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Scattering theory on graphs

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Abstract

We consider the scattering theory for the Schrödinger operator $-D_x^2 + V(x)$ on the graphs made of one-dimensional wires connected to external leads. We derive two expressions for the scattering matrix on arbitrary graphs. One involves matrices that couple arcs (oriented bonds), the other involves matrices that couple vertices. We discuss a simple way to tune the coupling between the graph and the leads. The efficiency of the formalism is demonstrated with a few known examples.

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1. Introduction

The study of graphs is a vast domain. Spectral theory of the Laplacian on graphs has been widely studied in the mathematical literature [1–4]. Here we are interested in the graphs made of one-dimensional wires identified with finite interval of \mathbb{R} and connected at vertices. A trace formula for the partition function of the Laplace operator on such graphs has been derived in a very nice work by Roth [5, 6] who expressed the partition function in terms of the contributions of periodic orbits. The study of the Laplace operator on graphs has been shown to be relevant in many physical situations. It has been first considered for the study of organic molecules [7]. It has also some interest in the context of superconducting networks [8], for the study of adiabatic quantum transport in networks [9, 10] and in the weak localization theory [11–15]. More precisely, several physical quantities of weak localization theory are related to the spectral determinant of the Laplace operator $S(\gamma) = \det(-D_x^2 + \gamma)$, which can be expressed in terms of the determinant of a $V \times V$ -matrix M coupling the vertices [14]. The relation between $S(\gamma)$ and the trace formula obtained by Roth has been examined in [16]. Graphs have also been a subject of several studies in the context of quantum chaos for their spectral properties [17–20] and also their scattering properties when they are connected to leads [21]. Scattering theory on graphs has been studied in [22] and is also frequently used in

the context of transport theory for mesoscopic networks (e.g. [23–26]; more recently graphs were considered [27] to describe mesoscopic 2D normal metal networks and superconducting networks realized experimentally to reveal the so-called Aharonov–Bohm cage effect [28, 29]. In order to describe disordered networks, for example, to understand how the Aharonov–Bohm cage effect is affected by disorder, it is important to have a simple and efficient formalism which incorporates a potential on the bonds.

In this paper we consider the scattering theory for a graph on the bonds of which lives a potential $V(x)$ and connected to external leads from which some wave is injected. Some spectral properties of the Schrödinger operator on graphs have already been studied in [30]. More recently, Desbois generalized the expression of the spectral determinant of the Laplace operator [14] in two ways: in the first step, he considered the case of the Schrödinger operator with a continuity condition of the wave function at the vertices [31, 32]. In the second step [33], he studied the case of the Schrödinger operator with general boundary conditions at the vertices and gave the corresponding expression for the spectral determinant. The scattering problem for graphs with potential has already attracted the attention of several authors (see [34–36] where other references are given). The aim of our study is to provide a general and systematic framework to construct the scattering matrix of a given graph in terms of matrices encoding the information on the topology and the potential on the graph.

This paper is organized as follows: in the next section we introduce the basic definitions. In section 3 we derive an expression of the scattering matrix of the graph in terms of arc matrices (24). In section 4 we take a different point of view and express the scattering matrix in terms of vertex matrices (43) and (48). Our results generalize the formulae known for the Schrödinger operator $-D_x^2$ in the absence of scattering by the bonds [10, 18]. We see that the second formulation of the scattering matrix with vertex matrices offers the advantage of compactness compared to the arc matrix formulation. We discuss, in section 5, simple modifications of the formalism to introduce tunable couplings between the leads and the graph in the most efficient way. Simple examples are developed.

2. Position of the problem

We first define the problem and recall the notations chosen in [16, 31]. We consider the Schrödinger operator

$$H = -D_x^2 + V(x) \quad (1)$$

where $D_x = d_x - iA(x)$ is the covariant derivative and the x coordinate lives on a graph \mathcal{G} made of B one-dimensional wires connected at V vertices. Throughout this paper we will designate the vertices with greek letters $(\alpha, \beta, \mu, \dots)$. We introduce the $V \times V$ -adjacency matrix $a_{\alpha\beta}$; if the vertices α and β are linked by a bond then $a_{\alpha\beta} = 1$ and $a_{\alpha\beta} = 0$ otherwise. The coordination of vertex α (number of bonds issuing from the vertex) is $m_\alpha = \sum_\beta a_{\alpha\beta}$. We call $x_{\alpha\beta} \in [0; l_{\alpha\beta}]$ the coordinate on the bond $(\alpha\beta)$ of length $l_{\alpha\beta}$ (note that by definition $x_{\beta\alpha} = l_{\alpha\beta} - x_{\alpha\beta}$).

The Schrödinger operator acts on scalar functions $\psi(x)$ living on \mathcal{G} that are represented by a set of B components $\psi_{(\alpha\beta)}(x_{\alpha\beta})$ satisfying appropriate boundary conditions at the vertices [9, 10, 37]:

(i) continuity

$$\psi_{(\alpha\beta_i)}(x_{\alpha\beta_i} = 0) = \psi_\alpha \quad \text{for } i = 1, \dots, m_\alpha. \quad (2)$$

The indice β_i designates a vertex neighbour of vertex α ; the wavefunction at the vertex is ψ_α .

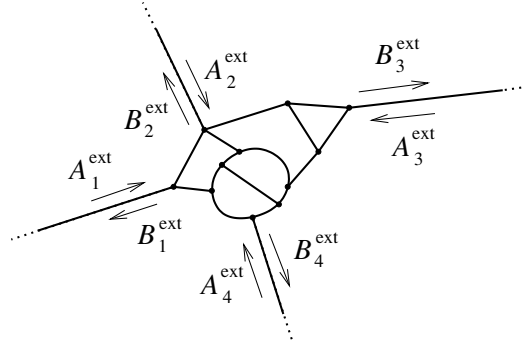


Figure 1. A graph made of $B = 15$ internal bonds and $V = 11$ vertices connected to $L = 4$ external leads.

- (ii) A second condition sufficient to ensure current conservation (i.e. unitarity of the scattering matrix)

$$\sum_{\beta} a_{\alpha\beta} D_{x_{\alpha\beta}} \psi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = \lambda_{\alpha} \psi_{\alpha} \quad (3)$$

where λ_{α} is a real parameter. Due to the presence of the connectivity matrix $a_{\alpha\beta}$, the sum runs over all neighbouring vertices linked with vertex α . To have a better understanding of the physical meaning of the parameter λ_{α} we remark that for a vertex of coordination number 2, equation (3) describes a potential $\lambda_{\alpha} \delta(x_{\alpha\beta})$ at the position of the vertex α . Note also that the limit $\lambda_{\alpha} \rightarrow \infty$ corresponds to the Dirichlet condition $\psi_{\alpha} = 0$ which means that no current is transmitted through this vertex.

It is also possible to consider more general boundary conditions than (2 and 3) and release the continuity condition as it was proposed in [22].

The magnetic flux along the bond is denoted by $\theta_{\alpha\beta} = \int_{\alpha}^{\beta} dx A(x) = -\theta_{\beta\alpha}$.

We also introduce the notion of *arc* which is an *oriented bond*. Each bond $(\alpha\beta)$ is associated with two arcs $\alpha\beta$ and $\beta\alpha$. Throughout this paper we label the arcs with roman letters (i, j, \dots) and designate the reversed arc of i with a bar: \bar{i} .

To describe the potential $V_{(\alpha\beta)}(x_{\alpha\beta})$ on the bond $(\alpha\beta)$ it will be appropriate to introduce reflection and transmission coefficients. We call $r_{\alpha\beta}(E)$ and $t_{\alpha\beta}(E)$ the reflection and transmission probability amplitudes associated with the transmission from vertex α to vertex β for a plane wave of energy E . The scattering 2×2 -matrix for the bond is

$$\begin{pmatrix} r_{\alpha\beta} & t_{\beta\alpha} \\ t_{\alpha\beta} & r_{\beta\alpha} \end{pmatrix}. \quad (4)$$

We consider a scattering problem, that is, a situation where the graph \mathcal{G} is connected to L external leads by which some wave is injected (see figure 1). The on-shell scattering matrix Σ is an $L \times L$ matrix that relates the incoming amplitudes in the L channels to the outgoing ones. We call A_{α}^{ext} (resp. B_{α}^{ext}) the incoming (resp. outgoing) amplitude on the external lead connected at the vertex α . By definition

$$B^{\text{ext}} = \Sigma A^{\text{ext}}. \quad (5)$$

The purpose of this paper is to express Σ by means of arc $2B \times 2B$ -matrices and vertex $V \times V$ -matrices. We generalize the expressions known in the absence of potential [10, 18, 21].

