Local Friedel sum rule on graphs

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Abstract

We consider graphs made of one-dimensional wires connected at vertices and on which may live a scalar potential. We are interested in a scattering situation where the graph is connected to infinite leads. We investigate relations between the scattering matrix and the continuous part of the local density of states, the injectivities, emissivities and partial local density of states. Those latter quantities can be obtained by attaching an extra lead at the point of interest and by investigating the transport in the limit of zero transmission into the additional lead. In addition to the continuous part related to the scattering states, the spectrum of graphs may present a discrete part related to states that remain uncoupled to the external leads. The theory is illustrated with the help of a few simple examples.

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1 Introduction

Thanks to the powerful experimental techniques used in mesoscopic physics during the past 20 years, many interesting and fundamental effects have been investigated on systems that can be modelized by graphs : networks of wires through which an electrical current can flow. The most famous example is of course the Aharonov-Bohm oscillations in a coherent metallic ring [1, 2, 3, 4] (see also the excellent review [5]), but there have also been many other realizations of graphs like the recent ones devoted to the Aharonov-Bohm cage effect [6, 7, 8, 9]. Graphs which could seem at first sight to be oversimplified models for mesoscopic networks, succeeded in those cases to describe the interesting physical effects, which explain why they are so widely used in many theoretical works.

Among all the useful concepts of mesoscopic physics the scattering approach plays a central role. It provides a powerful tool to study many physical quantities related to transport, noise, etc. A very important concept of the scattering theory is the one related to the Krein-Friedel relation, or Friedel sum rule [10, 11], which establishes a relation between the scattering and the spectral properties[1]. The use of this kind of relations in mesoscopic physics allows to express,

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[1] In fact the idea of relating the spectral properties to the scattering properties goes back to 1937 when Beth and Uhlenbeck [12] related the second virial coefficient of a gas of interacting particles to the phase shifts of the 2-body scattering problem (see also [13] or §77 of [14]).

for instance, the charge distribution in terms of the scattering properties. However it permits to consider only the total charge in the scattering region in an equilibrium situation. Several works have been devoted to build corresponding concepts to describe out-of-equilibrium situations and also to relate not only global but *local* quantities to the scattering (like the local density of states). This has lead to the introduction of the concepts of partial local density of states, injectivities, emissivities, etc [15, 16, 17]. Let us also mention the recent work on the relation between scattering and local density of states for the particular case of quasi-one-dimensional systems [18, 19].

The scattering theory on graphs has attracted the interest of many authors among which we can quote [20, 21, 22, 23, 24, 25, 26]. The purpose of this article is to discuss the relation between scattering properties of the graph and the local quantities mentioned above.

2 Motivation

The local density of states (LDoS) is by definition : $\rho(x; E) = \langle x | \delta(E - H) | x \rangle$. If we consider a graph $\mathcal{G}$ connected to infinite leads, its spectrum is continuous. We can define the DoS of the scattering region (the graph) as $\rho_{\mathcal{G}}(E) = \int_{\mathcal{G}} \mathrm{d}x \, \rho(x; E)$, where the integral runs over all the bonds of the graph (by convention, we do not include the infinite leads in what we call "graph $\mathcal{G}$"). It is well known that this object is related to the scattering properties through the Krein-Friedel relation (or Friedel sum rule). Graphs have the particularity (which does not occur in 1d for example) that due to certain symmetries some states may remain uncoupled to the external leads. The presence of such localized states leads to the existence of a discrete part in the spectrum, superimposed on the continuous part : $\rho_{\mathcal{G}}(E) = \rho_{\mathrm{reg}}(E) + \rho_{\mathrm{dis}}(E)$ where $\rho_{\mathrm{reg}}(E)$ is the contribution of the stationary scattering states and $\rho_{\mathrm{dis}}(E) = \sum_n g_n \delta(E - E_n)$ is the contribution of the localized states (see appendix A). The existence of these two contributions was already noticed by J.-P. Roth in a work [27] in which he extended the trace formula obtained for closed graphs without potential [28] to open graphs connected to semi infinite wires. What is rather unusual is that the continuous part and the discrete part live on the same intervals of energy. If the wave function is chosen continuous at the vertices, the absence of hybridization of the localized states with the states of the continuum occurs when some states vanish at all the vertices to which external leads are connected. It was shown in [26] that the Friedel sum rule has to be modified since, obviously, only the continuous part is related to the scattering matrix : $\rho_{\mathrm{reg}}(E) = \frac{1}{2\mathrm{i}\pi} \left(\frac{\mathrm{d}}{\mathrm{d}E} \ln \det \Sigma + \frac{1}{4E} \mathrm{Tr} \left\{ \Sigma - \Sigma^\dagger \right\} \right)$ where Σ is the scattering matrix of the graph.

Similarly, the LDoS can be separated into a continuous part related to the stationary scattering states and a discrete part given by the localized states (see appendix A) :

$$\rho(x; E) = \sum_\alpha |\tilde{\psi}_E^{(\alpha)}(x)|^2 + \sum_n \sum_{j=1}^{g_n} \delta(E - E_n) \, |\varphi_{n,j}(x)|^2 \tag{1}$$

(if $x \notin \mathcal{G}$, only the first term remains since the localized wave functions vanish outside the graph of course). $\tilde{\psi}_E^{(\alpha)}(x)$ is the stationary scattering state corresponding to the injection of a plane wave at lead α. The sum over α runs over the L vertices connected to leads. The normalization is chosen to associate to those states a measure $\mathrm{d}E$. The wave function $\varphi_{n,j}(x)$ is normalized to unity in the graph, j being a degeneracy label. g_n is the number of the localized states with energy E_n.

The modified Friedel sum rule is an example of a relation between a "global" quantity characterizing the graph (the regular part $\rho_{\mathrm{reg}}(E)$ of the DoS $\rho_{\mathcal{G}}(E)$) and the scattering matrix. The purpose of the present work is to demonstrate some relations between local quantities such as the local density of states (LDoS), injectivities, emissivities and partial LDoS, and the objects of scattering theory (stationary states, scattering matrix) in the context of graphs.

In particular we will show that the first term of the LDoS is related to a functional derivative of the scattering matrix. The second term of the LDoS, if it exists, cannot be probed from the scattering properties.

3 The scattering matrix

We consider a graph $\mathcal{G}$ being the domain of the Schrödinger operator $H = -\mathrm{D}_x^2 + V(x)$, where $\mathrm{D}_x = \mathrm{d}_x - \mathrm{i}A(x)$ is the covariant derivative. The graph is a network of B bonds joining V vertices (denoted by greek letters $\alpha, \beta, \ldots$). Each bond $(\alpha\beta)$ is identified with the interval $[0, l_{\alpha\beta}]$ of $\mathbb{R}$ so that a scalar function $\psi(x)$ defined on the graph is characterized by its B components $\psi_{(\alpha\beta)}(x)$. The Schrödinger operator acts on functions $\psi(x)$ which are chosen, in a first step, to be continuous at the vertices of the graph : $\psi_{(\alpha\beta)}(x = 0) = \psi_\alpha$ for all vertices β neighbours of α. We denote by ψ_α the value of the wave function at the vertex. Additionally we must add a constraint on the derivatives of ψ to ensure current conservation. As soon as continuity of $\psi(x)$ is required, the most general additional condition is $\sum_\beta a_{\alpha\beta} \mathrm{D}_x \psi_{(\alpha\beta)}(\alpha) = \lambda_\alpha \psi_\alpha$ where the presence of the connectivity matrix $a_{\alpha\beta}$ in the sum ensures that it runs over the neighbouring vertices of α. The connectivity (or adjacency) matrix describes the topology of the graph : $a_{\alpha\beta} = 1$ if α and β are connected by a bond, and 0 otherwise. The notation $\psi_{(\alpha\beta)}(\alpha) \equiv \psi_{(\alpha\beta)}(x = 0)$ designates the value of the component at the vertex. λ_α is a real parameter that affects the scattering at the vertex. It allows to interpolate between Neumann boundary conditions ($\lambda_\alpha = 0$) and Dirichlet boundary conditions ($\lambda_\alpha = \infty$, which imposes $\psi_\alpha = 0$). We can develop an intuition of the role of this parameter by noting that if the vertex has coordination 2, the boundary condition describes a potential $\lambda_\alpha \delta(x)$ at the vertex. Note that the transmission amplitude through the vertex is $2/(m_\alpha + \mathrm{i}\lambda_\alpha/k)$ where m_α is its coordination ; the transmission is maximized for $\lambda_\alpha = 0$.

Among the V vertices of the graph, L are connected to infinite leads. The couplings to the leads can be chosen arbitrary such that we can go continuously from a situation where the graph is coupled to the leads to a situation where it becomes decoupled from some leads. This procedure introduces some discontinuity between the wave function at the extremity of the lead and at the vertex of the graph to which the lead is connected [25]. The scattering matrix Σ is an $L \times L$ matrix that depends on the energy $E = k^2$. It can be constructed by manipulating matrices that encode the information about the graph (topology, potentials on the bonds, lengths of the bonds, magnetic fluxes, couplings to the leads) [25] :

$$\Sigma = -1 + 2W \left(M + W^\mathrm{T} W\right)^{-1} W^\mathrm{T} . \tag{2}$$

The rectangular matrix W encodes the information on the way the graph is connected to leads :

$$W_{\alpha\beta} = w_\alpha \, \delta_{\alpha\beta} \tag{3}$$

with $\alpha \in \mathcal{V}_\mathrm{ext}$ and $\beta \in \mathcal{V}$, where $\mathcal{V} = \{1, \cdots, V\}$ is the set of vertices and $\mathcal{V}_\mathrm{ext}$ the set of vertices connected to leads ($\mathrm{Card}(\mathcal{V}_\mathrm{ext}) = L$). The parameter $w_\alpha \in \mathbb{R}$ describes the coupling between the graph and the lead at vertex α. Its precise definition is given in [25] : the transmission amplitude between the lead and the graph is $2w_\alpha/(1 + w_\alpha^2)$.

