_{\alpha, \alpha} \otimes E_{\beta, \beta} \otimes E_{jj} \otimes \exp(-id_j^{\alpha\beta} p), \quad (2.46)$$

with

$$D(p)D(q) = D(p+q), \quad p, q \in \mathbb{C}. \quad (2.47)$$

3. Including loops

The case of loops attached to single vertices can be treated with minor modifications in our formalism. Essentially, the idea is again to see a loop attached to a given vertex α as arising from the gluing of two edges attached to this vertex. This will be most easily incorporated in the general formalism if we use the following trick for notations. Let $N_{\alpha\alpha} \neq 0$ be the number of loops attached to vertex α . To each loop j , $j = 1, \dots, N_{\alpha\alpha}$ correspond two modes⁴ $a_{2j-1}^{\alpha\alpha}(p)$ and $a_{2j}^{\alpha\alpha}(p)$ which are related by

$$a_{2j-1}^{\alpha\alpha}(p) = e^{-ipd_j^{\alpha\alpha}} a_{2j}^{\alpha\alpha}(-p), \quad j = 1, \dots, N_{\alpha\alpha}. \quad (3.1)$$

We collect these modes in two-component vectors

$$\mathbf{a}_j^{\alpha\alpha}(p) = \begin{pmatrix} a_{2j-1}^{\alpha\alpha}(p) \\ a_{2j}^{\alpha\alpha}(p) \end{pmatrix}, \quad j = 1, \dots, N_{\alpha\alpha}. \quad (3.2)$$

We denote all the components of the local scattering matrix $S_\alpha(p)$ related to the loop modes by $s_{\alpha; jk}^{\alpha\beta}(p)$, $j = 1, \dots, 2N_{\alpha\alpha}$, $k = 1, \dots, N_{\alpha\beta}$; $s_{\alpha; jk}^{\beta\alpha}(p)$, $j = 1, \dots, N_{\alpha\beta}$, $k = 1, \dots, 2N_{\alpha\alpha}$; and $s_{\alpha; jk}^{\alpha\alpha}(p)$, $j, k = 1, \dots, 2N_{\alpha\alpha}$. Mimicking (3.2), we then define, for $\alpha \neq \beta$,

⁴ Again, the choice of numbering is for convenience only and is irrelevant to the final results.

$$s_{\alpha;jk}^{\alpha\beta}(p) = \begin{pmatrix} s_{\alpha;2j-1,k}^{\alpha\beta}(p) \\ s_{\alpha;2j,k}^{\alpha\beta}(p) \end{pmatrix}, \quad j = 1, \dots, N_{\alpha\alpha}, \quad k = 1, \dots, N_{\alpha\beta}, \quad (3.3)$$

$$s_{\alpha;jk}^{\beta\alpha}(p) = (s_{\alpha;j,2k-1}^{\beta\alpha}(p) \quad s_{\alpha;j,2k}^{\beta\alpha}(p)), \quad j = 1, \dots, N_{\alpha\beta}, \quad k = 1, \dots, N_{\alpha\alpha}, \quad (3.4)$$

and also,

$$s_{\alpha;jk}^{\alpha\alpha}(p) = \begin{pmatrix} s_{\alpha;2j-1,2k-1}^{\alpha\alpha}(p) & s_{\alpha;2j-1,2k}^{\alpha\alpha}(p) \\ s_{\alpha;2j,2k-1}^{\alpha\alpha}(p) & s_{\alpha;2j,2k}^{\alpha\alpha}(p) \end{pmatrix}, \quad j, k = 1, \dots, N_{\alpha\alpha}. \quad (3.5)$$

Finally, we define

$$e_j^{\alpha\beta}(p) = \begin{cases} e^{ipd_j^{\alpha\beta}}, & \text{if } \beta \neq \alpha \text{ and } N_{\alpha\beta} \neq 0, \\ e^{ipd_j^{\alpha\alpha}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, & \text{if } \beta = \alpha \text{ and } N_{\alpha\alpha} \neq 0. \end{cases} \quad (3.6)$$

With all this, the relations defining scattering and propagation on the graph take the same form as before (cf. (2.1) and (2.2))

$$a_j^{\beta\alpha}(p) = \sum_{\gamma=0}^N \sum_{k=1}^{N_{\alpha\gamma}} s_{\alpha;jk}^{\beta\gamma}(p) a_k^{\alpha\gamma}(-p) \quad \forall j = 1, \dots, N_{\alpha\beta}; \quad \forall \beta = 0, 1, \dots, N \quad (3.7)$$

and

$$a_j^{\alpha\beta}(p) = e_j^{\alpha\beta}(-p) a_j^{\beta\alpha}(-p) \quad \forall j = 1, \dots, N_{\alpha\beta}; \quad \forall \beta = 0, 1, \dots, N. \quad (3.8)$$

Therefore, all the formalism and the results developed in Section 2.1 hold in the same form, provided one substitutes $e_j^{\alpha\beta}(-p)$ for $e^{-ipd_j^{\alpha\beta}}$ in (2.12). One should not be deceived by the apparent similarity of the results with or without loops. In general, the consequences of adding a loop in a given graph can be drastic.