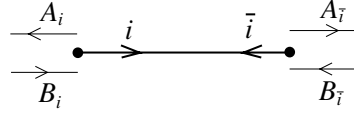


Figure 2. The amplitudes on the arcs i and \bar{i} .

3. Scattering matrix in terms of arc matrices

In this section we construct the scattering matrix by relating it to arc matrices.

3.1. Scattering by bonds

We have already explained in section 2 how to describe the scattering by the potential $V(x)$ on the bonds by 2×2 scattering matrices. We associate with each internal arc i two amplitudes A_i^{int} and B_i^{int} (see figure 2); this means that the component $\psi_i(x)$ of the wave function of energy k^2 matches with $A_i^{\text{int}}e^{-ikx} + B_i^{\text{int}}e^{ikx}$ at the node from which arc i issues. It follows that the amplitudes at the two boundaries of the arc i are related by

$$\begin{pmatrix} A_i^{\text{int}} \\ A_{\bar{i}}^{\text{int}} \end{pmatrix} = \begin{pmatrix} r_i & t_{\bar{i}} \\ t_i & r_{\bar{i}} \end{pmatrix} \begin{pmatrix} B_i^{\text{int}} \\ B_{\bar{i}}^{\text{int}} \end{pmatrix} \quad (6)$$

where \bar{i} is the reversed arc. This relation may be more conveniently written in terms of a matrix R that couples the $2B$ internal arcs

$$A_i^{\text{int}} = \sum_j R_{ij} B_j^{\text{int}} \quad (7)$$

with

$$R_{ij} = r_i \delta_{i,j} + t_{\bar{i}} \delta_{\bar{i},j} \quad (8)$$

where $\delta_{i,j}$ is the Kronecker symbol and indices i and j run over the labels of the $2B$ internal arcs $i, j \in \{1, \dots, B, \bar{1}, \dots, \bar{B}\}$.

If there is no potential on the bonds ($V(x) = 0$) we recover the R -matrix introduced in [16]:

$$R_{ij}^0 = e^{ikl_i} \delta_{\bar{i},j}. \quad (9)$$

The reflection and transmission coefficients characterize the scattering by the potential alone and if we introduce a magnetic field, the modification brought is straightforward: the transmission amplitudes receive additional phases $t_i \rightarrow t_i e^{i\theta_i}$ and the reflection amplitudes are not affected by the magnetic field. $\theta_{\alpha\beta} = \int_{\alpha}^{\beta} dx A(x) = -\theta_{\beta\alpha}$ is the magnetic flux along arc $\alpha\beta$. The bond scattering matrix then reads as

$$R_{ij} = r_i \delta_{i,j} + t_{\bar{i}} e^{-i\theta_i} \delta_{\bar{i},j}. \quad (10)$$

This matrix can also be written in a vertex notation (we identify i with $\alpha\beta$ and j with $\mu\nu$)

$$R_{\alpha\beta,\mu\nu} = a_{\alpha\beta} a_{\mu\nu} (r_{\alpha\beta} \delta_{\alpha\mu} \delta_{\beta\nu} + t_{\beta\alpha} e^{i\theta_{\beta\alpha}} \delta_{\alpha\nu} \delta_{\beta\mu}) \quad (11)$$

where the adjacency matrix elements $a_{\alpha\beta}$ and $a_{\mu\nu}$ ensure that α and β are connected by a bond, as well as μ and ν .

3.2. Scattering by vertices

The bond-scattering matrix only couples amplitudes A^{int} and B^{int} associated with internal arcs. On the other hand, some vertices (L) couple internal bonds and external leads. We write the wavefunction on the lead connected to the vertex α as (see figure 1)

$$\psi_{\text{lead}\alpha}(x) = A_{\alpha}^{\text{ext}} e^{-ikx} + B_{\alpha}^{\text{ext}} e^{ikx} \quad (12)$$

($x = 0$ coincides with the vertex). Since we have to introduce only one pair of amplitudes A_{α}^{ext} , B_{α}^{ext} per external lead, this means that each lead is described by one arc only. Adopting this convention implies that we are now dealing with $2B + L$ arcs. We group the internal and external amplitudes in a unique vector:

$$A = \begin{pmatrix} A^{\text{int}} \\ A^{\text{ext}} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} B^{\text{int}} \\ B^{\text{ext}} \end{pmatrix}. \quad (13)$$

If we consider a given vertex α of coordination m_{α} , it follows from (2) and (3) that the m_{α} incoming amplitudes A_i at the vertex are related to the outgoing amplitudes B_i by a $m_{\alpha} \times m_{\alpha}$ unitary matrix Q_{α} whose diagonal elements are $\frac{2}{m_{\alpha} + i\lambda_{\alpha}/k} - 1$, all others being $\frac{2}{m_{\alpha} + i\lambda_{\alpha}/k}$. We call Q the $(2B + L) \times (2B + L)$ -vertex scattering matrix of the whole graph with leads [16]:

$$B_i = \sum_j Q_{ij} A_j \quad (14)$$

with

$$Q_{ij} = \frac{2}{m_{\alpha} + i\lambda_{\alpha}/k} - 1 \quad \text{if } i = j \text{ (} i \text{ issues from the vertex } \alpha) \quad (15)$$

$$Q_{ij} = \frac{2}{m_{\alpha} + i\lambda_{\alpha}/k} \quad \text{if } i \neq j \text{ both issuing from the vertex } \alpha \quad (16)$$

$$Q_{ij} = 0 \quad \text{otherwise.} \quad (17)$$

We can also write the matrix elements for the internal arcs in a vertex notation:

$$Q_{\alpha\beta, \mu\nu} = a_{\alpha\beta} a_{\mu\nu} \delta_{\alpha\mu} \left(\frac{2}{m_{\alpha} + i\lambda_{\alpha}/k} - \delta_{\beta\nu} \right). \quad (18)$$

All the information on the topology of the graph is encoded in matrix Q .

3.3. Scattering by the full graph

We have seen that the scattering by bonds relates internal amplitudes

$$A^{\text{int}} = R B^{\text{int}} \quad (19)$$

and the scattering by vertices all amplitudes:

$$B = Q A. \quad (20)$$

We separate the Q matrix into four block matrices:

$$Q = \begin{pmatrix} Q^{\text{int}} & \tilde{Q}^{\text{T}} \\ \tilde{Q} & Q^{\text{ext}} \end{pmatrix} \quad (21)$$

where Q^{T} is the transposed matrix (Q^{int} is a $2B \times 2B$ -matrix, Q^{ext} is an $L \times L$ -matrix and \tilde{Q} is an $L \times 2B$ -matrix). In the following we will always choose to write the matrix Q according to this structure.

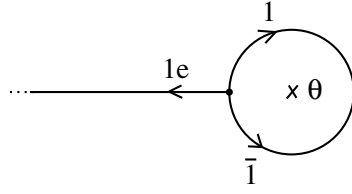


Figure 3. Scattering in a ring pierced by a magnetic flux.

Equation (20) becomes

$$B^{\text{int}} = Q^{\text{int}} A^{\text{int}} + \tilde{Q}^{\text{T}} A^{\text{ext}} \quad (22)$$

$$B^{\text{ext}} = \tilde{Q} A^{\text{int}} + Q^{\text{ext}} A^{\text{ext}}. \quad (23)$$

We can now eliminate the internal amplitudes from (19), (22) and (23) and relate A^{ext} to B^{ext} . Therefore, we obtain the scattering matrix of the graph

$$\Sigma = Q^{\text{ext}} + \tilde{Q}(R^{\dagger} - Q^{\text{int}})^{-1} \tilde{Q}^{\text{T}}. \quad (24)$$

We have used the unitarity of R

$$(R^{-1})_{ij} = (R^{\dagger})_{ij} = r_i^* \delta_{i,j} + t_i^* e^{-i\theta_i} \delta_{\bar{i},j}. \quad (25)$$

The expression (24) generalizes the result known in the absence of potential [21].