We call $x_{\alpha\beta} \in [0, l_{\alpha\beta}]$ the coordinate on the bond $(\alpha\beta)$, starting from α (note that $x_{\alpha\beta} + x_{\beta\alpha} = l_{\alpha\beta}$, the length of the bond). To describe the potentials on the bonds, we introduce two real functions $f_{\alpha\beta}(x_{\alpha\beta})$, $f_{\beta\alpha}(x_{\alpha\beta})$: the two linearly independent solutions of the Schrödinger equation $[E + \mathrm{d}_x^2 - V_{(\alpha\beta)}(x)]f(x) = 0$ on the bond, satisfying boundary conditions : $f_{\alpha\beta}(0) = 1$, $f_{\alpha\beta}(l_{\alpha\beta}) = 0$, $f_{\beta\alpha}(0) = 0$ and $f_{\beta\alpha}(l_{\alpha\beta}) = 1$. For example, in the free case ($V(x) = 0$), we have $f_{\alpha\beta}(x_{\alpha\beta}) = \frac{\sin k(l_{\alpha\beta} - x_{\alpha\beta})}{\sin k l_{\alpha\beta}}$ and $f_{\beta\alpha}(x_{\alpha\beta}) = \frac{\sin k x_{\alpha\beta}}{\sin k l_{\alpha\beta}}$.

The matrix M that contains all the information on the isolated graph (potential on the bond, topology) is :

$$M_{\alpha\beta}(-E) = \frac{\mathrm{i}}{\sqrt{E}} \left(\delta_{\alpha\beta} \left[\lambda_\alpha - \sum_\mu a_{\alpha\mu} \frac{\mathrm{d}f_{\alpha\mu}}{\mathrm{d}x_{\alpha\mu}}(\alpha) \right] + a_{\alpha\beta} \frac{\mathrm{d}f_{\alpha\beta}}{\mathrm{d}x_{\alpha\beta}}(\beta)\, \mathrm{e}^{\mathrm{i}\theta_{\alpha\beta}} \right) , \tag{4}$$

we introduced the obvious notation $f_{\alpha\beta}(0) \equiv f_{\alpha\beta}(\alpha)$, $f_{\alpha\beta}(l_{\alpha\beta}) \equiv f_{\alpha\beta}(\beta)$, etc. $\theta_{\alpha\beta}$ is the magnetic flux along the bond. This matrix was introduced in the study of the spectral determinant of isolated graphs [29, 30, 31]. Instead of encoding the information about the potential through the functions $f_{\alpha\beta}(x)$, it can be more conveniently related to the reflection and transmission coefficients of each bond [25] :

$$\begin{aligned} M_{\alpha\beta} &= \delta_{\alpha\beta} \left(\mathrm{i}\frac{\lambda_\alpha}{k} + \sum_\mu a_{\alpha\mu} \frac{(1 - r_{\alpha\mu})(1 + r_{\mu\alpha}) + t_{\alpha\mu}\, t_{\mu\alpha}}{(1 + r_{\alpha\mu})(1 + r_{\mu\alpha}) - t_{\alpha\mu}\, t_{\mu\alpha}} \right) \\ &\quad - a_{\alpha\beta} \frac{2\, t_{\alpha\beta}}{(1 + r_{\alpha\beta})(1 + r_{\beta\alpha}) - t_{\alpha\beta}\, t_{\beta\alpha}} . \end{aligned} \tag{5}$$

These equations generalize the result known in the absence of the potential [21]. In this latter case we recover from (5) the well-known matrix:

$$M_{\alpha\beta} = \mathrm{i}\, \delta_{\alpha\beta} \sum_\mu a_{\alpha\mu} \cotg kl_{\alpha\mu} - a_{\alpha\beta} \frac{\mathrm{i}\, \mathrm{e}^{\mathrm{i}\theta_{\alpha\beta}}}{\sin kl_{\alpha\beta}} . \tag{6}$$

We are now ready to discuss the extraction of local information from the scattering matrix.

4 Functional derivative of the scattering matrix

The scattering matrix is a functional of the potential $V(x)$ and we are now going to compute $\frac{\delta\Sigma}{\delta V(x)}$. As a starting point it is useful to note that if a δ potential at $x = x_0$ is added to the potential, the first perturbative correction to the scattering matrix is exactly the functional derivative [16]:

$$\Sigma^\lambda \stackrel{\mathrm{def}}{=} \Sigma[V(x) + \lambda\, \delta(x - x_0)] = \Sigma[V(x)] + \lambda \frac{\delta\Sigma}{\delta V(x_0)}[V(x)] + \cdots \tag{7}$$

The advantage with graphs is that the addition of a δ potential at x is easily implemented : it is done by adding a vertex of weight λ at x, obtaining a graph $\mathcal{G}^\lambda$. The "weight" is the real parameter involved in the mixed boundary conditions introduced above [21, 32, 29]. As a consequence, the construction of the matrix Σ^λ of $\mathcal{G}^\lambda$ in the vertex approach requires to consider matrices M and W of size $(V + 1) \times (V + 1)$ and $L \times (V + 1)$, respectively. We call W_x the matrix describing the coupling of the graph to the leads when the additional vertex is at x (the matrix W_x has only an additional column of 0's compare to W) and M^λ the new matrix M. We have :

$$\Sigma^\lambda = -1 + 2\, W_x \frac{1}{M^\lambda + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} \tag{8}$$

From (4,5) we see that the matrix M^λ depends linearly on λ :

$$M^\lambda = M_x + \frac{\mathrm{i}\lambda}{k} K_x \tag{9}$$

where M_x is the matrix of the graph $\mathcal{G}^{\lambda=0}$. This graph differs from $\mathcal{G}$ only by its number of vertices : it possesses an additional vertex of weight $\lambda = 0$ at x. Since no scattering occurs at

this vertex when $\lambda = 0$, we do not change the properties of the graph, but only the size of the matrices describing it. In the following we adopt notations such that all matrices with label x refer to the graph $\mathcal{G}_x \overset{\text{def}}{=} \mathcal{G}^{\lambda=0}$. The matrix K_x contains only one non zero element coupling the vertex x to itself :

$$(K_x)_{\alpha\beta} = \delta_{\alpha\beta}\delta_{\alpha x} \tag{10}$$

where the indices run over the V vertices of the initial graph and the additional vertex at x. Expanding the scattering matrix Σ^λ in powers of λ we get :

$$\Sigma^\lambda = -1 + 2\,W_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} - 2\,W_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} \frac{\mathrm{i}\lambda}{k} K_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} + \cdots \tag{11}$$

The first term is the scattering matrix $\Sigma = \Sigma^{\lambda=0}$

$$\Sigma = -1 + 2\,W_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} = -1 + 2\,W \frac{1}{M + W^{\mathrm{T}} W} W^{\mathrm{T}} \tag{12}$$

and the second gives the functional derivative. Then :

$$\frac{\delta\,\Sigma}{\delta V(x)} = -\frac{2\mathrm{i}}{k} W_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} K_x \frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} \tag{13}$$

This expression allows to compute explicitly the functional derivative by manipulating matrices.

5   Functional derivative and its relation to wave functions

We now show the relation between the functional derivative of the scattering matrix and the stationary scattering state wave functions. The wave function at the vertices of $\mathcal{G}_x$ is a solution of [25]

$$1 + \Sigma = W_x \Psi_x \tag{14}$$
$$W_x^{\mathrm{T}}(1 - \Sigma) = M_x \Psi_x \,, \tag{15}$$

where Ψ_x is the $(V+1) \times L$ matrix gathering the wave function $\psi_\mu^{(\alpha)}$ at vertex μ for the stationary scattering state $\psi^{(\alpha)}(x)$: the matrix element is by definition $\Psi_{\mu\alpha} \equiv \psi_\mu^{(\alpha)}$. The index μ runs over the V vertices and the additional vertex x. α runs over the L vertices connected to leads. The wave function with the correct normalization is :

$$\tilde{\psi}^{(\alpha)}(x) = \frac{1}{\sqrt{4\pi k}}\,\psi^{(\alpha)}(x)\,. \tag{16}$$

In the previous papers [25, 26] we have used the notation $\tilde{\psi}_E^{(\alpha)}(x)$. Here we omit the energy label E to lighten the expressions. It follows from the above equations that the wave function at the V vertices for the L stationary scattering states is encoded in the matrix :

$$\Psi_x = 2\frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}} \tag{17}$$

For the state associated to a measure $\mathrm{d}E$:

$$\tilde{\Psi}_x = \frac{1}{\sqrt{\pi k}}\,\frac{1}{M_x + W_x^{\mathrm{T}} W_x} W_x^{\mathrm{T}}\,. \tag{18}$$

These matrix expressions are useful if we want to establish a relation between the functional derivative of the scattering matrix and wave functions.

5.1 Time reversed graph

If we consider a graph described by a matrix $M(\{\theta_{\alpha\beta}\})$ depending on magnetic fluxes $\theta_{\alpha\beta}$, it follows from the construction of M (see formula (48) and appendix A of [25]) that the time reversed graph (with all fluxes reversed) is described by the matrix $M(\{-\theta_{\alpha\beta}\}) = M(\{\theta_{\alpha\beta}\})^{\mathrm{T}}$. The wave function at the vertices for the time-reversed graph is then :

$$\tilde{\Psi}^{t.r.} = \frac{1}{\sqrt{\pi k}} \frac{1}{M^{\mathrm{T}} + W^{\mathrm{T}}W} W^{\mathrm{T}} . \tag{19}$$

Important remark : $\tilde{\Psi}^{t.r.}$ gives the wave function at the vertices for the time-reversed graph, which is related to the original graph by reversing all the fluxes. It should not be confused with the wave function describing the time-reversed motion of the electron (see also appendix B).

5.2 A first result

We can now relate the functional derivative (13) to the wave function. From the above remark we get :

$$\frac{\delta\,\Sigma}{\delta V(x)} = -2\mathrm{i}\pi(\tilde{\Psi}_x^{t.r.})^{\mathrm{T}} K_x \tilde{\Psi}_x \tag{20}$$

The matrix K_x select the line in $\tilde{\Psi}_x$ associated with x and the corresponding column in $(\tilde{\Psi}_x^{t.r.})^{\mathrm{T}}$. Then the matrix elements read :

$$\frac{\delta\,\Sigma_{\alpha\beta}}{\delta V(x)} = -2\mathrm{i}\pi\,\tilde{\psi}_x^{t.r.(\alpha)}\,\tilde{\psi}_x^{(\beta)} . \tag{21}$$

Since $\tilde{\psi}_x^{(\alpha)}$ is the wave function at vertex x of the graph, we could write more elegantly :

$$\frac{\delta\,\Sigma_{\alpha\beta}}{\delta V(x)} = -2\mathrm{i}\pi\,\tilde{\psi}^{t.r.(\alpha)}(x)\,\tilde{\psi}^{(\beta)}(x) . \tag{22}$$

For the scattering matrix element with indices interchanged we have obviously

$$\frac{\delta\,\Sigma_{\beta\alpha}}{\delta V(x)} = -2\mathrm{i}\pi\,\tilde{\psi}^{t.r.(\beta)}(x)\,\tilde{\psi}^{(\alpha)}(x) \tag{23}$$

which shows that

$$\frac{\delta\,\Sigma_{\alpha\beta}^{t.r.}}{\delta V(x)} = \frac{\delta\,\Sigma_{\beta\alpha}}{\delta V(x)} \tag{24}$$

as required by the symmetry of the scattering matrix under flux reversal.