However, as the formalism suggests, allowing for loops in graphs opens the possibility that two topologically completely different graphs can have exactly the same total scattering matrix. This is illustrated on the example below. In particular, this shows that the uniqueness of the inverse scattering problem, as discussed in [9], does not extend to the case of graphs with loops.⁵ The equivalent statement in terms of the Schrödinger operator on a graph was discussed in [17] where it was shown that in general the knowledge of the scattering matrix of a noncompact graph is not enough to fix its topological structure and the boundary conditions at the vertices.

We consider the two graphs depicted in Fig. 1 below. To illustrate our notations, we have displayed the modes involved in the construction, dropping the p -dependence for conciseness. They are topologically completely different, one being a triangle with one external edge attached to each vertex and the other being a single vertex star graph with three external edges and three loops attached to it. Note that for the triangle, we drop the unnecessary Latin subscripts since $N_{\alpha\beta} = 1$ for all $\alpha = 1, 2, 3$ and $\beta = 0, 1, 2, 3, \beta \neq \alpha$.

We assume that the scattering and propagation data is given as follows (we drop again the p dependence for clarity),

⁵ Uniqueness is only guaranteed if one requires in addition that the number of vertices is maximal (cf. Theorem 4.6 in [9]).

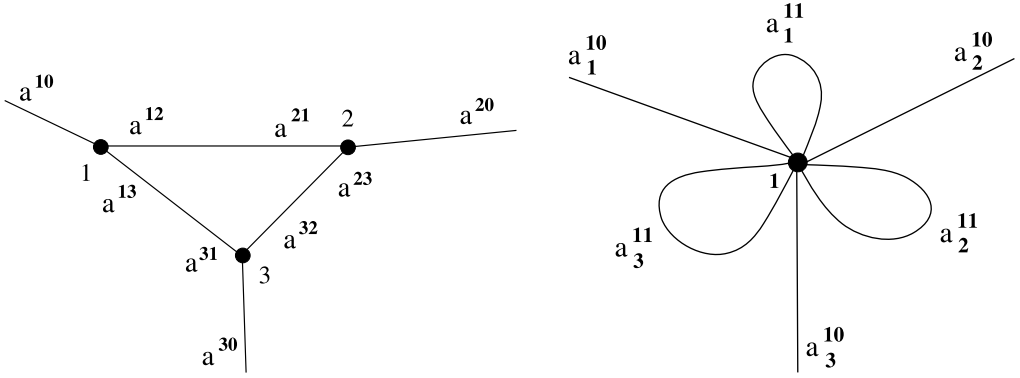


Fig. 1. Two topologically different graphs with the same total scattering matrix. Left: triangle. Right: star graph with loops.

For the triangle,

$$S_1 = \begin{pmatrix} s_1^{00} & s_1^{02} & s_1^{03} \\ s_1^{20} & s_1^{22} & s_1^{23} \\ s_1^{30} & s_1^{32} & s_1^{33} \end{pmatrix}, \quad S_2 = \begin{pmatrix} s_2^{00} & s_2^{01} & s_2^{03} \\ s_2^{10} & s_2^{11} & s_2^{13} \\ s_2^{30} & s_2^{31} & s_2^{33} \end{pmatrix}, \quad S_3 = \begin{pmatrix} s_3^{00} & s_3^{01} & s_3^{02} \\ s_3^{10} & s_3^{11} & s_3^{12} \\ s_3^{20} & s_3^{21} & s_3^{22} \end{pmatrix}, \quad (3.9)$$

giving the four blocks as defined in (2.14)–(2.17) in the form

$$S^{(11)} = \begin{pmatrix} s_1^{00} & 0 & 0 \\ 0 & s_2^{00} & 0 \\ 0 & 0 & s_3^{00} \end{pmatrix}, \quad S^{(22)} = \begin{pmatrix} s_1^{22} & s_1^{23} & 0 & 0 & 0 & 0 \\ s_1^{32} & s_1^{33} & 0 & 0 & 0 & 0 \\ 0 & 0 & s_2^{11} & s_2^{13} & 0 & 0 \\ 0 & 0 & s_2^{31} & s_2^{33} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_3^{11} & s_3^{12} \\ 0 & 0 & 0 & 0 & s_3^{21} & s_3^{22} \end{pmatrix}, \quad (3.10)$$