Example. As an example we consider the scattering on the ring of perimeter l pierced by a flux θ (figure 3) without potential, a simple geometry studied in many studies like [26, 36, 38]. This graph possesses one internal bond (arcs 1 and $\bar{1}$); the external lead is associated with an arc called $1e$. The bond-scattering matrix (10) and (11) is

$$R = \begin{pmatrix} 0 & e^{ikl-i\theta} \\ e^{ikl+i\theta} & 0 \end{pmatrix} \quad (26)$$

and the vertex-scattering matrix (15)–(18), expressed in a basis of arcs $\{1, \bar{1}, 1e\}$ (see figure 3) for $\lambda_{\alpha} = 0$, reads as

$$Q = \left(\begin{array}{cc|c} -1/3 & 2/3 & 2/3 \\ 2/3 & -1/3 & 2/3 \\ \hline 2/3 & 2/3 & -1/3 \end{array} \right). \quad (27)$$

Applying (24) we find

$$\Sigma = -\frac{3e^{ikl} - 4 \cos \theta + e^{-ikl}}{3e^{-ikl} - 4 \cos \theta + e^{ikl}}. \quad (28)$$

With one lead, the scattering matrix is given by a unique phase $\Sigma(E) = e^{i\delta(E)}$ with

$$\cot \frac{\delta}{2} = \frac{\sin kl}{2(\cos \theta - \cos kl)}. \quad (29)$$

We recover a result obtained by relating the scattering matrix to the ratio of spectral determinants in the one-channel case [16].

Remark: multichannel wires. We remark that the formulation of the scattering in terms of arc matrices can be generalized for multichannel wires: the matrix elements Q_{ij} and R_{ij} would then become submatrices coupling channels.

3.4. Multiple-scattering expansion

It is sometimes interesting to expand the quantities of interest in terms of contributions of paths in the graph (we call *path* an ordered set of arcs). Since the matrices Q and R contain the scattering amplitudes on vertices and bonds, respectively, it is obvious that the expansion of (24) expresses the contributions of paths to the transmission amplitudes from one lead to another:

$$\Sigma = Q^{\text{ext}} + \tilde{Q}R\tilde{Q}^{\text{T}} + \tilde{Q}RQ^{\text{int}}R\tilde{Q}^{\text{T}} + \dots + \tilde{Q}R(Q^{\text{int}}R)^n\tilde{Q}^{\text{T}} + \dots \quad (30)$$

The first term is associated with transmission from leads without entering the graph. The term $\tilde{Q}R\tilde{Q}^{\text{T}}$ corresponds to paths that contain only one bond of the graph. More generally, the element $(\tilde{Q}R(Q^{\text{int}}R)^n\tilde{Q}^{\text{T}})_{ij}$ is the sum of all amplitudes associated with the paths made of $n + 1$ internal arcs and going from lead j to lead i .

4. Scattering matrix in terms of vertex matrices

The approach presented in the previous section has the advantage of considering only scattering matrices for bonds and vertices but presents the disagreement to manipulate rather big matrices ($2B \times 2B$). In this section we follow a different methodology by constructing the stationary scattering states in the graph which leads to dealing with vertex matrices ($V \times V$) that are usually smaller.

For convenience, we label the vertices connected to leads with the L -first indices: $\alpha = 1, \dots, L$; however, the final result will be completely independent of the way the basis of vertices is organized.

We introduce the $L \times V$ matrix W [18] containing the information about the way the graph is connected: $W_{\alpha\beta} = \delta_{\alpha\beta}$ with $\alpha \in \{1, \dots, L\}$ and $\beta \in \{1, \dots, V\}$,

$$W = \left(\begin{array}{cccc|cccc} 1 & 0 & \dots & 0 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & 0 & 1 & 0 & \dots & 0 \end{array} \right). \quad (31)$$

We now turn to the construction of the stationary scattering states $\psi^{(\alpha)}(x)$ of energy k^2 which describes a plane wave entering the graph from the lead connected at vertex α and being scattered by the graph into all leads. We consider the case without a magnetic field since the addition of a magnetic field is straightforward by adding the appropriate phases in the transmission coefficients of the bonds.

On the lead connected to vertex μ , the wave function is

$$\psi_{\text{lead } \mu}^{(\alpha)}(x) = \delta_{\mu\alpha}e^{-ikx} + \Sigma_{\mu\alpha}e^{ikx} \quad (32)$$

with $x \in [0; +\infty[$.

To construct a wavefunction on the internal bond $(\mu\beta)$ of the graph, it is convenient to introduce two linearly independent solutions $f_{\mu\beta}(x_{\mu\beta})$ and $f_{\beta\mu}(x_{\mu\beta})$ of the differential equation

$$\left(-\frac{d^2}{dx_{\mu\beta}^2} + V_{(\mu\beta)}(x_{\mu\beta}) + \gamma \right) f(x_{\mu\beta}) = 0 \quad (33)$$

for $x \in [0, l_{\mu\beta}]$, satisfying the following boundary conditions at the edges of the interval:

$$\begin{cases} f_{\mu\beta}(\mu) = 1 \\ f_{\mu\beta}(\beta) = 0 \end{cases} \quad \text{and} \quad \begin{cases} f_{\beta\mu}(\mu) = 0 \\ f_{\beta\mu}(\beta) = 1 \end{cases}. \quad (34)$$

We follow here the construction of the spectral determinant for the Schrödinger operator in [31]. To lighten the expressions we have introduced the obvious notation $f(\mu) \equiv f(x_{\mu\beta} = 0)$ and $f(\beta) \equiv f(x_{\mu\beta} = l_{\mu\beta})$. The spectral parameter is

$$\gamma = -k^2 - i0^+. \quad (35)$$

For example, if $V_{(\mu\beta)}(x) = 0$ the two functions are $f_{\mu\beta}(x_{\mu\beta}) = \frac{\text{sh}\sqrt{\gamma}(l_{\mu\beta} - x_{\mu\beta})}{\text{sh}\sqrt{\gamma}l_{\mu\beta}}$ and $f_{\beta\mu}(x_{\mu\beta}) = \frac{\text{sh}\sqrt{\gamma}x_{\mu\beta}}{\text{sh}\sqrt{\gamma}l_{\mu\beta}}$.

We call $\psi_{\mu}^{(\alpha)}$ the wavefunction at the vertex μ when the plane wave is injected at vertex α . The solution of the Schrödinger equation (33) on the bond $(\mu\beta)$

$$\psi_{(\mu\beta)}^{(\alpha)}(x_{\mu\beta}) = \psi_{\mu}^{(\alpha)} f_{\mu\beta}(x_{\mu\beta}) + \psi_{\beta}^{(\alpha)} f_{\beta\mu}(x_{\mu\beta}) \quad (36)$$

already satisfies the continuity condition (2).

If we impose condition (2) for the wave function on the lead $(\psi_{\text{lead}\mu}^{(\alpha)}(0) = \psi_{\mu}^{(\alpha)})$ we get

$$\delta_{\mu\alpha} + \Sigma_{\mu\alpha} = \psi_{\mu}^{(\alpha)} \quad \text{for } \mu = 1, \dots, L. \quad (37)$$

The solution $\psi^{(\alpha)}(x)$ must also satisfy condition (3), that is

$$\sum_{\beta} a_{\mu\beta} \frac{d\psi_{(\mu\beta)}^{(\alpha)}}{dx_{\mu\beta}}(\mu) + (W^T W)_{\mu\mu} \frac{d\psi_{\text{lead}\mu}^{(\alpha)}}{dx}(\mu) = \lambda_{\mu} \psi_{\mu}^{(\alpha)} \quad \text{for } \mu = 1, \dots, V. \quad (38)$$

The $(W^T W)_{\mu\mu}$ ensures that this contribution to current from leads vanishes if μ is an internal vertex. This equation can be rewritten as

$$(W^T W)_{\mu\mu} (\delta_{\mu\alpha} - \Sigma_{\mu\alpha}) = \sum_{\beta} M_{\mu\beta} \psi_{\beta}^{(\alpha)} \quad \text{for } \mu = 1, \dots, V \quad (39)$$

where M is the matrix appearing in the expression of the spectral determinant¹ [31]

$$M_{\mu\beta}(\gamma) = \frac{1}{\sqrt{\gamma}} \left(\delta_{\mu\beta} \left[\lambda_{\mu} - \sum_v a_{\mu v} \frac{df_{\mu v}}{dx_{\mu v}}(\mu) \right] + a_{\mu\beta} \frac{df_{\mu\beta}}{dx_{\mu\beta}}(\beta) \right). \quad (40)$$