5.3 A compact formulation of the functional derivative

All above formulae (13,20) expressing the functional derivative of the scattering matrix involve matrices describing the graph $\mathcal{G}_x$. The purpose of this paragraph is to simplify (13) and express the functional derivative in terms of matrices of smaller size, related to the original graph $\mathcal{G}$.

We suppose that x belongs to the bond $(\alpha\beta)$ and we choose to organize the basis of $V+1$ vertices of $\mathcal{G}_x$ as $\{\cdots, \alpha, \beta\,|x\}$ to help the discussion. The matrix of interest has the following structure :

$$M_x + W_x^{\mathrm{T}}W_x = \begin{pmatrix} & & & \vdots \\ & & & 0 \\ & (M_x)_{\alpha\alpha} + w_\alpha^2 & 0 & (M_x)_{\alpha x} \\ & 0 & (M_x)_{\beta\beta} + w_\beta^2 & (M_x)_{\beta x} \\ \hline \cdots & 0 & (M_x)_{x\alpha} & (M_x)_{x\beta} & (M_x)_{xx} \end{pmatrix} = \left(\begin{array}{c|c} A & B \\ \hline C & (M_x)_{xx} \end{array} \right) \tag{25}$$

Since the vertex x is the only neighbour of α and β, the part which is not written in the block A is precisely the same as in $M + W^\mathrm{T}W$. We have separated by a line the matrices into blocks related to the vertices of $\mathcal{G}$ and the additional vertex x. The matrices W_x and K_x read :

$$W_x = \left(\ W\ \middle|\ 0\ \right) \qquad\qquad K_x = \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & 1 \end{array}\right) . \tag{26}$$

To express the inverse of the matrix $M_x + W_x^\mathrm{T}W_x$, we note that $A - B(M_x)_{xx}^{-1}C = M + W^\mathrm{T}W$. Then :

$$\left(M_x + W_x^\mathrm{T}W_x\right)^{-1} = \left(\begin{array}{c|c} (M + W^\mathrm{T}W)^{-1} & -(M + W^\mathrm{T}W)^{-1}B(M_x)_{xx}^{-1} \\ \hline -(M_x)_{xx}^{-1}C(M + W^\mathrm{T}W)^{-1} & \cdots \end{array}\right) . \tag{27}$$

After a little bit of algebra, we obtain from (13) :

$$\frac{\delta\,\Sigma}{\delta V(x)} = -\frac{2\mathrm{i}}{k}W\frac{1}{M + W^\mathrm{T}W}K(x)K(x)^\dagger\frac{1}{M + W^\mathrm{T}W}W^\mathrm{T} \tag{28}$$

where the $V \times V$ matrix $K(x)K(x)^\dagger$ couples only the vertices α and β :

$$K(x)K(x)^\dagger = \frac{1}{(M_x)_{xx}^2}\begin{pmatrix} \vdots \\ 0 \\ (M_x)_{\alpha x} \\ (M_x)_{\beta x} \end{pmatrix}\begin{pmatrix} \cdots & 0 & (M_x)_{x\alpha} & (M_x)_{x\beta} \end{pmatrix} . \tag{29}$$

We can also derive a more transparent expression of the matrix $K(x)K(x)^\dagger$ in terms of the two functions $f_{\alpha\beta}(x)$ and $f_{\beta\alpha}(x)$ introduced above. On the bond $(\alpha\beta)$ the wave function is

$$\tilde{\psi}_{(\alpha\beta)}(x) = \tilde{\psi}_\alpha\mathrm{e}^{\mathrm{i}\theta_{\alpha\beta}x/l_{\alpha\beta}}f_{\alpha\beta}(x) + \tilde{\psi}_\beta\mathrm{e}^{-\mathrm{i}\theta_{\alpha\beta}(1-x/l_{\alpha\beta})}f_{\beta\alpha}(x) , \tag{30}$$

where $x \equiv x_{\alpha\beta} \in [0, l_{\alpha\beta}]$ measures the distance from the vertex α. The wave function of the time-reversed graph is obtained by changing the sign of flux (the wave function at vertices is of course also affected by this operation). Then we can write $\tilde{\psi}_{(\alpha\beta)}^{(\mu)}(x_{\alpha\beta}) = (K(x)^\dagger\tilde{\Psi})_\mu$ where

$$K(x)^\dagger = \begin{pmatrix} \cdots & 0 & f_{\alpha\beta}(x_{\alpha\beta})\mathrm{e}^{\mathrm{i}\theta_{\alpha x}} & f_{\beta\alpha}(x_{\alpha\beta})\mathrm{e}^{\mathrm{i}\theta_{\beta x}} \end{pmatrix} . \tag{31}$$

We have also : $\tilde{\psi}_{(\alpha\beta)}^{t.r.(\mu)}(x_{\alpha\beta}) = ((\tilde{\Psi}^{t.r.})^\mathrm{T}K(x))_\mu$.
If we now write

$$-\frac{1}{2\mathrm{i}\pi}\frac{\delta\,\Sigma}{\delta V(x)} = (\tilde{\Psi}^{t.r.})^\mathrm{T}K(x)K(x)^\dagger\tilde{\Psi} \tag{32}$$

We find from (22) the new expression of the matrix involved in (28) :

$$K(x)K(x)^\dagger = \begin{pmatrix} \vdots \\ 0 \\ f_{\alpha\beta}(x_{\alpha\beta})\mathrm{e}^{-\mathrm{i}\theta_{\alpha x}} \\ f_{\beta\alpha}(x_{\alpha\beta})\mathrm{e}^{-\mathrm{i}\theta_{\beta x}} \end{pmatrix}\begin{pmatrix} \cdots & 0 & f_{\alpha\beta}(x_{\alpha\beta})\mathrm{e}^{\mathrm{i}\theta_{\alpha x}} & f_{\beta\alpha}(x_{\alpha\beta})\mathrm{e}^{\mathrm{i}\theta_{\beta x}} \end{pmatrix} . \tag{33}$$

We can extract some nontrivial relations between the elements of M_x and the functions $f_{\alpha\beta}(x_{\alpha\beta})$ and $f_{\beta\alpha}(x_{\alpha\beta})$:

$$f_{\alpha\beta}(x_{\alpha\beta}) = -\frac{(M_x)_{x\alpha}}{(M_x)_{xx}} = \frac{\frac{\mathrm{d}f_{x\alpha}}{\mathrm{d}x_{x\alpha}}(\alpha)}{\frac{\mathrm{d}f_{x\alpha}}{\mathrm{d}x_{x\alpha}}(x) + \frac{\mathrm{d}f_{x\beta}}{\mathrm{d}x_{x\beta}}(x)} , \tag{34}$$

which could have been demonstrated more directly by constructing $f_{\alpha\beta}(x_{\alpha\beta})$ in terms of $f_{\alpha x}(x_{\alpha x})$, $f_{x\alpha}(x_{x\alpha})$ and $f_{x\beta}(x_{x\beta})$.

6   Partial LDoS, injectivies, emissivities and LDoS

Partial LDoS. The partial LDoS is defined as [15, 16]

$$\rho(\alpha, x, \beta) \overset{\text{def}}{=} -\frac{1}{4i\pi}\left(\Sigma_{\alpha\beta}^* \frac{\delta\,\Sigma_{\alpha\beta}}{\delta V(x)} - \frac{\delta\,\Sigma_{\alpha\beta}^*}{\delta V(x)}\Sigma_{\alpha\beta}\right)\,. \tag{35}$$

It follows from (22) that :

$$\rho(\alpha, x, \beta) = \text{Re}\left[\Sigma_{\alpha\beta}^* \tilde{\psi}^{t.r.(\alpha)}(x)\,\tilde{\psi}^{(\beta)}(x)\right]\,. \tag{36}$$

Injectivies and emissivities. The injectivies are defined as

$$\rho(x, \beta) \overset{\text{def}}{=} \sum_{\alpha} \rho(\alpha, x, \beta) \tag{37}$$

and the emissivities as

$$\rho(\alpha, x) \overset{\text{def}}{=} \sum_{\beta} \rho(\alpha, x, \beta)\,. \tag{38}$$

They can be rewritten as :

$$\rho(x, \alpha) = -\frac{1}{2i\pi}\left(\Sigma^\dagger \frac{\delta\,\Sigma}{\delta V(x)}\right)_{\alpha\alpha} \tag{39}$$

and

$$\rho(\alpha, x) = -\frac{1}{2i\pi}\left(\frac{\delta\,\Sigma}{\delta V(x)}\Sigma^\dagger\right)_{\alpha\alpha}\,. \tag{40}$$

These two quantities are real thanks to the relations $\frac{\delta\,\Sigma^\dagger}{\delta V(x)}\Sigma + \Sigma^\dagger \frac{\delta\,\Sigma}{\delta V(x)} = 0$ and $\frac{\delta\,\Sigma}{\delta V(x)}\Sigma^\dagger + \Sigma\frac{\delta\,\Sigma^\dagger}{\delta V(x)} = 0$ coming from the unitariry : $\Sigma^\dagger\Sigma = \Sigma\Sigma^\dagger = 1$.