$$S^{(12)} = \begin{pmatrix} s_1^{02} & s_1^{03} & 0 & 0 & 0 & 0 \\ 0 & 0 & s_2^{01} & s_2^{03} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_3^{01} & s_3^{02} \end{pmatrix}, \quad S^{(21)} = \begin{pmatrix} s_1^{20} & 0 & 0 \\ s_1^{30} & 0 & 0 \\ 0 & s_2^{10} & 0 \\ 0 & s_2^{30} & 0 \\ 0 & 0 & s_3^{10} \\ 0 & 0 & s_3^{20} \end{pmatrix}, \quad (3.11)$$

and

$$E_t = \begin{pmatrix} 0 & 0 & e^{-ipd^{12}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{-ipd^{13}} & 0 \\ e^{-ipd^{12}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-ipd^{23}} \\ 0 & e^{-ipd^{13}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-ipd^{23}} & 0 & 0 \end{pmatrix}. \quad (3.12)$$

For the star graph,

$$T = \begin{pmatrix} t_{1;11}^{00} & 0 & 0 & t_{1;11}^{01} & t_{1;12}^{01} & t_{1;13}^{01} \\ 0 & t_{1;22}^{00} & 0 & t_{1;21}^{01} & t_{1;22}^{01} & t_{1;23}^{01} \\ 0 & 0 & t_{1;33}^{00} & t_{1;31}^{01} & t_{1;32}^{01} & t_{1;33}^{01} \\ t_{1;11}^{10} & t_{1;12}^{10} & t_{1;13}^{10} & t_{1;11}^{11} & t_{1;12}^{11} & t_{1;13}^{11} \\ t_{1;21}^{10} & t_{1;22}^{10} & t_{1;23}^{10} & t_{1;21}^{11} & t_{1;22}^{11} & t_{1;23}^{11} \\ t_{1;31}^{10} & t_{1;32}^{10} & t_{1;33}^{10} & t_{1;31}^{11} & t_{1;32}^{11} & t_{1;33}^{11} \end{pmatrix} \equiv \left(\frac{T^{(11)}}{T^{(21)}} \middle| \frac{T^{(12)}}{T^{(22)}} \right), \quad (3.13)$$

and

$$E_s = \begin{pmatrix} 0 & e^{-ipd_1^{11}} & 0 & 0 & 0 & 0 \\ e^{-ipd_1^{11}} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-ipd_2^{11}} & 0 & 0 \\ 0 & 0 & e^{-ipd_2^{11}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{-ipd_3^{11}} \\ 0 & 0 & 0 & 0 & e^{-ipd_3^{11}} & 0 \end{pmatrix}. \quad (3.14)$$

The lengths of the internal edges of the triangle are related to the lengths of the loop in the star graph by

$$d^{12} = d_1^{11}, \quad d^{23} = d_3^{11}, \quad d^{23} = d_2^{11}, \quad (3.15)$$

and the following relations for the scattering data hold, showing in particular the matrix structure defined in (3.3)–(3.5) in the case of loops,

$$t_{1;11}^{00} = s_1^{00}, \quad t_{1;22}^{00} = s_2^{00}, \quad t_{1;33}^{00} = s_3^{00}, \quad (3.16)$$

$$t_{1;11}^{01} = (s_1^{02} \ 0), \quad t_{1;12}^{01} = (0 \ 0), \quad t_{1;13}^{01} = (s_1^{03} \ 0), \quad (3.17)$$

$$t_{1;21}^{01} = (0 \ s_2^{01}), \quad t_{1;22}^{01} = (s_2^{03} \ 0), \quad t_{1;23}^{01} = (0 \ 0), \quad (3.18)$$

$$t_{1;31}^{01} = (0 \ 0), \quad t_{1;32}^{01} = (0 \ s_3^{02}), \quad t_{1;33}^{01} = (0 \ s_3^{01}), \quad (3.19)$$

$$t_{1;11}^{10} = \begin{pmatrix} s_1^{20} \\ 0 \end{pmatrix}, \quad t_{1;12}^{10} = \begin{pmatrix} 0 \\ s_2^{10} \end{pmatrix}, \quad t_{1;13}^{10} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad (3.20)$$

$$t_{1;21}^{10} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t_{1;22}^{10} = \begin{pmatrix} s_2^{30} \\ 0 \end{pmatrix}, \quad t_{1;23}^{10} = \begin{pmatrix} 0 \\ s_3^{20} \end{pmatrix}, \quad (3.21)$$