If we consider $\psi_{\mu}^{(\alpha)}$ as the matrix elements (μ, α) of a $V \times L$ -matrix Ψ , (37) and (39) can be rewritten in a matrix form

$$1 + \Sigma = W\Psi \quad (41)$$

$$W^T(1 - \Sigma) = M\Psi. \quad (42)$$

We obtain the scattering matrix by eliminating Ψ from (41) and (42) (with the help of the identity recalled in appendix C). Finally we get

$$\Sigma = -1 + 2W(M + W^T W)^{-1} W^T. \quad (43)$$

The last step is to relate the matrix M to the reflection and transmission coefficients of the bonds. For this purpose we note that we could have chosen a different basis of solutions of equation (33) to construct the stationary state (36) on the bond. In particular, we could have chosen the right $\phi_{\beta\mu}(x)$ and left $\phi_{\mu\beta}(x)$ stationary scattering states solely associated with the

¹ We have used the fact that the Wronskian is equal to

$$\mathcal{W}[f_{\mu\beta}, f_{\beta\mu}] = f_{\mu\beta} \frac{df_{\beta\mu}}{dx_{\mu\beta}} - \frac{df_{\mu\beta}}{dx_{\mu\beta}} f_{\beta\mu} = \frac{df_{\beta\mu}}{dx_{\mu\beta}}(\mu) = -\frac{df_{\mu\beta}}{dx_{\mu\beta}}(\beta).$$

potential $V_{(\mu\beta)}(x)$ of the bond. If we think of the bond potential $V_{\beta\mu}(x)$ with support $[0, l_{\mu\beta}]$ embedded in an infinite line (\mathbb{R}), these states would be written outside the interval as

$$\begin{aligned} \phi_{\mu\beta}(x) &= e^{ikx} + r_{\mu\beta}e^{-ikx} && \text{for } x \leq 0 \\ &= t_{\mu\beta}e^{ik(x-l_{\mu\beta})} && \text{for } x \geq l_{\mu\beta} \\ \phi_{\beta\mu}(x) &= t_{\beta\mu}e^{-ikx} && \text{for } x \leq 0 \\ &= e^{-ik(x-l_{\mu\beta})} + r_{\beta\mu}e^{ik(x-l_{\mu\beta})} && \text{for } x \geq l_{\mu\beta}. \end{aligned} \tag{44}$$

It is easy to see that the functions $f_{\mu\beta}(x)$ are related to those stationary scattering states by

$$f_{\mu\beta}(x_{\mu\beta}) = \frac{(1 + r_{\beta\mu})\phi_{\mu\beta}(x_{\mu\beta}) - t_{\mu\beta}\phi_{\beta\mu}(x_{\mu\beta})}{(1 + r_{\mu\beta})(1 + r_{\beta\mu}) - t_{\mu\beta}t_{\beta\mu}}. \tag{45}$$

Then

$$\frac{df_{\mu\beta}}{dx_{\mu\beta}}(\mu) = ik \frac{(1 - r_{\mu\beta})(1 + r_{\beta\mu}) + t_{\mu\beta}t_{\beta\mu}}{(1 + r_{\mu\beta})(1 + r_{\beta\mu}) - t_{\mu\beta}t_{\beta\mu}} \tag{46}$$

and

$$\frac{df_{\mu\beta}}{dx_{\mu\beta}}(\beta) = ik \frac{2t_{\mu\beta}}{(1 + r_{\mu\beta})(1 + r_{\beta\mu}) - t_{\mu\beta}t_{\beta\mu}}. \tag{47}$$

We can now express the matrix M for $\gamma = -k^2 - i0^+$ in terms of bond reflections and transmissions as

$$M_{\alpha\beta} = \delta_{\alpha\beta} \left(i \frac{\lambda_\alpha}{k} + \sum_{\mu} a_{\alpha\mu} \frac{(1 - r_{\alpha\mu})(1 + r_{\mu\alpha}) + t_{\alpha\mu}t_{\mu\alpha}}{(1 + r_{\alpha\mu})(1 + r_{\mu\alpha}) - t_{\alpha\mu}t_{\mu\alpha}} \right) - a_{\alpha\beta} \frac{2t_{\alpha\beta}}{(1 + r_{\alpha\beta})(1 + r_{\beta\alpha}) - t_{\alpha\beta}t_{\beta\alpha}}. \tag{48}$$

This equation with (43) generalizes the result known in the absence of the potential [10, 18]. In appendix A we rewrite the matrix M with real parameters replacing the complex reflection and transmission coefficients of the bonds, and in appendix B we discuss how it is modified if the graph contains loops that we do not want to describe with several vertices.

We repeat that the addition of a magnetic field implies the substitution $t_{\alpha\beta} \rightarrow t_{\alpha\beta}e^{i\theta_{\alpha\beta}}$, the reflections being unchanged.

Note that if $V(x) = 0$ we have $r_{\alpha\beta} = 0$ and $t_{\alpha\beta} = e^{ikl_{\alpha\beta} + i\theta_{\alpha\beta}}$ and we recover the well-known matrix [7, 8, 37] that appears in the search of the eigenvalues of the closed graph (if $\lambda_\alpha = 0$):

$$M_{\alpha\beta}^0 = i \delta_{\alpha\beta} \sum_{\mu} a_{\alpha\mu} \cot kl_{\alpha\mu} - a_{\alpha\beta} \frac{ie^{i\theta_{\alpha\beta}}}{\sin kl_{\alpha\beta}}. \tag{49}$$

Example. We consider again the case of the ring (figure 3); this example has been studied in [10]. The graph can be described with only one vertex to which one loop is attached. In this case the matrix M reduces to a scalar (see [15, 16] and appendix B):

$$M = 2i \left(\cot kl - \frac{\cos \theta}{\sin kl} \right). \tag{50}$$

The matrix W reduces to 1 and we recover from (43) the result (28) in a straightforward manner:

$$\Sigma = \frac{i \sin kl + 2(\cos kl - \cos \theta)}{i \sin kl - 2(\cos kl - \cos \theta)}. \tag{51}$$

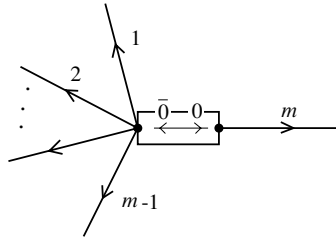


Figure 4. The box on the arc 0 represents a potential characterized by the scattering matrix (53). The arc m can be decoupled from the other external arcs by tuning the transmission through the bond (0).

Remark: spectral determinant. Note that the spectral determinant $S(\gamma) = \prod_n (E_n + \gamma)$ characterizing the spectrum of the isolated graph can also be expressed in terms of the reflection and transmission coefficients by using equations (46)–(48) with the result of Desbois [31]:

$$S(\gamma) = \gamma^{V/2} \prod_{(\alpha\beta)} \left(\frac{df_{\beta\alpha}}{dx_{\alpha\beta}}(\alpha) \right)^{-1} \det M(\gamma). \tag{52}$$

5. Tuning the coupling of the graph to the leads

In this section we consider the situation where a graph \mathcal{G} can be decoupled from the leads at which it is connected by tuning some parameters. One way to proceed is to add a bond with a tunable transmission between each lead and the corresponding vertex to which it is plugged in (figure 5); this can be described with the formalism we have presented above in the two previous sections but requires consideration of a new graph $\tilde{\mathcal{G}}$ with $V + L$ vertices and $B + L$ bonds (if \mathcal{G} has V vertices, B bonds and L leads). The purpose of this section is to demonstrate that the problem can be reduced, in the sense that we can keep considering the original graph \mathcal{G} with V vertices and B bonds, provided some modifications of the above formalism are made: (i) in the ‘arc matrices’ formulation we have to modify the vertex-scattering matrix for vertices connected to leads. (ii) In the ‘vertex matrices’ formulation, formulae (43) and (48) still hold using the matrix M of \mathcal{G} if we modify the matrix W in a way that appears to be very natural.

5.1. A vertex-scattering matrix including arbitrary coupling of one arc

We construct the scattering matrix of the graph of figure 4 made of one bond (two arcs 0 and $\bar{0}$). To describe the scattering on the bond (0) we choose a simple bond-scattering matrix (10)

$$R = \begin{pmatrix} \cos \xi & \sin \xi \\ \sin \xi & -\cos \xi \end{pmatrix} \tag{53}$$

that allows tuning of the transmission probability through the bond $T = \sin^2 \xi$. At one side of the bond, $m - 1$ arcs are connected and there is only one at the other side. The scattering matrix we obtain is the scattering matrix for a vertex with m arcs among which one can be disconnected by tuning the parameter ξ , all other arcs being equivalent.