We can now compute :

$$\Sigma^\dagger \frac{\delta\,\Sigma}{\delta V(x)} = -2i\pi\,\Sigma^\dagger(\tilde{\Psi}_x^{t.r.})^{\text{T}}K_x\tilde{\Psi}_x = -2i\pi\,\tilde{\Psi}_x^\dagger K_x\tilde{\Psi}_x\,, \tag{41}$$

where we have used (122). Since

$$(\tilde{\Psi}_x^\dagger K_x \tilde{\Psi}_x)_{\alpha\beta} = \sum_{\mu,\nu}\tilde{\psi}_\mu^{(\alpha)*}\delta_{\mu\nu}\delta_{\mu x}\tilde{\psi}_\nu^{(\beta)} = \tilde{\psi}_x^{(\alpha)*}\tilde{\psi}_x^{(\beta)} \tag{42}$$

it follows that :

$$-\frac{1}{2i\pi}\left(\Sigma^\dagger \frac{\delta\,\Sigma}{\delta V(x)}\right)_{\alpha\beta} = \tilde{\psi}^{(\alpha)}(x)^*\,\tilde{\psi}^{(\beta)}(x) \tag{43}$$

a relation that has been demonstrated in a different context and by different means in Ref. [33]. From (39) we finally get for the injectivies :

$$\rho(x, \alpha) = |\tilde{\psi}^{(\alpha)}(x)|^2\,. \tag{44}$$

The physical meaning of the injectivies is now clear : it is the contribution of the stationary scattering state incoming from α to the continuous part of the LDoS.

We proceed similarly as above :

$$\frac{\delta\,\Sigma}{\delta V(x)}\Sigma^\dagger = -2i\pi\,(\tilde{\Psi}_x^{t.r.})^{\text{T}}K_x\tilde{\Psi}_x\Sigma^\dagger = -2i\pi\,(\tilde{\Psi}_x^{t.r.})^{\text{T}}K_x(\tilde{\Psi}_x^{t.r.})^*\,. \tag{45}$$

Then

$$\rho(\alpha, x) = \left(\tilde{\Psi}_x^{t.r.\mathrm{T}} K_x \tilde{\Psi}_x^{t.r.*} \right)_{\alpha\alpha} \tag{46}$$

and we finally get

$$\rho(\alpha, x) = |\tilde{\psi}^{t.r.(\alpha)}(x)|^2 . \tag{47}$$

Obviously we have recovered in the particular case of graphs the Onsager-Casimir relation relating injectivities and emissivities [15] :

$$\rho(\alpha, x; \{\theta_{\mu\nu}\}) = \rho(x, \alpha; \{-\theta_{\mu\nu}\}) . \tag{48}$$

Injectivities and emissivities are related by reversing the sign of the magnetic field.
LDoS. If we sum the injectivities or the emissivities, we get the same result, the contribution of the continuous part of the spectrum to the LDoS of the graph :

$$\sum_\alpha \rho(\alpha, x) = \sum_\alpha \rho(x, \alpha) = -\frac{1}{2\mathrm{i}\pi} \operatorname{Tr} \left\{ \Sigma^\dagger \frac{\delta \Sigma}{\delta V(x)} \right\} \tag{49}$$

From (44) we demonstrate that :

$$-\frac{1}{2\mathrm{i}\pi} \frac{\delta}{\delta V(x)} \ln \det \Sigma = \sum_\alpha |\tilde{\psi}^{(\alpha)}(x)|^2 . \tag{50}$$

Once again, we insist that one of the interest of graphs is the fact that the functional derivatives involved in the injectivities, emissivities or the LDoS can be computed with algebraic calculations :

$$-\frac{1}{2\mathrm{i}\pi} \frac{\delta}{\delta V(x)} \ln \det \Sigma$$

$$= \operatorname{Tr} \left\{ \tilde{\Psi}_x^\dagger K_x \tilde{\Psi}_x \right\} = \frac{1}{\pi k} \operatorname{Tr} \left\{ W_x \frac{1}{-M_x + W_x^\mathrm{T} W_x} K_x \frac{1}{M_x + W_x^\mathrm{T} W_x} W_x^\mathrm{T} \right\} \tag{51}$$

$$= \operatorname{Tr} \left\{ \tilde{\Psi}^\dagger K(x) K(x)^\dagger \tilde{\Psi} \right\} = \frac{1}{\pi k} \operatorname{Tr} \left\{ W \frac{1}{-M + W^\mathrm{T} W} K(x) K(x)^\dagger \frac{1}{M + W^\mathrm{T} W} W^\mathrm{T} \right\} . \tag{52}$$

Relation between $d\Sigma/dE$ and $\delta \Sigma/\delta V(x)$

If the relation (43) is integrated over the whole graph, we get the following exact relation (see [16] for the one-dimensional case and the demonstration in an appendix of [34] for graphs) :

$$-\int_{\mathrm{Graph}} \mathrm{d}x \, \Sigma^\dagger \frac{\delta \Sigma}{\delta V(x)} = \Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E} + \frac{1}{4E} \left(\Sigma - \Sigma^\dagger \right) . \tag{53}$$

If we trace this relation between matrices we obtain :

$$-\int_{\mathrm{Graph}} \mathrm{d}x \, \frac{\delta}{\delta V(x)} \ln \det \Sigma = \frac{\mathrm{d}}{\mathrm{d}E} \ln \det \Sigma + \frac{1}{4E} \operatorname{Tr} \left\{ \Sigma - \Sigma^\dagger \right\} . \tag{54}$$

Note that in the usual formulation of the Friedel sum rule [10, 11, 13, 14] only the first term appears. This is due to the fact that what is considered in this case is the variation of the total density of states (the LDoS integrated over the whole space) due to the introduction of a potential, whereas what we consider in the above formulae is the LDoS integrated in the scattering region only (the graph). This point is discussed in detail in the appendix B of [26].

Example : The ring

We apply in this section the above considerations to a ring [2, 3] of perimeter l threaded by an Aharonov-Bohm flux θ. The upper arm (arc a) is of length l_a and the lower arm (arc b) of length l_b (we have $l = l_a + l_b$). We consider the situation without potential for simplicity. The ring is coupled to two leads at the two vertices 1 and 2 by arbitrary couplings described by the two real parameters w_1 and w_2 (The maximum coupling is $w_i = 1$; in this case the scattering at the vertex is symmetric. The decoupling of the ring occurs for $w_i \to 0$). We call $\theta_{a,b}$ the line integral of the vector potential due to the flux along the two arcs : $\theta = \theta_a + \theta_b$.
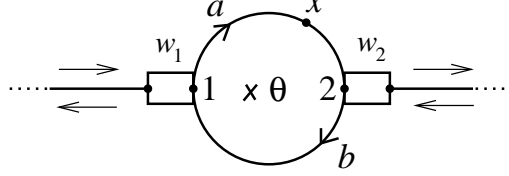

Figure 1: Ring penetrated by an Aharonov-Bohm flux coupled to two leads. The functional derivative of the scattering matrix at x determines the local quantities: partial density of states, injectivities, emissivities and the local density of states.

The matrix M of the ring is :

$$M = \begin{pmatrix} i cot_a + i cot_b & -\frac{i e^{-i\theta_a}}{s_a} - \frac{i e^{i\theta_b}}{s_b} \\ -\frac{i e^{i\theta_a}}{s_a} - \frac{i e^{-i\theta_b}}{s_b} & i cot_a + i cot_b \end{pmatrix} \tag{55}$$

where $cot_{a,b} \equiv \cot kl_{a,b}$ and $s_{a,b} \equiv \sin kl_{a,b}$. The matrix W is :

$$W = \begin{pmatrix} w_1 & 0 \\ 0 & w_2 \end{pmatrix}. \tag{56}$$

From (2) we obtain :

$$\Sigma = -1 + \frac{2}{\tilde{S}} \begin{pmatrix} i w_1^2 \sin kl + w_1^2 w_2^2 s_a s_b & i w_1 w_2 (s_b e^{-i\theta_a} + s_a e^{i\theta_b}) \\ i w_2 w_1 (s_b e^{i\theta_a} + s_a e^{-i\theta_b}) & i w_2^2 \sin kl + w_1^2 w_2^2 s_a s_b \end{pmatrix} \tag{57}$$

where

$$\tilde{S} = s_a s_b \det(M + W^{\mathrm{T}} W) = 2(\cos \theta - \cos kl) + i(w_1^2 + w_2^2)\sin kl + w_1^2 w_2^2 s_a s_b \tag{58}$$

is the modified spectral determinant (the spectral determinant $S(-E)$ is obtained by taking $w_{1,2} = 0$).

Figure 2: Scattering states incident from the left and the right.

The two components of the stationary state (1) wave function on the two arcs read :

$$\tilde{\psi}_a^{(1)}(x) \;=\; \frac{\mathrm{i}w_1}{\sqrt{\pi k}\,\tilde{S}}\mathrm{e}^{\mathrm{i}\theta_a x/l_a}\left[\sin k(l-x)+\mathrm{e}^{-\mathrm{i}\theta}\sin kx-\mathrm{i}w_2^2 s_b\sin k(l_a-x)\right] \tag{59}$$

$$\tilde{\psi}_{\bar{b}}^{(1)}(x) \;=\; \frac{\mathrm{i}w_1}{\sqrt{\pi k}\,\tilde{S}}\mathrm{e}^{-\mathrm{i}\theta_b x/l_b}\left[\sin k(l-x)+\mathrm{e}^{\mathrm{i}\theta}\sin kx-\mathrm{i}w_2^2 s_a\sin k(l_b-x)\right] \tag{60}$$

and the stationary state (2) :

$$\tilde{\psi}_a^{(2)}(x) \;=\; \frac{\mathrm{i}w_2}{\sqrt{\pi k}\,\tilde{S}}\mathrm{e}^{\mathrm{i}\theta_a(x/l_a-1)}\left[\sin k(l-l_a+x)+\mathrm{e}^{\mathrm{i}\theta}\sin k(l_a-x)-\mathrm{i}w_1^2 s_b\sin kx\right] \tag{61}$$

$$\tilde{\psi}_{\bar{b}}^{(2)}(x) \;=\; \frac{\mathrm{i}w_2}{\sqrt{\pi k}\,\tilde{S}}\mathrm{e}^{\mathrm{i}\theta_b(1-x/l_b)}\left[\sin k(l-l_b+x)+\mathrm{e}^{-\mathrm{i}\theta}\sin k(l_b-x)-\mathrm{i}w_1^2 s_a\sin kx\right]\,. \tag{62}$$

From the choice of orientations of the arcs a and b (see figure) we see that for the two components, the coordinate x measures the distance from the vertex 1 (this is why we consider the component $\psi_{\bar{b}}(x)$ instead of $\psi_b(x)$). Then $\psi_a^{(\alpha)}(0)=\psi_{\bar{b}}^{(\alpha)}(0)$ and $\psi_a^{(\alpha)}(l_a)=\psi_{\bar{b}}^{(\alpha)}(l_b)$.