$$t_{1;31}^{10} = \begin{pmatrix} s_1^{30} \\ 0 \end{pmatrix}, \quad t_{1;32}^{10} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad t_{1;33}^{10} = \begin{pmatrix} 0 \\ s_3^{10} \end{pmatrix}, \quad (3.22)$$

$$t_{1;11}^{11} = \begin{pmatrix} s_1^{22} & 0 \\ 0 & s_2^{11} \end{pmatrix}, \quad t_{1;12}^{11} = \begin{pmatrix} 0 & 0 \\ s_2^{13} & 0 \end{pmatrix}, \quad t_{1;13}^{11} = \begin{pmatrix} s_1^{23} & 0 \\ 0 & 0 \end{pmatrix}, \quad (3.23)$$

$$t_{1;21}^{11} = \begin{pmatrix} 0 & s_2^{31} \\ 0 & 0 \end{pmatrix}, \quad t_{1;22}^{11} = \begin{pmatrix} s_2^{33} & 0 \\ 0 & s_3^{22} \end{pmatrix}, \quad t_{1;23}^{11} = \begin{pmatrix} 0 & 0 \\ 0 & s_3^{21} \end{pmatrix}, \quad (3.24)$$

$$t_{1;31}^{11} = \begin{pmatrix} s_1^{32} & 0 \\ 0 & 0 \end{pmatrix}, \quad t_{1;32}^{11} = \begin{pmatrix} 0 & 0 \\ 0 & s_3^{12} \end{pmatrix}, \quad t_{1;33}^{11} = \begin{pmatrix} s_1^{33} & 0 \\ 0 & s_3^{11} \end{pmatrix}. \quad (3.25)$$

The fact that these two graphs give rise to the same total scattering matrix follows from the fact that their scattering data are related by an internal permutation

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad (3.26)$$

such that

$$\begin{aligned} PS^{(22)}P^{-1} &= T^{(22)}, & PE_tP^{-1} &= E_s, \\ S^{(12)}P^{-1} &= T^{(12)}, & PS^{(21)} &= T^{(21)}. \end{aligned} \quad (3.27)$$

Then,

$$\begin{aligned} S_{tot}^{triangle} &= S^{(11)} + S^{(12)}(E_t - S^{(22)})^{-1}S^{(21)} \\ &= S^{(11)} + S^{(12)}P^{-1}(PE_tP^{-1} - PS^{(22)}P^{-1})^{-1}PS^{(21)} \\ &= T^{(11)} + T^{(12)}(E_s - T^{(22)})^{-1}T^{(21)} \\ &= S_{tot}^{star}. \end{aligned} \quad (3.28)$$

4. Platonic solids

In this section, we illustrate the freedom on numbering and the use of formula (2.22) on the convex regular polyhedra known as Platonic solids (tetrahedron, cube, octahedron, dodecahedron, icosahedron) [18]. Once the scattering matrix is known, physical quantities associated to the graph can easily be computed, such as the conductance, using the formalism developed in [3]. The calculation essentially relies on the pole structure and the general techniques have been explicated in [15].

We carry out explicit calculations in the case of the tetrahedron and the cube. This choice is primarily motivated by aesthetic and academic criteria rather than any particular practical application. It also shows the computational advantage of our method over recursive ones on rather involved graphs. More precisely, we consider graphs whose internal edges and vertices correspond to Platonic solids and for which exactly one external edge is attached to each vertex. This corresponds to $N_{\alpha\beta} = 1$, $\alpha = 1, \dots, N$, $\beta = 0, \dots, N$, $\alpha \neq \beta$. Note that the condition of regularity yields $d_1^{\alpha\beta} \equiv d$ for all $\alpha, \beta = 1, \dots, N$. Also, all the vertices are connected to the same number of vertices so $v_\alpha \equiv v$ is the same for all $\alpha = 1, \dots, N$. N is even for all those graphs. Finally, from the general theory of graph colouring, see *e.g.* [19], it is known that we can assign a label (or colour) $a \in \{1, \dots, v\}$ to the edges connected to the same vertex in a way compatible with the graph, *i.e.* in colour terms, such that no two edges connected to the same vertex have the same colour and each edge can only have one colour. This allows us to define functions n_α , $\alpha \in \{1, \dots, N\}$ from $\{1, \dots, v\}$ to $\{1, \dots, N\}$ such that $n_\alpha(a) = \beta$ if and only if β is connected to α by the edge labelled a . We use the convention $a = 0$ for external edges and set $n_\alpha(0) = 0$ for all $\alpha \in \{1, \dots, N\}$. By construction, we have the following properties

$$\begin{aligned} n_\alpha(a) = \beta &\Leftrightarrow n_\beta(a) = \alpha, & n_\alpha(a) = n_\beta(a) &\Leftrightarrow \alpha = \beta, \\ n_\alpha(a) = n_\alpha(b) &\Leftrightarrow a = b. \end{aligned} \quad (4.1)$$