On the basis of arcs $\{0, \bar{0}, 1, 2, \dots, m\}$, the matrix Q (15)–(17) is

$$Q = \left(\begin{array}{cc|ccc} \frac{2}{m} - 1 & 0 & \frac{2}{m} & \frac{2}{m} & \dots & \frac{2}{m} & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 1 \\ \hline \frac{2}{m} & 0 & \frac{2}{m} - 1 & \frac{2}{m} & \dots & \frac{2}{m} & 0 \\ \frac{2}{m} & 0 & \frac{2}{m} & \frac{2}{m} - 1 & \dots & \frac{2}{m} & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \frac{2}{m} & 0 & \frac{2}{m} & \frac{2}{m} & \dots & \frac{2}{m} - 1 & 0 \\ 0 & 1 & 0 & 0 & \dots & 0 & 0 \end{array} \right). \tag{54}$$

The matrix has been written with the parameter $\lambda = 0$ to lighten the expressions. This parameter is re-introduced by performing the following substitution in a straightforward manner:

$$m \rightarrow m + i \frac{\lambda}{k}. \tag{55}$$

We now use equation (24) to express the $m \times m$ scattering matrix of the graph

$$\Sigma = \left(\begin{array}{c|c} \rho & \tau^T \\ \hline \tau & \rho' \end{array} \right) \tag{56}$$

where ρ is a $(m - 1) \times (m - 1)$ matrix, τ a line vector of dimension $m - 1$ and ρ' a number:

$$\rho_{ij} = \frac{2}{m} \frac{1 + \cos \xi}{1 + (1 - \frac{2}{m}) \cos \xi} - \delta_{i,j} \tag{57}$$

$$\tau_i = \frac{2}{m} \frac{\sin \xi}{1 + (1 - \frac{2}{m}) \cos \xi} \tag{58}$$

$$\rho' = -\frac{1 - \frac{2}{m} + \cos \xi}{1 + (1 - \frac{2}{m}) \cos \xi}. \tag{59}$$

The indices i, j run over the first $m - 1$ equivalent arcs.

A more convenient parametrization is obtained by relating $\xi \in] - \pi, \pi]$ to a parameter $w \in \mathbb{R}$:

$$w = \tan(\xi/2). \tag{60}$$

We emphasize that the parameter w characterizes only the scattering through the bond (0) (figure 4). With this new parameter the scattering matrix takes the simpler form

$$\rho_{ij} = \frac{2}{m^*} - \delta_{i,j} \tag{61}$$

$$\tau_i = \frac{2w}{m^*} \tag{62}$$

$$\rho' = \frac{2w^2}{m^*} - 1 \tag{63}$$

where we have re-introduced the parameter λ in

$$m^* = m - 1 + w^2 + i \frac{\lambda}{k}. \tag{64}$$

m^* plays the role of an effective coordination number. The expressions (61)–(63) generalize the vertex-scattering matrix introduced in [5] to the case of tunable couplings to the leads. These transmission coefficients were used to calculate the weights of the periodic orbits involved in the trace formula [5, 6] and later in [17, 18, 21].

Let us examine several limiting cases to have a better understanding of the role of parameter w :

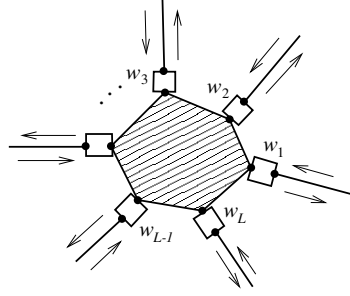


Figure 5. Graph with arbitrary coupling to leads. The couplings w_α 's are represented by boxes; we recall that they are defined by $w_\alpha = \tan(\xi_\alpha/2)$ where the transmission through the box is $T_\alpha = \sin^2 \xi_\alpha$. The dashed area schematizes the internal structure of the graph.

- If $w = 1$, the matrix Σ is the symmetric $m \times m$ -scattering matrix for a vertex of coordination m given by (15)–(18). In this case the transmission of the bond (0) is $T = 1$.
- If $w = 0$, the last arc is decoupled from the others and no current is transmitted to this arc. The scattering between $m - 1$ other arcs, described by the $(m - 1) \times (m - 1)$ matrix ρ , is given by the usual scattering matrix (15)–(18) for a coordination $m - 1$.
- If $w = \sqrt{m - 1}$ and $\lambda = 0$, the scattering matrix coincides with the one introduced by Shapiro [23] up to an inessential change of the sign of ρ (this case corresponds to $\cos \xi = -1 + \frac{2}{m}$, i.e. a transmission $T = \frac{4(m-1)}{m^2}$).
- If $w = \pm\infty$, all the arcs are decoupled: $\rho_{ij} = -\delta_{i,j}$, $\tau_i = 0$ and $\rho' = 1$. From the point of view of the $m - 1$ first arcs, this limit is equivalent to $\lambda = \pm\infty$.

Here we have given a generalization of the scattering matrix proposed in [25] for the case of coordination $m = 3$ and $\lambda = 0$. A generalization to any m of the parametrization of Büttiker *et al* is

$$\Sigma = \left(\begin{array}{ccc|c} b & b & \dots & \sqrt{\epsilon} \\ b & b & \dots & \sqrt{\epsilon} \\ \vdots & \vdots & \ddots & \vdots \\ \hline \sqrt{\epsilon} & \sqrt{\epsilon} & \dots & c \end{array} \right) - 1 \quad (65)$$

where $b = \frac{1}{m-1} (1 + \sqrt{1 - (m-1)\epsilon})$ and $c = 2 - (m-1)b = 1 - \sqrt{1 - (m-1)\epsilon}$. The relation with our parametrization with w is given by $\sqrt{\epsilon} = \frac{2w}{m^*}$ (then $b = \frac{2}{m^*}$), valid for $\lambda = 0$. Note, however, that the parametrization with $\epsilon \in [0, 1/(m-1)]$ does not allow covering of the full range of the parameter $w \in \mathbb{R}$, but only the interval $w \in [0, \sqrt{m-1}]$.

5.2. Scattering matrix of the graph with arbitrary coupling to the leads

We now consider the graph \mathcal{G} of figure 5. Each external lead is connected to vertices $\alpha \in \{1, 2, \dots, L\}$ of the graph through a barrier which is described by a parameter $w_\alpha \in \mathbb{R}$; we call those vertices ‘external vertices’. The scattering matrix of the full graph can be constructed with (24). Let us discuss the structure of the vertex-scattering matrix. Q couples arcs issuing from the same vertex; to help the discussion, let us imagine for a moment that the basis of the arcs is organized so that the arcs issuing from the same vertex are grouped. The matrix Q is a block-diagonal matrix in such a basis. As above, we call Q_α the $m_\alpha \times m_\alpha$ block coupling the arcs issuing from the vertex α . The blocks related to internal vertices

$\alpha \in \{L + 1, \dots, V\}$ are unchanged, still given by (15)–(17), whereas the blocks coupling arcs issuing from external vertices $\alpha \in \{1, \dots, L\}$ are now given by (56) and (61)–(63)

$$Q_\alpha = \frac{2}{m_\alpha^*} \left(\begin{array}{cccc|c} 1 & 1 & \cdots & 1 & w_\alpha \\ 1 & 1 & \cdots & 1 & w_\alpha \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 & w_\alpha \\ \hline w_\alpha & w_\alpha & \cdots & w_\alpha & w_\alpha^2 \end{array} \right) - 1 \tag{66}$$

where $m_\alpha^* \equiv m_\alpha - 1 + w_\alpha^2 + i\lambda_\alpha/k$. The introduction of the couplings in this way does not increase the size of the matrices we have to deal with by using (24).