Now we show how the local FSR is applied. The matrix M_x describes the same graph with an additional vertex x on arc a :

$$M_x=\begin{pmatrix} \mathrm{i}cot_{1x}+\mathrm{i}cot_b & -\frac{\mathrm{i}}{s_b}\mathrm{e}^{\mathrm{i}\theta_b} & -\frac{\mathrm{i}}{s_{1x}}\mathrm{e}^{-\mathrm{i}\theta_{x1}} \\ -\frac{\mathrm{i}}{s_b}\mathrm{e}^{-\mathrm{i}\theta_b} & \mathrm{i}cot_{2x}+\mathrm{i}cot_b & -\frac{\mathrm{i}}{s_{2x}}\mathrm{e}^{\mathrm{i}\theta_{2x}} \\ -\frac{\mathrm{i}}{s_{1x}}\mathrm{e}^{\mathrm{i}\theta_{x1}} & -\frac{\mathrm{i}}{s_{2x}}\mathrm{e}^{-\mathrm{i}\theta_{2x}} & \mathrm{i}cot_{1x}+\mathrm{i}cot_{2x} \end{pmatrix} \tag{63}$$

in the basis of vertices $\{1,2,x\}$. The notations $1x$ and $x2$ designate the two arcs replacing the arc a. In particular : $l=l_{1x}+l_{2x}+l_b$ and $\theta=\theta_b+\theta_{2x}+\theta_{x1}$. The coupling matrix is :

$$W_x=\begin{pmatrix} w_1 & 0 & 0 \\ 0 & w_2 & 0 \end{pmatrix} \tag{64}$$

and

$$K_x=\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\,. \tag{65}$$

After a little of algebra, we can check that (13) gives (22). The wave function of the time-reversed graph is obtained by changing the signs of all fluxes : $\psi^{t.r.(\alpha)}(x)=\psi^{(\alpha)}(x)|_{\theta_i\to-\theta_i}$.

A more direct derivation follows from (28). We can use more efficiently (28). x belongs to the arc a, then we have :

$$K(x)K(x)^\dagger=\frac{1}{s_a^2}\begin{pmatrix} \sin k(l_a-x) \\ \mathrm{e}^{\mathrm{i}\theta_a}\sin kx \end{pmatrix}\begin{pmatrix} \sin k(l_a-x) & \mathrm{e}^{-\mathrm{i}\theta_a}\sin kx \end{pmatrix}\,. \tag{66}$$

Using (28) we can check easily that

$$-\frac{1}{2\mathrm{i}\pi}\frac{\delta\,\Sigma}{\delta V(x)}=\begin{pmatrix} \tilde{\psi}_a^{t.r.\,(1)}(x) \\ \tilde{\psi}_a^{t.r.\,(2)}(x) \end{pmatrix}\begin{pmatrix} \tilde{\psi}_a^{(1)}(x) & \tilde{\psi}_a^{(2)}(x) \end{pmatrix} \tag{67}$$

Together with Σ this permits to calculate the density of states of interest.
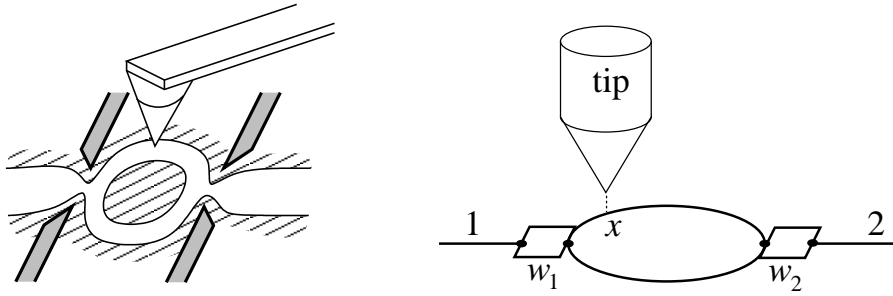
Figure 3: *Left figure* : Ahronov-Bohm ring probed by an STM. The dashed region is forbidden to the electron gas at the interface of 2 semiconductors. The couplings to the contacts can be adjusted with the help of gate voltages. *Right figure* : the graph that models this situation.

A ring out-of-equilibrium studied by STM

We now give a physical application : a ring probed by scanning tunneling microscopy (STM).

It is well known that if the system is at equilibrium, the tunneling current is related to the LDoS through the Bardeen formula. If now the device under consideration is put in an out-of-equilibrium situation by taking different potentials at the various contacts, which induces current flow, the Bardeen formula has to be generalized. We have to consider the conductances between the contact α and the STM tip. According to Refs. [17, 35] the corresponding transmission probabilities are

$$T_{\text{tip},\alpha} = 4\pi^2 \rho_{\text{tip}} |t_{\text{tip}}|^2 \rho(x,\alpha) . \tag{68}$$

Here ρ_{tip} is the DoS in the tip, t_{tip} the transmission amplitude between the system and the tip and $\rho(x,\alpha)$ is the injectivity from contact α into the point x.

In the case of the ring threaded by a flux θ, the injectivities were calculated above. Transmission from the tip into contact α are related to the emissivities :

$$T_{\alpha,\text{tip}} = 4\pi^2 \rho_{\text{tip}} |t_{\text{tip}}|^2 \rho(\alpha,x) \tag{69}$$

whereas the modification of the conductances (transmission probabilities) of the system due to the presence of the tip involves the partial LDoS :

$$T_{\alpha\beta}^{\text{tip}} = T_{\alpha\beta} - 4\pi^2 \rho_{\text{tip}} |t_{\text{tip}}|^2 \rho(\alpha,x,\beta) \tag{70}$$

where $T_{\alpha\beta}$ is the transmission amplitude from lead β to α in the absence of the tip.

We consider in detail the case where the ring is also weakly coupled to the two leads : $w_{1,2} \ll 1$. Transmission sepctroscopy of a weakly coupled ring was already investigated in Ref. [3]. In this case the scattering matrix presents sharp resonant (Breit-Wigner or Fano) structures. It is shown in [34] that, if the spectrum is non degenerate, the modulus of the stationary scattering state near an energy E_n of the isolated graph is

$$\rho(x,\alpha) = |\tilde{\psi}_E^{(\alpha)}(x)|^2 \underset{E \sim E_n}{\simeq} \frac{1}{\pi} \frac{\Gamma_{n,\alpha}}{(E-E_n)^2 + \Gamma_n^2} |\varphi_n(x)|^2 \tag{71}$$

where $\varphi_n(x)$ is the eigenstate of the isolated graph. $\Gamma_{n,\alpha} = \sqrt{E_n} w_\alpha^2 |\varphi_n(\alpha)|^2$ is the contribution of the coupling to the lead α to the resonance width $\Gamma_n = \sum_\alpha \Gamma_{n,\alpha}$. From the appendix B we also see that the emissivity is equal to the injectivity in the case of the ring $\rho(x,\alpha) = \rho(\alpha,x)$, then the conductances are equal : $T_{\text{tip},\alpha} = T_{\alpha,\text{tip}}$. [Note that in general these two transmissions

are not equal but $T_{\text{tip},\alpha}(\theta) = T_{\alpha,\text{tip}}(-\theta)$]. Using the equations of appendix B and the definition of the PLDoS we show

$$\rho(\alpha, x, \beta) \underset{E \sim E_n}{\simeq} \frac{1}{\pi} \frac{\delta_{\alpha\beta}\Gamma_{n,\alpha}[(E - E_n)^2 - \Gamma_n^2] + 2\Gamma_n\Gamma_{n,\alpha}\Gamma_{n,\beta}}{[(E - E_n)^2 + \Gamma_n^2]^2} |\varphi_n(x)|^2 . \tag{72}$$

For the perfect ring (no potential), since the eigenstates of the isolated graph are $\varphi_n(x) = \frac{1}{\sqrt{l}}e^{2ni\pi x/l}$ with $n \in \mathbb{Z}$, none of the conductances depend on the position x of the tip and they only present a resonant structure as a function of the Fermi energy E_F :

$$T_{\text{tip},\alpha} \propto \sum_n \frac{\Gamma_{n,\alpha}}{(E_F - E_n)^2 + \Gamma_n^2} \tag{73}$$

with $E_n = \left(\frac{2n\pi - \theta}{l}\right)^2$ and $\Gamma_{n,\alpha} = \frac{1}{l}\sqrt{E_n}w_\alpha^2$. As a function of the magnetic flux θ, the level $E_n(\theta)$ shifts and the conductance presents also a resonant structure as a function of the flux. If we increase the couplings $w_{1,2}$ to the leads, the resonance peaks are broadened and oscillations in the injectivities are generated, and thus an x-dependence of $T_{\text{tip},\alpha}$, since the original eigenstates of the isolated ring become strongly perturbed by the couplings to the leads.

7 Functional derivative of Σ in the arc language

We have demonstrated above how the functional derivative of the scattering matrix with respect to the potential is calculated. We have adopted a vertex point of view: all the matrices considered were matrices coupling the vertices of the graph. The vertex language is rather efficient in the sense that it leads to the consideration of compact matrices of the smallest possible size. However this approach supposes that one can introduce vertex variables, which can be achieved only if the wave function is continuous at the vertices inside the graph (the introduction of tunable couplings to the leads implies that the wave function at the end of the lead is different from the wave function at the vertex, however the wave function is still continuous inside the graph). The continuity of the wave function at the vertices implies a particular choice for the scattering at the vertices: the transmission amplitudes between all the leads issuing from the same vertex are equal, a description that may not be absolutely satisfactory in all cases. To describe the most general situation one has to abandon the constraint of continuity of the wave function at the vertices. In this case it is not anymore possible to define vertex variables and one has to introduce arc variables. We recall here some notions presented in [25]. On each arc i we introduce an amplitude A_i arriving at the vertex from which i issues and an amplitude B_i departing from it (see figure). That is to say that the wave function $\psi_i(x)$ on the bond is matched with $A_i e^{-ikx} + B_i e^{ikx}$ at the extremity of the arc.
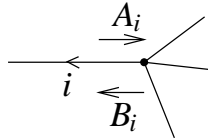

Figure 4: The two amplitudes associated to the arc i.