In view of formula (2.22), the main object of interest is $E(p) - S^{(22)}(p)$ which we seek to invert. With our notations, we get

$$\begin{aligned} E(p) &= e^{-ipd} \sum_{\alpha=1}^N \sum_{a=1}^v E_{\alpha, n_{\alpha}(a)} \otimes E_{aa}, \\ S^{(22)}(p) &= \sum_{\alpha=1}^N \sum_{a,b=1}^v E_{\alpha, \alpha} \otimes E_{ab} \otimes \mathfrak{s}_{\alpha}^{ab}(p), \end{aligned} \quad (4.2)$$

where the local matrices read

$$S_{\alpha}(p) = \sum_{a,b=0}^v E_{a+1, b+1} \otimes \mathfrak{s}_{\alpha}^{ab}(p), \quad \alpha = 1, \dots, N. \quad (4.3)$$

For later convenience, we define a reduced scattering matrix containing only the information about scattering on the internal edges

$$S_{\alpha}^{red}(p) = \sum_{a,b=1}^v E_{a,b} \otimes \mathfrak{s}_{\alpha}^{ab}(p), \quad \alpha = 1, \dots, N. \quad (4.4)$$

Let us also define

$$\mathcal{E}_{\alpha} = \sum_{a=1}^N E_{\alpha, n_{\alpha}(a)}. \quad (4.5)$$

Then $E(p) = e^{-ipd} \sum_{a=1}^v \mathcal{E}_a \otimes E_{aa}$ and from the general properties of E (or by direct calculation) we find

$$\mathcal{E}_a = \mathcal{E}_a^t = \mathcal{E}_a^{-1}, \quad a = 1, \dots, v. \quad (4.6)$$

Therefore \mathcal{E}_a is diagonalizable with eigenvalues ± 1 each degenerate $\frac{N}{2}$ times and with eigenvectors $v_{\alpha}^{\epsilon} = \frac{1}{\sqrt{2}}(e_{\alpha} + \epsilon e_{n_{\alpha}(a)})$, $\epsilon = \pm 1$, $\alpha < n_{\alpha}(a)$, forming an orthonormal basis.

4.1. Tetrahedron

For the tetrahedron, $N = 4$, $v = 3$ and the matrices \mathcal{E}_a enjoy the additional property

$$\mathcal{E}_a \mathcal{E}_b = \mathcal{E}_b \mathcal{E}_a, \quad \forall a, b = 1, 2, 3, \quad (4.7)$$

due to the fact that

$$\forall \beta \in \{1, 2, 3, 4\}, \quad \forall a, b \in \{1, 2, 3\}, \quad n_{n_{\beta}(a)}(b) = n_{n_{\beta}(b)}(a). \quad (4.8)$$

This can be seen to hold by direct inspection on Fig. 2 and holds also for other inequivalent numberings.

From (4.7), they can be diagonalized simultaneously. As already explained, to fix ideas we can fix a numbering without loss of generality since we work up to permutations. In the present case, changing the edges and or vertices numbering amounts to interchanging the \mathcal{E}_a 's. From the figure we obtain

$$\mathcal{E}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{E}_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{E}_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (4.9)$$

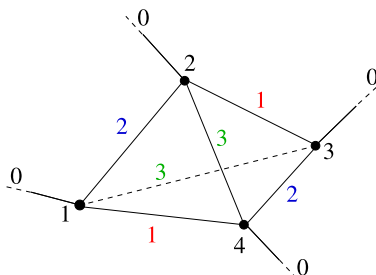


Fig. 2. Tetrahedron with an example of numbering.

and a diagonalizing matrix is

$$T = \frac{1}{2} \begin{pmatrix} -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} = T^{-1} = T^t. \quad (4.10)$$

So far, we haven't taken advantage of the geometry and its symmetries. The scattering can still be different from vertex to vertex (as labelled by the index α on the local matrices) and at a given vertex, the scattering from edge a to edge b needs not be the same as the scattering from edge a to edge c say. Clearly, this does not respect the natural symmetry of the underlying graph. One can impose that the local scattering matrices be the same for all vertices *i.e.* $S_\alpha(p) \equiv S(p)$ and in particular $S_\alpha^{red}(p) \equiv S^{red}(p)$ for all $\alpha = 1, 2, 3, 4$. This already greatly simplifies the problem of inversion. Let $\tau = T \otimes \mathbb{1}_3$ and $D_a = T \mathcal{E}_a T^{-1}$ then

$$\tau(E(p) - S^{(22)}(p))\tau^{-1} = e^{-ipd} \sum_{a=1}^3 D_a \otimes E_{aa} - \mathbb{1}_4 \otimes S^{red}(p). \quad (4.11)$$