Now we would like to generalize formula (43) without increasing the difficulty of the calculation of Σ . The construction of the scattering matrix Σ using vertex matrices uses the continuity of the wave function as a basic ingredient at the vertices. If we now describe the scattering at the external vertices with (66), this means that the wave function is not continuous anymore at those vertices due to their internal structure (but still continuous at vertices inside the graph). For a moment we focus on the vertex α with m_α arcs among which $m_\alpha - 1$ are internal arcs of the graph, the remaining arc being a lead. We call $A_1, A_2, \dots, A_{m_\alpha-1}$ the $m_\alpha - 1$ incoming amplitudes from the graph and A_{m_α} the incoming amplitude from the lead. Let us examine the value of the wavefunction on the arcs i : $\psi_i(x) = A_i e^{-ikx} + B_i e^{ikx}$. We have $B_i = \sum_{j=1}^{m_\alpha} (Q_\alpha)_{ij} A_j$; on the arc i , if $x \rightarrow 0$ the wavefunction goes to $\psi_i(0) = A_i + B_i$. It follows from expression (66) that we still have the continuity for the wavefunction on the arcs inside the graph

$$\psi_1(0) = \dots = \psi_{m_\alpha-1}(0) = \frac{2}{m_\alpha^*} \mathcal{A} + \frac{2 w_\alpha}{m_\alpha^*} \mathcal{A}' \tag{67}$$

and the wavefunction at the extremity of the lead is

$$\psi_{m_\alpha}(0) = \frac{2 w_\alpha}{m_\alpha^*} \mathcal{A} + \frac{2 w_\alpha^2}{m_\alpha^*} \mathcal{A}' \tag{68}$$

where $\mathcal{A} = A_1 + \dots + A_{m_\alpha-1}$ and $\mathcal{A}' = A_{m_\alpha}$. It is straightforward to see that the matrix involved in the two equations has an eigenvalue zero associated with the eigenvector $(w_\alpha, -1)$. It follows that

$$\psi_1(0) = \dots = \psi_{m_\alpha-1}(0) = \frac{1}{w_\alpha} \psi_{m_\alpha}(0). \tag{69}$$

This equation replaces the continuity condition for the vertices coupled to the leads.

We now consider the full graph and follow the same lines as in the previous section to construct the scattering matrix by constructing the stationary scattering state $\psi^{(\alpha)}(x)$ of energy $E = k^2$ corresponding to a plane wave injected from the lead α . The wavefunction on the lead connected to the vertex μ is (32) and (36) on the internal bonds. By virtue of (69) the continuity condition (37) is now replaced by

$$\delta_{\mu\alpha} + \Sigma_{\mu\alpha} = w_\mu \psi_\mu^{(\alpha)} \quad \text{for } \mu = 1, \dots, L. \tag{70}$$

The current conservation reads as

$$\psi_\mu^{(\alpha)*} \sum_\beta a_{\mu\beta} d_x \psi_{(\mu\beta)}^{(\alpha)}(\mu) + \psi_{\text{lead } \mu}^{(\alpha)*}(\mu) d_x \psi_{\text{lead } \mu}^{(\alpha)}(\mu) = \lambda_\mu |\psi_\mu^{(\alpha)}|^2 \quad \text{for } \mu = 1, \dots, L \tag{71}$$

$$\sum_\beta a_{\mu\beta} d_x \psi_{(\mu\beta)}^{(\alpha)}(\mu) = \lambda_\mu \psi_\mu^{(\alpha)} \quad \text{for } \mu = L + 1, \dots, V \tag{72}$$

which is now rewritten as

$$w_\mu(\delta_{\mu\alpha} - \Sigma_{\mu\alpha}) = \sum_{\beta} M_{\mu\beta} \psi_{\beta}^{(\alpha)} \quad \text{for } \mu = 1, \dots, L \quad (73)$$

$$0 = \sum_{\beta} M_{\mu\beta} \psi_{\beta}^{(\alpha)} \quad \text{for } \mu = L + 1, \dots, V. \quad (74)$$

Equations (70), (73) and (74) have the same form as (41) and (42) provided that the $L \times V$ -matrix W is now defined as

$$W_{\alpha\beta} = w_\alpha \delta_{\alpha\beta} \quad (75)$$

with $w_\alpha \in \mathbb{R}$. The introduction of tunable couplings² between the graph and the leads in (43) and (48) is thus a simple modification of matrix W with (75). Looking at equation (43), this modification seems very natural. However, we stress that we have given in the above paragraph a precise physical meaning to the parameters w_α 's by relating them to the scattering matrix (53) and equation (60).

5.3. Resonances

It is easy to see from the above formalism how the spectrum of resonances of the graph connected to external leads is related to the eigenvalues spectrum of the same isolated graph. The spectrum of resonances is given by the poles of the scattering matrix, the real part of the pole being the energy of the resonance and the imaginary part its width.

- (i) In the vertex matrix formulation, the poles of Σ are the complex zeros of $\det(M + W^T W)$. The matrix M encodes all the information on the isolated graph (topology of the graph and potential on the bonds) whereas the information on the way the graph is coupled to the external leads is contained in W . If we turn off the couplings $w_\alpha \rightarrow 0$, it is clear that we recover the energies of the isolated graph, solutions³ of $\det M(-k^2) = 0$ (see [31] and remark of section 4).
- (ii) In the arc matrix formulation, the poles are the zeros of $\det(1 - RQ^{\text{int}})$. Now the information on the topology of the graph and the couplings is mixed in Q^{int} whereas R encodes the information on the potential. Again, if the couplings are switched off, the matrix Q^{int} is equal to the matrix Q of the isolated graph whose spectrum is given by $\det(1 - RQ) = 0$.

Example 1. We compute the scattering matrix of a ring connected to one lead (figure 6). This is the situation considered in [26]. The result is obtained by replacing (27) by (66) in the calculation we have already made. A more direct way is to use (43) and (75), $\Sigma = -1 + 2\frac{w^2}{M+w^2}$, the matrix M being given by (50).

² The question of tunable couplings has also been studied in [36]. It is interesting to point out the relation between the coupling parameter w and the parameters α , $\tilde{\alpha}$ and γ introduced in [36] where the continuity equation and 'current conservation' are written for the external node with one lead and M internal bonds: $\psi_{\text{lead}}(0) = \frac{1}{\alpha} \psi'_{\text{lead}}(0) + \gamma \sum_{i=1}^M \psi'_i(0)$ and $\psi_1(0) = \dots = \psi_M(0) = \gamma^* \psi'_{\text{lead}}(0) + \frac{1}{\tilde{\alpha}} \sum_{i=1}^M \psi'_i(0)$. Comparing these equations with (69) and (71) we immediately see that $\alpha = \frac{\lambda}{w^2}$, $\tilde{\alpha} = \lambda$ and $\gamma = \frac{w}{\lambda}$.

³ Note that in certain cases, the equation $\det M(-k^2) = 0$ is not sufficient to construct all the eigenstates of the graph. However, the states missed by this equation are found by solving $\det(1 - RQ) = 0$ for the isolated graph. Such a situation occurs, for example, for the complete graph K_V (a graph with V vertices all connected by bonds of same length) considered in [16].

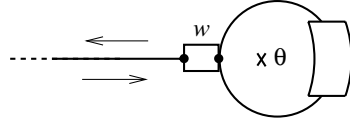


Figure 6. Ring with arbitrary coupling w to the lead.

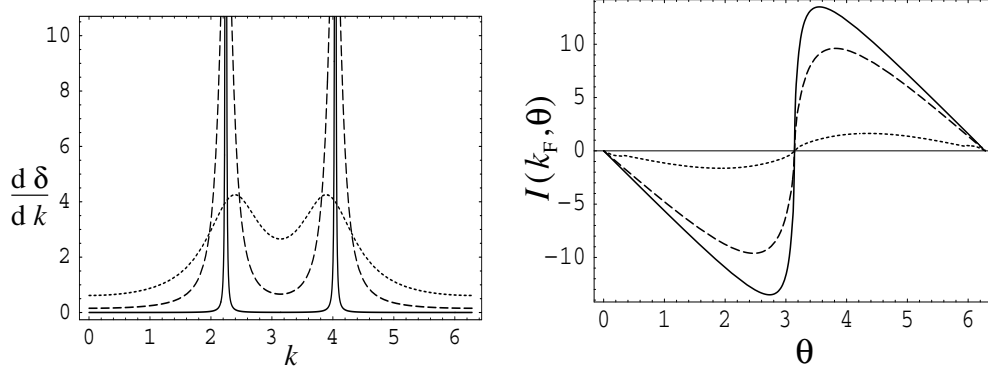


Figure 7. Left: $\frac{d\delta}{dk}$ for the ring of figure 6 for different values of the coupling w . Dotted lines: $w = 1$, dashed lines: $w = 0.5$ and solid lines: $w = 0.05$. The flux is $\theta = 5\pi/7$ and the length $l = 1$. Right: persistent current $I(k_F, \theta) = \int_0^{k_F} dk 2k j(k^2, \theta)$ for $w = 0.5$ (solid line), $w = 1$ (dashed lines) and $w = 5$ (dotted lines). We have chosen $k_F l = 3\pi$.