It is clear that we have to introduce L such couples of amplitudes, one for each external lead. These external amplitudes are gathered in L-column vectors A^{ext} and B^{ext}. By definition the scattering matrix relates these amplitudes : $B^{\text{ext}} = \Sigma A^{\text{ext}}$. On the other hand we must introduce two couples of amplitudes A_i, B_i per bond of the graph, *i.e.* one couple per arc. We gather

these $2B$ amplitudes into the column vectors A^{int} and B^{int}. Finally we group all amplitudes, internal and external, in two $2B + L$ column vectors A and B.

The scattering by the bonds is described by a matrix R coupling reversed internal arcs : $A^{\text{int}} = RB^{\text{int}}$. The scattering at the vertices is described by a matrix Q coupling arcs issuing from the same vertex : $B = QA$. If the basis of arcs is organized as {internal arcs, external arcs}, the matrix Q is separated into blocks:

$$Q = \left(\begin{array}{c|c} Q^{\text{int}} & \tilde{Q}^{\text{T}} \\ \hline \tilde{Q} & Q^{\text{ext}} \end{array} \right) \tag{74}$$

For simplicity we suppose here that the vertex scattering matrix is symmetric, that is the scattering at the vertices is not influenced by the presence of a magnetic field. However it is straightforward to extend the results to the more general situation: one has to make a disctinction between the two off-diagonal blocks of Q. The scattering matrix reads [25]:

$$\Sigma = Q^{\text{ext}} + \tilde{Q} \, (R^{\dagger} - Q^{\text{int}})^{-1} \, \tilde{Q}^{\text{T}} \, . \tag{75}$$

We now follow the same methodology as in the vertex approach to derive an expression of the functional derivative of Σ involving arc matrices. We consider a new graph $\mathcal{G}^{\lambda}$ which is similar to the original graph $\mathcal{G}$, apart from the fact that it possesses an additional vertex at x of weight λ (we recall that $\mathcal{G}$ and $\mathcal{G}_x = \mathcal{G}^{\lambda=0}$ possess the same properties). We call R_x the new bond scattering matrix. It describes the same physics as R. The vertex scattering matrix is Q^{λ}. Compared to Q, Q^{λ} has an additional 2×2 block describing the scattering at the vertex x. This block couples the two arcs issuing from x :

$$\frac{2}{2 + \text{i}k/\lambda} \left(\begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right) - 1 \, . \tag{76}$$

We introduce the notation $Q_x = Q^{\lambda=0}$. This matrix describes the same physical situation as Q. If we expand Q^{λ} in powers of λ we get for the internal part, at first order :

$$(Q^{\lambda})^{\text{int}} = Q_x^{\text{int}} - \frac{\text{i}\lambda}{2k}\kappa_x + \cdots \tag{77}$$

(κ_x couples the internal arcs). The only non vanishing elements are those associated to the two arcs issuing from x:

$$\kappa_x = \left(\begin{array}{ccc|cc|c} \ddots & \vdots & \vdots & \vdots & \vdots & \\ \cdots & 0 & 0 & 0 & 0 & \cdots \\ \hline \cdots & 0 & 1 & 1 & 0 & \cdots \\ \cdots & 0 & 1 & 1 & 0 & \cdots \\ \hline \cdots & 0 & 0 & 0 & 0 & \cdots \\ & \vdots & \vdots & \vdots & \vdots & \ddots \end{array} \right) = \left(\begin{array}{c} \vdots \\ 0 \\ \hline 1 \\ 1 \\ \hline 0 \\ \vdots \end{array} \right) \left(\begin{array}{ccccccc} \cdots & 0 & | & 1 & 1 & | & 0 & \cdots \end{array} \right) \, . \tag{78}$$

The functional derivative of Σ is equal to the first order term of Σ^{λ}. We get :

$$\frac{\delta \Sigma}{\delta V(x)} = -\frac{\text{i}}{2k}\tilde{Q}_x(R_x^{\dagger} - Q_x^{\text{int}})^{-1}\kappa_x(R_x^{\dagger} - Q_x^{\text{int}})^{-1}\tilde{Q}_x^{\text{T}} \, . \tag{79}$$

This expression allows to compute the functional derivative of Σ in terms of matrices describing the graph $\mathcal{G}_x$. The component of the stationary scattering state on the bond $(\alpha\beta)$ to which x belongs is given by

$$\sqrt{4\pi k} \, \tilde{\psi}_{(\alpha\beta)}^{(\mu)}(x) = \left[\left(\begin{array}{ccccccc} \cdots & 0 & 1 & 1 & 0 & \cdots \end{array} \right) (R_x^{\dagger} - Q_x^{\text{int}})^{-1}\tilde{Q}_x^{\text{T}} \right]_{\mu} \, . \tag{80}$$

With these results we can recover the relation (22) within the arc approach.

We are now going to simplify this expression in the sense that we will relate the functional derivative to the matrices of the original graph $\mathcal{G}$, of smaller size than those of $\mathcal{G}_x$.

We suppose that x belongs to the bond $(\alpha\beta)$ of $\mathcal{G}$. We show the structure of the matrices describing $\mathcal{G}$ in a basis {other internal arcs, $\alpha\beta, \beta\alpha \,||$external arcs}. The vertex scattering matrix is given by

$$Q = \left(\begin{array}{c|c} Q^{\mathrm{int}} & \tilde{Q}^{\mathrm{T}} \\ \hline \hat{Q} & Q^{\mathrm{ext}} \end{array} \right) \tag{81}$$

where we separate by a double line the internal and external vertices. The bond scattering matrix is

$$R = \left(\begin{array}{cc} R_{\mathrm{oia}} & 0 \\ 0 & \left(\begin{array}{cc} r_{\alpha\beta} & t_{\beta\alpha} \\ t_{\alpha\beta} & r_{\beta\alpha} \end{array} \right) \end{array} \right) \tag{82}$$

where R_{oia} is the block coupling all internal arcs apart from $\alpha\beta$ and $\beta\alpha$.

We now examine the structure of the matrices describing the graph $\mathcal{G}_x$. The bond $(\alpha\beta)$ of $\mathcal{G}$ is replaced by two bonds (αx) and $(x\beta)$ in $\mathcal{G}_x$.
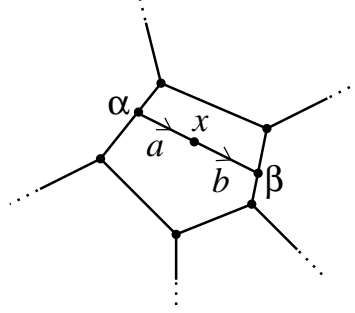

Figure 5: Auxiliary bonds $a \equiv \alpha x$ and $b \equiv \beta x$ on the $\alpha\beta$.

The two arcs will be also denoted by : $a \equiv \alpha x$ and $b \equiv x\beta$ (see Fig. 5). For simplicity we chose to organize the basis of arcs as : {other internal arcs, $a, \bar{b} \,|\, \bar{a}, b \,||$external arcs}. The vertex scattering matrix reads :

$$Q_x = \left(\begin{array}{cc|c} Q^{\mathrm{int}} & 0 & \tilde{Q}^{\mathrm{T}} \\ \hline 0 & \left(\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) & 0 \\ \hline \hat{Q} & 0 & Q^{\mathrm{ext}} \end{array} \right) \tag{83}$$

where the blocks of Q appear. We separate by a single line the part reminiscent of $\mathcal{G}$ and the one added by considering $\mathcal{G}_x$. The bond scattering matrix is

$$R_x = \left(\begin{array}{cc|c} R_{\mathrm{oia}} & 0 & 0 \\ 0 & \left(\begin{array}{cc} r_a & 0 \\ 0 & r_{\bar{b}} \end{array} \right) & \left(\begin{array}{cc} t_{\bar{a}} & 0 \\ 0 & t_b \end{array} \right) \\ \hline 0 & \left(\begin{array}{cc} t_a & 0 \\ 0 & t_{\bar{b}} \end{array} \right) & \left(\begin{array}{cc} r_{\bar{a}} & 0 \\ 0 & r_b \end{array} \right) \end{array} \right) . \tag{84}$$

Note that the transmission and reflexion coefficients of the arcs $a = \alpha x$ and $b = x\beta$ are related to the ones of the arc $\alpha\beta$ through the following relation :

$$\left(\begin{array}{cc} r_{\alpha\beta} & t_{\beta\alpha} \\ t_{\alpha\beta} & r_{\beta\alpha} \end{array} \right)^{-1} = \left(\begin{array}{cc} r_a^* & 0 \\ 0 & r_{\bar{b}}^* \end{array} \right) - \left(\begin{array}{cc} t_a^* & 0 \\ 0 & t_{\bar{b}}^* \end{array} \right) \left(\begin{array}{cc} r_{\bar{a}}^* & -1 \\ -1 & r_b^* \end{array} \right)^{-1} \left(\begin{array}{cc} t_{\bar{a}}^* & 0 \\ 0 & t_b^* \end{array} \right) . \tag{85}$$

It implies the expected relations : $r_{\alpha\beta} = r_a + \frac{t_{\bar{a}} r_b t_a}{1 - r_{\bar{a}} r_b}$, $t_{\alpha\beta} = \frac{t_a t_b}{1 - r_{\bar{a}} r_b}$, etc. (A remark about notations : $t_{\alpha\beta}$ is the transmission amplitude from α to β since it is the transmission of the arc $\alpha\beta$ connecting α to β.) To compute the functional derivative of the scattering matrix, we need to find the inverse of

$$
R_x^\dagger - Q_x^{\text{int}} = \left(
\begin{array}{c|c}
\cdots & \begin{array}{c} 0 \\ \left(\begin{array}{cc} t_a^* & 0 \\ 0 & t_b^* \end{array}\right) \end{array} \\
\hline
0 \quad \left(\begin{array}{cc} t_{\bar{a}}^* & 0 \\ 0 & t_b^* \end{array}\right) & \left(\begin{array}{cc} r_{\bar{a}}^* & -1 \\ -1 & r_b^* \end{array}\right)
\end{array}
\right) = \left(\begin{array}{c|c} A & B \\ \hline C & D \end{array}\right) .
\tag{86}
$$