The matrix on the right-hand side is a block diagonal matrix made of four 3×3 blocks essentially determined by S^{red}

$$\tau(E(p) - S^{(22)}(p))\tau^{-1} = \sum_{\alpha=1}^4 E_{\alpha\alpha} \otimes (e^{-ipd} I_\alpha - S^{red}(p)), \quad (4.12)$$

with

$$\begin{aligned} I_1 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, & I_2 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \\ I_3 &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, & I_4 &= \mathbb{1}_3. \end{aligned} \quad (4.13)$$

Thus, the problem is reduced to inverting 3×3 matrices. In particular, the poles of S_{tot} are solutions of

$$\det(e^{-ipd} I_\alpha - S^{red}(p)) = 0, \quad \alpha = 1, 2, 3, 4. \quad (4.14)$$

We now turn to the explicit calculation of S_{tot} in the case where the vertices are described by scale invariant local matrices (independent of p) capturing universal features of scattering. In

our case, each local matrix is the same 4×4 scale invariant matrix whose explicit form has been classified in [3]. Note also that we can take further advantage of the symmetries of the underlying geometry here by imposing for instance that the scattering be invariant under a rotation of $\pi/3$ around the axis passing through a vertex and the centre of the opposite face. Physically, this means that an incoming particle from the external edge of a vertex has the same probability of being transmitted to any one of the internal edges attached to this vertex. Mathematically, this amounts to requiring that S satisfies

$$\begin{pmatrix} 1 & 0 \\ 0 & J \end{pmatrix} S \begin{pmatrix} 1 & 0 \\ 0 & J^{-1} \end{pmatrix} = S, \quad (4.15)$$

where

$$J = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad J^3 = \mathbb{1}_3. \quad (4.16)$$

Putting everything together, we find two possible local scattering matrices

$$S_1 = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \quad S_2 = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{5}{6} & -\frac{1}{6} & -\frac{1}{6} \\ \frac{1}{2} & -\frac{1}{6} & \frac{5}{6} & -\frac{1}{6} \\ \frac{1}{2} & -\frac{1}{6} & -\frac{1}{6} & \frac{5}{6} \end{pmatrix}. \quad (4.17)$$

In the first case, we compute $S_{tot}(p)$ as

$$S_{tot}^1(p) = \frac{1}{G_1(p)} (-2(e^{-3ipd} + e^{-ipd} - 1)\mathbb{1}_4 + e^{-ipd}(e^{-ipd} + 1)A), \quad (4.18)$$

where $G_1(p) = (2e^{-2ipd} + e^{-ipd} + 1)(2e^{-ipd} - 1)$ and

$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}. \quad (4.19)$$

The poles of this matrix are given by

$$e^{-ipd} = x \quad \text{with } x \in \left\{ \frac{1}{2}, \frac{-1 + i\sqrt{7}}{4}, \frac{-1 - i\sqrt{7}}{4} \right\}. \quad (4.20)$$

In the second case, we obtain

$$S_{tot}^2(p) = \frac{1}{G_2(p)} (-2(-6e^{-3ipd} + 4e^{-2ipd} + 10e^{-ipd} - 6)\mathbb{1}_4 + 3e^{-ipd}(e^{-ipd} - 1)A), \quad (4.21)$$

where $G_2(p) = (6e^{-2ipd} - e^{-ipd} - 3)(2e^{-ipd} - 1)$, leading to the poles

$$e^{-ipd} = x \quad \text{with } x \in \left\{ \frac{1}{2}, \frac{1 + \sqrt{73}}{12}, \frac{1 - \sqrt{73}}{12} \right\}. \quad (4.22)$$

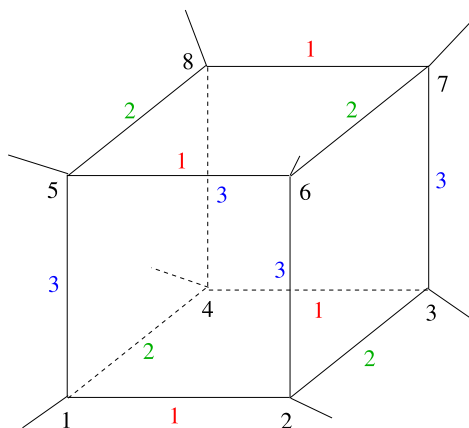


Fig. 3. Cube with an example of numbering.