If we consider the case of a ring with a potential on the bond like in figure 6, M is given by $M = 2i \frac{\cos \Phi - \sqrt{T} \cos \theta}{\sin \Phi - \sqrt{1-T} \cos \varphi}$, as explained in appendix B. We obtain $\Sigma = e^{i\delta}$ with

$$\cot \frac{\delta}{2} = w^2 \frac{\sin \Phi - \sqrt{1-T} \cos \varphi}{2(\sqrt{T} \cos \theta - \cos \Phi)}. \quad (76)$$

For $w = 0$, the ring is disconnected from the arm and the phase shift is constant ($\delta = \pi$). We now consider the case without a potential on the ring: $T = 1$, $\Phi = kl$.

$$\cot \frac{\delta}{2} = w^2 \frac{\sin kl}{2(\cos \theta - \cos kl)}. \quad (77)$$

If $w = 1$ we recover the result (29). The effect of the parameter w can clearly be seen if we compute $\frac{d\delta}{dk}$ (see figure 7):

$$\frac{d\delta}{dk} = lw^2 \frac{1 - \cos \theta \cos kl}{(\cos \theta - \cos kl)^2 + \frac{1}{4}w^4 \sin^2 kl}. \quad (78)$$

We now discuss the two ways to decouple the lead from the ring.

- In the limit $w \rightarrow 0$, the width of the resonance peaks is $\Delta k = \frac{w^2}{2l}$, the peaks being centred on the eigen-energies of the isolated ring of perimeter l : $k_n^\pm l = \pm \theta + 2n\pi$, with $n \in \mathbb{N}$ for the sign $+$ and $n \in \mathbb{N}^*$ for the sign $-$. We have $\frac{d\delta}{dk} \simeq 2\pi \frac{\Delta k/\pi}{(k - k_n^\pm)^2 + \Delta k^2}$ if $k \sim k_n^\pm$.
- In the limit $w \rightarrow \infty$ the three arcs decouple, the ring is open and $\frac{d\delta}{dk}$ presents peaks of width $\Delta k = \frac{2}{w^2 l} (1 - (-1)^m \cos \theta)$ centred on the eigen-energies of the isolated line of length l : $\kappa_m l = m\pi$, for $m \in \mathbb{N}$.

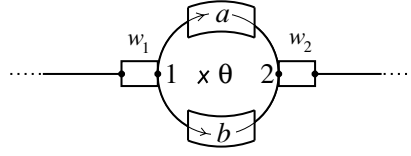


Figure 8. Ring pierced by a magnetic flux θ with potentials on the bonds.

The physical difference between the two limits may also be seen in the persistent current [38] (see also [39]): $j(k^2, \theta) = \frac{1}{2\pi} \frac{\partial}{\partial \theta} \delta(k^2, \theta)$ is the current density, i.e. $j(E, \theta) dE$ is the current of the states in the energy range $[E, E + dE]$. We get

$$j(k^2, \theta) = -\frac{1}{2\pi l} \frac{\sin \theta \sin kl}{1 - \cos \theta \cos kl} \frac{d\delta}{dk}. \quad (79)$$

- If $w \rightarrow 0$, the current density presents sharp peaks of alternate signs at the position of the resonances: $j(k^2, \theta) \simeq \mp \frac{1}{2\pi l} \frac{d\delta}{dk}$ for $k \sim k_n^\pm$. We define the contribution of the peak at k_n^\pm as $I_n^\pm = \int_{k_n^\pm - \delta K}^{k_n^\pm + \delta K} dk 2k j(k^2, \theta)$ with δK being a large quantity compared to the resonance width but small compared to the distance between peaks: $w^2 \ll \delta Kl \ll \min(\theta, \pi - \theta)$. We immediately see that $I_n^\pm \simeq \frac{4\pi}{l^2} (\mp n - \frac{\theta}{2\pi})$; we have recovered the persistent current of the isolated ring $\mathcal{I}_n^\pm = -\frac{\partial}{\partial \theta} (k_n^\pm)^2$.
- In the limit $w \rightarrow \infty$, the current density behaves like $j(k^2, \theta) \propto (k - \kappa_m) \frac{d\delta}{dk}$ in the neighbourhood of the resonance $k \sim \kappa_m$. It follows that the contributions of the resonance peaks vanish (due to the opening of the ring): $I_m = \int_{\kappa_m - \delta K}^{\kappa_m + \delta K} dk 2k j(k^2, \theta) \simeq 0$ (the right part of figure 7 indeed shows that the persistent current decreases as w increases).

Example 2. We consider a ring pierced by a flux θ and connected to two leads (see figure 8). This arrangement has been considered in several works to study the Aharonov–Bohm oscillations of the conductance of a normal metal ring; the authors of [24] considered a particular coupling of the leads whereas Büttiker *et al* [25] examined more general couplings.

The ring is made of two arcs a and b . We use the parameters of appendix A to write the matrix M . Using (89) matrix M is given by

$$M_{11} = i \frac{\lambda_1}{k} + i \frac{\cos \Phi_a + \sqrt{1 - T_a} \sin \varphi_a}{\sin \Phi_a - \sqrt{1 - T_a} \cos \varphi_a} + i \frac{\cos \Phi_b + \sqrt{1 - T_b} \sin \varphi_b}{\sin \Phi_b - \sqrt{1 - T_b} \cos \varphi_b} \quad (80)$$

$$M_{21}(\theta) = -\frac{i \sqrt{T_a} e^{i\theta/2}}{\sin \Phi_a - \sqrt{1 - T_a} \cos \varphi_a} - \frac{i \sqrt{T_b} e^{-i\theta/2}}{\sin \Phi_b - \sqrt{1 - T_b} \cos \varphi_b} \quad (81)$$

$$M_{12}(\theta) = M_{21}(-\theta) \quad (82)$$

$$M_{22} = i \frac{\lambda_2}{k} + i \frac{\cos \Phi_a - \sqrt{1 - T_a} \sin \varphi_a}{\sin \Phi_a - \sqrt{1 - T_a} \cos \varphi_a} + i \frac{\cos \Phi_b - \sqrt{1 - T_b} \sin \varphi_b}{\sin \Phi_b - \sqrt{1 - T_b} \cos \varphi_b}. \quad (83)$$

When several bonds link the two vertices α and β , we have to sum the contributions of each bond in $M_{\alpha\alpha}$ and $M_{\alpha\beta}$ (see [15] and appendix C of [16]). Since the two vertices are connected to leads, matrix W is the 2×2 diagonal matrix: $W = \text{diag}(w_1, w_2)$. We can get the scattering matrix from (43) as

$$\Sigma = -1 + \frac{2}{\det(M + W^2)} \begin{pmatrix} w_1^2 M_{22} + w_1^2 w_2^2 & -w_1 w_2 M_{12} \\ -w_1 w_2 M_{21} & w_2^2 M_{11} + w_1^2 w_2^2 \end{pmatrix}. \quad (84)$$

Now we concentrate on the case of perfect transmissions through the bonds $T_{a,b} = 1$ and $\Phi_{a,b} = kl_{a,b}$, with $\lambda_{1,2} = 0$. We have

$$\det(M + W^2) = -\frac{2(\cos kl - \cos \theta)}{\sin kl_a \sin kl_b} + i(w_1^2 + w_2^2) \frac{\sin kl}{\sin kl_a \sin kl_b} + w_1^2 w_2^2 \quad (85)$$

where $l = l_a + l_b$ is the perimeter of the ring. If we consider the limit of weak coupling $w_{1,2} \rightarrow 0$ we can expand the scattering matrix in the neighbourhood of the eigen-energies of the ring. We obtain the well-known Breit–Wigner form

$$\Sigma_{\alpha\beta} \underset{k \sim k_n^\pm}{\simeq} -\delta_{\alpha\beta} + \frac{i\sqrt{\Delta k_\alpha \Delta k_\beta} e^{i\chi_{\alpha\beta}}}{k - k_n^\pm + \frac{i}{2}(\Delta k_1 + \Delta k_2)} \quad (86)$$

where $\Delta k_{1,2} = \frac{w_{1,2}^2}{l}$, $\chi_{11} = \chi_{22} = 0$ and $\chi_{12} = -\chi_{21} = n\pi \pm \frac{1}{2}k_n^\pm(l_a - l_b)$. Note that a detailed analysis of the resonance structure of the transmission probability through the ring has already been done in [25].