One can see that

$$
A - B D^{-1} C = R^\dagger - Q^{\text{int}}
\tag{87}
$$

involves the matrices of $\mathcal{G}$. We have :

$$
(R_x^\dagger - Q_x^{\text{int}})^{-1} = \left(
\begin{array}{c|c}
(R^\dagger - Q^{\text{int}})^{-1} & -(R^\dagger - Q^{\text{int}})^{-1} B D^{-1} \\
\hline
-D^{-1} C (R^\dagger - Q^{\text{int}})^{-1} & \cdots
\end{array}
\right) .
\tag{88}
$$

Then after a little bit of algebra, (79) gives :

$$
\frac{\delta \Sigma}{\delta V(x)} = -\frac{\mathrm{i}}{2k} \tilde{Q} (R^\dagger - Q^{\text{int}})^{-1} \mathcal{L}(x) (R^\dagger - Q^{\text{int}})^{-1} \tilde{Q}^{\mathrm{T}}
\tag{89}
$$

where we have introduced the matrix $\mathcal{L}(x)$, that couples only the two arcs $\alpha\beta$ on which is put the vertex x :

$$
\mathcal{L}(x) = \left(
\begin{array}{c}
\vdots \\
0 \\
\frac{t_{\alpha x}^*(1 + r_{x\beta}^*)}{1 - r_{x\alpha}^* r_{x\beta}^*} \\
\frac{t_{\beta x}^*(1 + r_{x\alpha}^*)}{1 - r_{x\alpha}^* r_{x\beta}^*}
\end{array}
\right)
\left(
\begin{array}{cccc}
\cdots & 0 & \frac{(1 + r_{x\beta}^*) t_{x\alpha}^*}{1 - r_{x\alpha}^* r_{x\beta}^*} & \frac{(1 + r_{x\alpha}^*) t_{x\beta}^*}{1 - r_{x\alpha}^* r_{x\beta}^*}
\end{array}
\right) .
\tag{90}
$$

We have now achieved our program since (89) involves matrices of the original graph $\mathcal{G}$, and not bigger matrices of the graph $\mathcal{G}_x$ (describing however the same situation as $\mathcal{G}$) with an additional vertex at x.

Note that in the free case (no potential) the transmissions are $t_{\mu\nu} = \mathrm{e}^{\mathrm{i}k l_{\mu\nu} + \mathrm{i}\theta_{\mu\nu}}$ and the above matrix takes the simple form :

$$
\mathcal{L}(x) = \left(
\begin{array}{cccc}
\ddots & \vdots & \vdots & \vdots \\
\cdots & 0 & 0 & 0 \\
\cdots & 0 & \mathrm{e}^{-2\mathrm{i}k x_{\alpha\beta}} & \mathrm{e}^{-\mathrm{i}k l_{\alpha\beta} - \mathrm{i}\theta_{\alpha\beta}} \\
\cdots & 0 & \mathrm{e}^{-\mathrm{i}k l_{\alpha\beta} + \mathrm{i}\theta_{\alpha\beta}} & \mathrm{e}^{-2\mathrm{i}k x_{\beta\alpha}}
\end{array}
\right) .
\tag{91}
$$

Following what has been done previously we try to obtain a more transparent expression of $\mathcal{L}(x)$. The starting point is to express the wave function on a given bond $(\alpha\beta)$ in terms of the arc amplitudes. In the arc language, the appropriate basis of solutions of the Schrödinger equation on the bond $[E + \mathrm{d}_x^2 - V_{(\alpha\beta)}(x)] f(x) = 0$ is not anymore the functions $f_{\alpha\beta}(x)$ and $f_{\beta\alpha}(x)$, but the couple of stationary scattering states $\phi_{\alpha\beta}(x)$ and $\phi_{\beta\alpha}(x)$ associated with the potential $V_{(\alpha\beta)}(x)$ on the bond $(\alpha\beta)$. The function $\phi_{\alpha\beta}(x)$ is the scattering state incoming on the bond from the vertex α and is matched out of the bond like : $\phi_{\alpha\beta}(x) = \mathrm{e}^{\mathrm{i}kx} + r_{\alpha\beta} \mathrm{e}^{-\mathrm{i}kx}$ for $x < 0$ and $\phi_{\alpha\beta}(x) = t_{\alpha\beta} \mathrm{e}^{\mathrm{i}k(x - l_{\alpha\beta})}$ for $x > l_{\alpha\beta}$ [25].

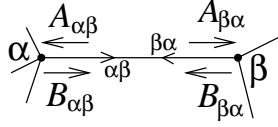Figure 6: The two couples of amplitudes $A_{\alpha\beta}$, $B_{\alpha\beta}$ and $A_{\beta\alpha}$, $B_{\beta\alpha}$ related to the arcs $\alpha\beta$ and $\beta\alpha$.

Then the component of the wave function on the bond reads :

$$\psi_{(\alpha\beta)}(x_{\alpha\beta}) = B_{\alpha\beta}\,\phi_{\alpha\beta}(x_{\alpha\beta}) + B_{\beta\alpha}\,\phi_{\beta\alpha}(x_{\alpha\beta})\,. \tag{92}$$

If we introduce the $2B$-vector

$$\mathcal{K}(x)^\dagger = \begin{pmatrix} \cdots & 0 & \phi_{\alpha\beta}(x_{\alpha\beta}) & \phi_{\beta\alpha}(x_{\alpha\beta}) \end{pmatrix} \tag{93}$$

we can write

$$\psi_{(\alpha\beta)}(x_{\alpha\beta}) = \mathcal{K}(x)^\dagger B^{\text{int}}\,. \tag{94}$$

We have now to specify the value of the amplitudes $B_{\alpha\beta}$ and $B_{\beta\alpha}$ for the stationary scattering state. If we consider the scattering state $\tilde{\psi}^{(\mu)}$, it is described by external incoming amplitudes $\tilde{A}^{(\mu)\text{ext}}$ whose components $\tilde{A}_\nu^{(\mu)\text{ext}} = \frac{1}{\sqrt{4\pi k}}\delta_{\mu\nu}$ describe a plane wave entering the graph from the lead connected to the vertex μ. From the two equations $A^{\text{int}} = RB^{\text{int}}$ and $B = QA$ we get

$$\tilde{B}^{(\mu)\text{int}} = (1 - Q^{\text{int}}R)^{-1}\tilde{Q}^{\text{T}}\tilde{A}^{(\mu)\text{ext}} \tag{95}$$

then

$$\tilde{\psi}_{(\alpha\beta)}^{(\mu)}(x_{\alpha\beta}) = \mathcal{K}(x)^\dagger(1 - Q^{\text{int}}R)^{-1}\tilde{Q}^{\text{T}}\tilde{A}^{(\mu)\text{ext}} = \frac{1}{\sqrt{4\pi k}}\left[\mathcal{K}(x)^\dagger(1 - Q^{\text{int}}R)^{-1}\tilde{Q}^{\text{T}}\right]_\mu\,. \tag{96}$$

Therefore, using (22) we obtain :

$$-\frac{1}{2\mathrm{i}\pi}\frac{\delta\,\Sigma}{\delta V(x)} = \frac{1}{4\pi k}\tilde{Q}(1 - RQ^{\text{int}})^{-1}R\mathcal{K}(x)\mathcal{K}(x)^\dagger(1 - Q^{\text{int}}R)^{-1}\tilde{Q}^{\text{T}} \tag{97}$$

which shows that

$$\mathcal{L}(x)R = \mathcal{K}(x)\mathcal{K}(x)^\dagger\,. \tag{98}$$

We have derived here non trivial relations between the reflection and transmission coefficients for the bonds (αx) and (βx) on one hand, and the functions $\phi_{\alpha\beta}(x)$ and $\phi_{\beta\alpha}(x)$ on the other hand.

7.1 Injectivities and emissivities

To compute the objects involved in the injectivities and emissivities, one needs to use the following relations :

$$\Sigma^\dagger\,\tilde{Q}\,(R^\dagger - Q^{\text{int}})^{-1} = \tilde{Q}^*\,(R - Q^{\text{int}\,\dagger})^{-1}R \tag{99}$$

and

$$(R^\dagger - Q^{\text{int}})^{-1}\,\tilde{Q}^{\text{T}}\,\Sigma^\dagger = R\,(R - Q^{\text{int}\,\dagger})^{-1}\,\tilde{Q}^\dagger\,. \tag{100}$$

The demonstration of these two relations uses (75) and relations between the blocks of Q coming from its unitarity. The computation of injectivities requires an expression for :

$$-\frac{1}{2\mathrm{i}\pi}\Sigma^\dagger\frac{\delta\,\Sigma}{\delta V(x)} = \frac{1}{4\pi k}\tilde{Q}^*\,(1 - R^\dagger Q^{\text{int}\,\dagger})^{-1}\mathcal{K}(x)\mathcal{K}(x)^\dagger(1 - Q^{\text{int}}R)^{-1}\tilde{Q}^{\text{T}} \tag{101}$$

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and the emissivities require :

$$-\frac{1}{2\mathrm{i}\pi}\frac{\delta\Sigma}{\delta V(x)}\Sigma^\dagger = \frac{1}{4\pi k}\tilde{Q}(R^\dagger - Q^{\mathrm{int}})^{-1}\mathcal{K}(x)\mathcal{K}(x)^\dagger\,(R - Q^{\mathrm{int}\,\dagger})^{-1}\,\tilde{Q}^\dagger\,. \tag{102}$$

7.2 Example : the ring with one lead

We consider the ring with only one lead. This geometry has been used to illustrate the decoherence introduced into a closed graph (here a ring) by the coupling to an external lead [4]. We now apply to this geometry the arc approach.
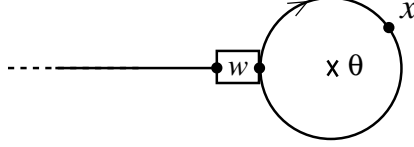
Figure 7:

We have :

$$Q = \frac{2}{2+w^2}\left(\begin{array}{cc|c} 1 & 1 & w \\ 1 & 1 & w \\ \hline w & w & w^2 \end{array}\right) - 1 \tag{103}$$

and

$$R = \left(\begin{array}{cc} 0 & \mathrm{e}^{\mathrm{i}kl-\mathrm{i}\theta} \\ \mathrm{e}^{\mathrm{i}kl+\mathrm{i}\theta} & 0 \end{array}\right)\,. \tag{104}$$