4.2. Cube

For the cube, $N = 8$ and $\nu = 3$ and the matrices \mathcal{E}_a also commute. So one can perform the same analysis as before.

Based on Fig. 3, we get explicitly

$$\mathcal{E}_1 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathcal{E}_2 = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}, \quad (4.23)$$

$$\mathcal{E}_3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (4.24)$$

and a diagonalizing matrix is

$$V = \frac{1}{2\sqrt{2}} \begin{pmatrix} 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & -1 & 1 & -1 & -1 & 1 \\ -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} = (V^{-1})^t. \quad (4.25)$$

Again assuming that the local scattering matrices are the same at all vertices, we get

$$\mathcal{V}(E(p) - S^{(22)}(p))\mathcal{V}^{-1} = e^{-ipd} \sum_{a=1}^3 \Delta_a \otimes E_{aa} - \mathbb{1}_8 \otimes S^{red}(p), \quad (4.26)$$

where $\Delta_a = V\mathcal{E}_a V^{-1}$ and $\mathcal{V} = V \otimes \mathbb{1}_3$. This is a block diagonal matrix and the problem is reduced to inverting 3×3 matrices,

$$(E(p) - S^{(22)}(p))^{-1} = \mathcal{V}^{-1} \left[\sum_{\alpha=1}^8 E_{\alpha\alpha} \otimes (e^{-ipd} \mathcal{I}_{\alpha} - S^{red}(p))^{-1} \right] \mathcal{V}, \quad (4.27)$$

where

$$\mathcal{I}_1 = \mathbb{1}_3, \quad \mathcal{I}_2 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\mathcal{I}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{I}_4 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (4.28)$$

$$\mathcal{I}_5 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathcal{I}_6 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$\mathcal{I}_7 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathcal{I}_8 = -\mathbb{1}_3. \quad (4.29)$$

We turn to the explicit computation of the total scattering matrix in the two cases (4.17) describing scale and rotation invariant local scattering at the vertices. In both cases, we find the following structures for S_{tot} : it is a linear combination of matrices in the Abelian group generated by the \mathcal{E} 's with coefficients being polynomials in e^{-ipd} . For $j = 1, 2$,

$$S_{tot}^j(p) = a_0^j(p) \mathbb{1}_8 + a_1^j(p) \mathcal{E}_1 + a_2^j(p) \mathcal{E}_2 + a_3^j(p) \mathcal{E}_3 + a_4^j(p) \mathcal{E}_1 \mathcal{E}_2 + a_5^j(p) \mathcal{E}_1 \mathcal{E}_3 \\ + a_6^j(p) \mathcal{E}_2 \mathcal{E}_3 + a_7^j(p) \mathcal{E}_1 \mathcal{E}_2 \mathcal{E}_3. \quad (4.30)$$

In the first case, we find

$$a_0^1(p) = \frac{8 + e^{-ipd} - 8e^{-2ipd} - 5e^{-3ipd} - 40e^{-4ipd} + 4e^{-5ipd} - 32e^{-6ipd}}{4(-1 + e^{-2ipd} + 8e^{-4ipd} + 16e^{-6ipd})}, \quad (4.31)$$

$$a_1^1(p) = \frac{-5e^{-ipd} + e^{-3ipd} - 20e^{-5ipd}}{4(-1 + e^{-2ipd} + 8e^{-4ipd} + 16e^{-6ipd})}, \quad (4.32)$$

$$a_2^1(p) = \frac{3e^{-ipd}}{4 - 16e^{-2ipd}}, \quad (4.33)$$

$$a_3^1(p) = \frac{3e^{-ipd}}{4 - 16e^{-2ipd}}, \quad (4.34)$$

$$a_4^1(p) = -\frac{e^{-ipd}(1 - 9e^{-ipd} + 2e^{-2ipd})}{4(-1 + e^{-ipd} + 2e^{-2ipd} - 4e^{-3ipd} + 8e^{-4ipd})}, \quad (4.35)$$

$$a_5^1(p) = -\frac{e^{-ipd}(1 - 9e^{-ipd} + 2e^{-2ipd})}{4(-1 + e^{-ipd} + 2e^{-2ipd} - 4e^{-3ipd} + 8e^{-4ipd})}, \quad (4.36)$$

$$a_6^1(p) = \frac{e^{-ipd}(1 + 9e^{-ipd} + 2e^{-2ipd})}{4(-1 - e^{-ipd} + 2e^{-2ipd} + 4e^{-3ipd} + 8e^{-4ipd})}, \quad (4.37)$$

$$a_7^1(p) = -\frac{e^{-ipd} + 19e^{-3ipd} + 4e^{-5ipd}}{4(-1 + e^{-2ipd} + 8e^{-4ipd} + 16e^{-6ipd})}. \quad (4.38)$$