6. Summary

We have given systematic procedures to construct the scattering matrix of graphs made of one-dimensional wires on which lives a potential, and connected to external leads.

In a first approach we used as basic ingredients a scattering matrix (10) describing scattering by the potentials on the bonds and a scattering matrix (15)–(17) providing information on the scattering by vertices and coupling to the external leads. This approach is quite natural in the sense that we combine the scattering matrices of parts of the system to construct the whole scattering matrix (24); however, it can become cumbersome since we have to deal with rather big matrices.

One way to reduce the problem is to reformulate it in terms of vertex matrices, which is possible if the scattering at vertices describes wavefunctions continuous at the vertices, which allows dealing with vertex variables instead of arc variables.

We have described an efficient way to introduce some tunable couplings between the leads and the graph (75), which permits to go continuously from a connected graph to an isolate graph.

We have generalized the results known in the absence of the potential [10, 18, 21] by adding scattering on bonds and allowing to tune the couplings to the external leads.

Acknowledgments

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Appendix A. Reformulating the matrix M

Here we would like to use some relations between the reflection and transmission coefficients on a bond to rewrite the result (48) in terms of parameters whose physical meanings are more clear. In the core of the paper we have considered that the reflection and transmission coefficients describe the effect of the scalar potential $V(x)$ only. In this appendix we adopt another point of view and consider that these coefficients describe the effect of both the scalar potential $V(x)$ and the vector potential $A(x)$.

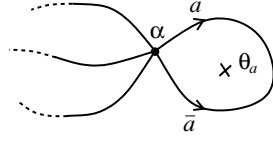


Figure 9. A loop at the vertex α .

Due to the unitarity of the scattering matrix for a given bond $(\alpha\beta)$, it follows that the four complex parameters describing the left ($r_{\alpha\beta}$ and $t_{\alpha\beta}$) and right ($r_{\beta\alpha}$ and $t_{\beta\alpha}$) scattering can be parametrized in terms of four real parameters:

$$\begin{pmatrix} r_{\alpha\beta} & t_{\beta\alpha} \\ t_{\alpha\beta} & r_{\beta\alpha} \end{pmatrix} = e^{i\Phi_{\alpha\beta}} \begin{pmatrix} ie^{i\varphi_{\alpha\beta}} \sqrt{1-T_{\alpha\beta}} & e^{-i\chi_{\alpha\beta}} \sqrt{T_{\alpha\beta}} \\ e^{i\chi_{\alpha\beta}} \sqrt{T_{\alpha\beta}} & ie^{-i\varphi_{\alpha\beta}} \sqrt{1-T_{\alpha\beta}} \end{pmatrix}. \quad (87)$$

$\Phi_{\alpha\beta}$ is a global phase. $T_{\alpha\beta} \in [0, 1]$ is the transmission probability through the barrier. In the absence of a magnetic field, we know that the scattering matrix is symmetric (it is well known that the symmetry of the scattering matrix in the presence of a magnetic field \mathcal{B} is $\Sigma(-\mathcal{B}) = \Sigma(\mathcal{B})^T$); it follows that we can identify the asymmetric part of the phase of the transmission coefficients with the magnetic flux

$$\chi_{\alpha\beta} = \theta_{\alpha\beta}. \quad (88)$$

The last phase $\varphi_{\alpha\beta}$ is related to the asymmetry of the potential (for $V_{(\alpha\beta)}(x) = V_{(\alpha\beta)}(l_{\alpha\beta} - x)$ we have $r_{\alpha\beta} = r_{\beta\alpha}$, i.e. $\varphi_{\alpha\beta} = 0$ or π).

Due to these definitions we have the following obvious relations: $T_{\alpha\beta} = T_{\beta\alpha}$, $\Phi_{\alpha\beta} = \Phi_{\beta\alpha}$, $\varphi_{\alpha\beta} = -\varphi_{\beta\alpha}$ and recall that $\theta_{\alpha\beta} = -\theta_{\beta\alpha}$.

We can now rewrite (48) in terms of these parameters as

$$M_{\alpha\beta} = i \delta_{\alpha\beta} \left(\frac{\lambda_{\alpha}}{k} + \sum_{\mu} a_{\alpha\mu} \frac{\cos \Phi_{\alpha\mu} + \sqrt{1-T_{\alpha\mu}} \sin \varphi_{\alpha\mu}}{\sin \Phi_{\alpha\mu} - \sqrt{1-T_{\alpha\mu}} \cos \varphi_{\alpha\mu}} \right) - i a_{\alpha\beta} \frac{\sqrt{T_{\alpha\beta}} e^{i\theta_{\alpha\beta}}}{\sin \Phi_{\alpha\beta} - \sqrt{1-T_{\alpha\beta}} \cos \varphi_{\alpha\beta}}. \quad (89)$$

As a by-product, it shows that the matrix M is anti-Hermitian: $M^{\dagger} = -M$. To end this appendix, we note that if the potential on the bond vanishes $V_{(\alpha\beta)}(x) = 0$, then $T_{\alpha\beta} = 1$ and $\Phi_{\alpha\beta} = kl_{\alpha\beta}$.

Appendix B. Matrix M for a graph with loops

We explain in this appendix how the matrix M is modified when we want to describe with the minimum number of vertices a graph possessing loops. We consider a graph with a loop threatened by a flux θ_a at the vertex α (see figure 9). The potential on arc a of the loop is described by four reflection and transmission coefficients: r_a, t_a for the arc a and $r_{\bar{a}}, t_{\bar{a}}$ for the reversed arc \bar{a} .

If we follow the lines of section 4 we can see that only the diagonal part of the matrix M (48) is affected by the loops

$$M_{\alpha\beta} \rightarrow M_{\alpha\beta} + \delta_{\alpha\beta} M_{\alpha\alpha}^{\text{loop}} \quad (90)$$

where the contribution of the loop is

$$M_{\alpha\alpha}^{\text{loop}} = \frac{(1-r_a)(1+r_{\bar{a}}) + t_a t_{\bar{a}}}{(1+r_a)(1+r_{\bar{a}}) - t_a t_{\bar{a}}} - \frac{2t_a}{(1+r_a)(1+r_{\bar{a}}) - t_a t_{\bar{a}}} + \frac{(1+r_a)(1-r_{\bar{a}}) + t_a t_{\bar{a}}}{(1+r_a)(1+r_{\bar{a}}) - t_a t_{\bar{a}}} - \frac{2t_{\bar{a}}}{(1+r_a)(1+r_{\bar{a}}) - t_a t_{\bar{a}}}. \quad (91)$$

This result is rather natural: $M_{\alpha\alpha}$ receives two contributions from each arc a and \bar{a} of the kind present in the diagonal elements of (48) and since the arc comes back to the same vertex we also get two contributions of the kind present in the off-diagonal elements of (48). After simplification we obtain

$$M_{\alpha\alpha}^{\text{loop}} = 2 \frac{1 - r_a r_{\bar{a}} + t_a t_{\bar{a}} - t_a - t_{\bar{a}}}{(1+r_a)(1+r_{\bar{a}}) - t_a t_{\bar{a}}}. \quad (92)$$

We can also express this contribution with the real parameters introduced in appendix A to describe the scattering by the arc a : $\Phi_a = \Phi_{\bar{a}}$, $T_a = T_{\bar{a}}$, $\varphi_a = -\varphi_{\bar{a}}$ and $\theta_a = -\theta_{\bar{a}}$. We obtain

$$M_{\alpha\alpha}^{\text{loop}} = 2i \frac{\cos \Phi_a - \sqrt{T_a} \cos \theta_a}{\sin \Phi_a - \sqrt{1-T_a} \cos \varphi_a}. \quad (93)$$

Appendix C. Inversion of block matrices

We recall in this appendix a result that can be found in standard textbooks. Consider the square matrix

$$\mathcal{M} = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array} \right) \quad (94)$$

where A and D are square matrices of arbitrary dimensions. Then

$$\mathcal{M}^{-1} = \left(\begin{array}{c|c} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ \hline -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{array} \right) \quad (95)$$

$$= \left(\begin{array}{c|c} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ \hline -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{array} \right). \quad (96)$$

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