The poles of the scattering matrix can be then computed. They are given by

$$e^{-ipd} = x \quad \text{with } x \in \left\{ \pm \frac{1}{2}, \pm \frac{1 + i\sqrt{7}}{4}, \pm \frac{1 - i\sqrt{7}}{4} \right\}. \quad (4.39)$$

In the second case, we find

$$a_0^2(p) = \frac{72 + 9e^{-ipd} - 440e^{-2ipd} - 45e^{-3ipd} + 728e^{-4ipd} + 36e^{-5ipd} - 288e^{-6ipd}}{4(-9 + 73e^{-2ipd} - 184e^{-4ipd} + 144e^{-6ipd})}, \quad (4.40)$$

$$a_1^2(p) = -\frac{3e^{-ipd}(15 - 67e^{-2ipd} + 60e^{-4ipd})}{4(-9 + 73e^{-2ipd} - 184e^{-4ipd} + 144e^{-6ipd})}, \quad (4.41)$$

$$a_2^2(p) = \frac{3e^{-ipd}}{4 - 16e^{-2ipd}}, \quad (4.42)$$

$$a_3^2(p) = \frac{3e^{-ipd}}{4 - 16e^{-2ipd}}, \quad (4.43)$$

$$a_4^2(p) = -\frac{3e^{-ipd}(-1 + 3e^{-ipd} + 2e^{-2ipd})}{4(3 - e^{-ipd} - 18e^{-2ipd} + 4e^{-3ipd} + 24e^{-4ipd})}, \quad (4.44)$$

$$a_5^2(p) = -\frac{3e^{-ipd}(-1 + 3e^{-ipd} + 2e^{-2ipd})}{4(3 - e^{-ipd} - 18e^{-2ipd} + 4e^{-3ipd} + 24e^{-4ipd})}, \quad (4.45)$$

$$a_6^2(p) = \frac{3e^{-ipd}(-1 - 3e^{-ipd} + 2e^{-2ipd})}{4(3 + e^{-ipd} - 18e^{-2ipd} - 4e^{-3ipd} + 24e^{-4ipd})}, \quad (4.46)$$

$$a_7^2(p) = \frac{3e^{-ipd}(3 - 7e^{-2ipd} + 12e^{-4ipd})}{4(9 - 73e^{-2ipd} + 184e^{-4ipd} - 144e^{-6ipd})}. \quad (4.47)$$

The poles of the scattering matrix are given by

$$e^{-ipd} = x \quad \text{with } x \in \left\{ \pm \frac{1}{2}, \pm \frac{1 + \sqrt{73}}{12}, \pm \frac{1 - \sqrt{73}}{12} \right\}. \quad (4.48)$$

5. Conclusion and outlooks

In this paper, we have presented a direct method for the computation of the total scattering matrix of an arbitrary finite noncompact connected graph given its topology, metric structure and local scattering data at each vertex. The method uses the formalism of quantum modes as our initial motivation was the study of quantum fields on graphs. This resulted in a simple and direct algebraic derivation of formula (2.22). We have also shown that the case of loops is easily incorporated in our method. This has been illustrated with an explicit example whose purpose was also to point out that the inverse scattering problem on graphs does not have a unique solution in general for graphs with loops.

We want to stress that in the present paper, the *modes* as we called them, appear more as convenient labels than true quantum field theoretic objects. This has two consequences. First, our results are ready to use for applications in quantum field theory on graphs by simply promoting the modes to generators of the RT-algebra [13], as briefly discussed in Section 2.2. Second, it means that our results hold in complete generality for abstract graphs with or without loops. In this respect, the present results provide an extension of the results in [10] to the case of loops.⁶

Finally, this paper lays the ground to applications to transport problems on arbitrary graphs in the spirit of the studies performed in *e.g.* [3–6] using quantum field theory and bosonization techniques. Indeed, it provides one with the central ingredient which is the total scattering matrix together with its pole structure. Once this structure is known, the calculation of physical data such as the conductance between external edges is rather direct, see *e.g.* [15]. We will return to these questions in the near future. Let us note that some of them have been addressed in the first quantization approach, where the scattering matrix was computed for continuous wave functions [20], and then used to compute local conserved quantities [21].

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⁶ The more general case where relations (2.2) are replaced by a general invertible connecting matrix is easily implemented in our context.

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