The matrix $\mathcal{L}(x)$ is :

$$\mathcal{L}(x) = \left(\begin{array}{cc} \mathrm{e}^{-2\mathrm{i}kx} & \mathrm{e}^{-\mathrm{i}kl-\mathrm{i}\theta} \\ \mathrm{e}^{-\mathrm{i}kl+\mathrm{i}\theta} & \mathrm{e}^{-2\mathrm{i}k(l-x)} \end{array}\right)\,. \tag{105}$$

We have $\det(R^\dagger - Q^{\mathrm{int}}) = \frac{2}{2+w^2}\mathrm{e}^{-\mathrm{i}kl}\,\tilde{S}$ where the modified spectral determinant is

$$\tilde{S} = 2(\cos\theta - \cos kl) + \mathrm{i}w^2\sin kl\,. \tag{106}$$

After a little bit of algebra we get, using (89) :

$$\frac{\delta\Sigma}{\delta V(x)} = \frac{2\mathrm{i}w^2}{k\tilde{S}^2}\left[\sin^2 kl + 2\sin kx\sin k(l-x)(\cos\theta - \cos kl)\right]\,. \tag{107}$$

We can check that this expression coincides with the one proven above

$$\frac{\delta\Sigma}{\delta V(x)} = -2\mathrm{i}\pi\,\tilde{\psi}^{t.r.}(x)\,\tilde{\psi}(x) \tag{108}$$

by using the wave function $\tilde{\psi}(x)$ that has been computed before (it is given by the wave function of the ring with two leads $\tilde{\psi}_a^{(1)}(x)$ in which we set $w_2 = 0$) : $\tilde{\psi}(x) = \frac{\mathrm{i}w}{\sqrt{\pi k}\,\tilde{S}}\mathrm{e}^{\mathrm{i}\theta x/l}(\sin k(l-x) + \mathrm{e}^{-\mathrm{i}\theta}\sin kx)$.

8   Conclusion

In this article, we have discussed the local Friedel sum rule which allows to extract local information (the local density of states, injectivities, emissivities, and partial density of states) from the scattering matrix. For this purpose one has to be able to compute functional derivatives of the scattering matrix, which can be achieved for graphs by algebraic calculations. We have presented a discussion both within the vertex language and the arc language. The former is appropriate when we consider wave functions which are continuous at the vertices of the graph, whereas the latter is needed for the most general graphs with arbitrary vertex scattering. We have emphasized that the scattering can only give information about the states of the graph coupled to the external leads. If the graph possesses some states that remain uncoupled to the leads, this part of the spectrum (discrete part) is not probed by elastic single particle scattering. Local information on density of states is important for the solution of physical problems which involve a changing charge distribution, like non-linear transport and frequency dependent transport. Here we have given several examples to demonstrate the applications of our formalism and in particular have considered the experimental situation in which the local properties of a system are probed by scanning tunneling microscopy.

The local density of states and its generalizations investigated here are not the only quantities related to functional derivatives of the scattering matrix. Off-diagonal elements of the functional derivatives of the scattering matrix are related to (dynamic) charge fluctuations [36] which play an important role in the description of dephasing in mesoscopic conductors [33, 37, 38]. Furthermore low frequency parametric pumping of electrical conductors [39, 40] and the fluctuations associated with it [41] can be related to functional derivatives. Thus the work presented here can be expected to be useful in a wide range of physical problems.

Acknowledgement

A   Spectrum of open graphs - Continuous and discrete parts

We have already mentioned in the introduction that certain graphs may possess some localized states that are not coupled to the leads. Since such states are not manifesting themselves in the scattering properties, the usual state counting method from the scattering (Friedel sum rule) fails [26]. The purpose of the appendix is to discuss the structure of the LDoS when such a situation occurs.

For each arc i of a graph, we introduce an amplitude A_i arriving at the vertex from which i issues, and an outgoing amplitude B_i (figure 4). Those amplitudes are related by vertex scattering $B = Q\,A$. The amplitudes associated with internal arcs are also related through the bond scattering matrix $A^{\mathrm{int}} = R\,B^{\mathrm{int}}$. If we eliminate B^{int} we get

$$\tilde{Q}^{\mathrm{T}} A^{\mathrm{ext}} 0 = (R^{\dagger} - Q^{\mathrm{int}})\,A^{\mathrm{int}} \tag{109}$$

$$B^{\mathrm{ext}} = \tilde{Q}\,A^{\mathrm{int}} + Q^{\mathrm{ext}}\,A^{\mathrm{ext}}\,. \tag{110}$$

Two cases occur :

(i) In general $\det(R^{\dagger} - Q^{\mathrm{int}}) \neq 0$. Then at any energy k^2, the solution of the above equations has components on all bonds of the graph and on the leads. All the solutions of the Schrödinger equation are the stationary scattering states. In this case, the FSR gives the correct information on the number of states of the graph[2].

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[2] Note that $\det(R^{\dagger} - Q^{\mathrm{int}}) \neq 0$ for the one-dimensional case. The 1d case may be viewed as a single bond

(*ii*) For certain graphs $\det(R^\dagger - Q^{\text{int}}) = 0$ possesses a discrete set of solutions $E = E_1, E_2, \cdots$. At those energies one can construct solutions of the Schrödinger equation such that $A^{\text{ext}} = B^{\text{ext}} = 0$ while the internal amplitudes satisfy $(R^\dagger - Q^{\text{int}})A^{\text{int}} = 0$ and $\tilde{Q}A^{\text{int}} = 0$. These relations describe a wave function localized inside the graph. In this case, the continuous spectrum related with the stationary scattering states coexists with a discrete spectrum of localized states. The LDoS takes the form :

$$\rho(x; E) = \underbrace{\sum_\alpha |\tilde{\psi}_E^{(\alpha)}(x)|^2}_{\text{continuous spectrum}} + \underbrace{\sum_n \sum_{j=1}^{g_n} \delta(E - E_n) |\varphi_{n,j}(x)|^2}_{\text{discrete spectrum}} \tag{111}$$

for x in the graph (if x belongs to a lead, the second part of course vanishes). $\varphi_{n,j}(x)$ is a wave function localized in the graph and normalized to unity and j a degeneracy label. The number of uncoupled states at energy E_n is $g_n = \dim \operatorname{Ker}(R^\dagger - Q^{\text{int}})|_{E=E_n}$.

We emphasize that what is unusual here is that the discrete and continous parts of the spectrum coexist at the same energies, due to the absence of hybridization of the localized states with the states of the continuous spectrum.

The second situation may occur if the spectrum of the isolated graph is degenerate. In the space of the parameters of the graph (lengths, fluxes,...) this occur in a volume of measure zero. This "violation" of the FSR occurs for discrete values of the parameters and signals a discontinuous behaviour of the scattering matrix as a function of those parameters.

A.1 Example

Let us consider the case of the ring coupled to one lead. This example has already been studied in [26] in the vertex language. Here we adopt an arc language needed to construct all the solutions of the Schrödinger equation in the case (*ii*) and compute the LDoS. The matrices R and Q are given above (103,104).

$$R^\dagger - Q^{\text{int}} = \begin{pmatrix} \frac{w^2}{2+w^2} & e^{-ikl-i\theta} - \frac{2}{2+w^2} \\ e^{-ikl+i\theta} - \frac{2}{2+w^2} & \frac{w^2}{2+w^2} \end{pmatrix}, \tag{112}$$

whose determinant is

$$\det(R^\dagger - Q^{\text{int}}) = \frac{2}{2+w^2} e^{-ikl} \left[2(\cos\theta - \cos kl) + iw^2 \sin kl \right]. \tag{113}$$

(*i*) If $\boldsymbol{\theta \neq 0}$, the equation $\det(R^\dagger - Q^{\text{int}}) = 0$ doesn't have a solution. The only solution of the Schrödinger equation is the stationary scattering state. Then the LDoS is

$$\rho(x; E) = \left| \tilde{\psi}(x) \right|^2 = \left| \frac{w}{\sqrt{\pi k}} \frac{\sin k(l-x) + e^{-i\theta} \sin kx}{2(\cos\theta - \cos kl) + iw^2 \sin kl} \right|^2. \tag{114}$$

In the limit $w \to 0$, the wave function $\tilde{\psi}(x)$ gives the wave functions of the isolated ring.
(*ii*) $\boldsymbol{\theta = 0}$: However if the flux is zero (or a multiple of the flux quantum),

$$\det(R^\dagger - Q^{\text{int}}) = \frac{4}{2+w^2} e^{-ikl} \left[2\sin(kl/2) + iw^2 \cos(kl/2) \right] \sin(kl/2) \tag{115}$$

(two arcs a and $\bar{a}$) connected at its extremities to two leads (arcs 1 and 2). The corresponding 4×4 vertex scattering matrix Q is decomposed into the four 2×2 blocks which can always be chosen as : $Q^{\text{ext}} = Q^{\text{int}} = 0$ and $\tilde{Q} = \tilde{Q}^{\text{T}} = 1$. Then $|\det(R^\dagger - Q^{\text{int}})| = 1$. The FSR always counts correctly the states in 1d, as it should.

vanishes for all energies of the isolated ring : $k_n = 2n\pi/l$ for $n \in \mathbb{N}$. At $k \neq k_n$ the solutions of (109,110) give the stationary scattering state. At $k = k_n$, (109,110) possesses a solution $A^{\text{int}} = (1,1) \times A^{\text{ext}}/w$ coupled to the lead (the scattering state), and a solution $A^{\text{int}} = (1,-1)$ with $A^{\text{ext}} = B^{\text{ext}} = 0$ localized in the ring. The LDoS is then :

$$\rho(x;E) = \left| \frac{w}{\sqrt{\pi k}} \frac{\cos k(x - l/2)}{2\sin(kl/2) + \mathrm{i}w^2\cos(kl/2)} \right|^2 + \sum_{n=1}^{\infty} \delta(E - k_n^2) \left| \sqrt{\frac{2}{l}} \sin k_n x \right|^2 . \tag{116}$$

The first term is $-\frac{1}{2\mathrm{i}\pi} \frac{\delta}{\delta V(x)} \ln \Sigma$.

Continuity of Σ

To end the section, let us discuss the question of continuity of Σ. The scattering matrix should be a continuous function of the energy obviously, however it has no reason to be continuous as a function of parameters such as fluxes, lengths,... In the case of the ring we have :

$$\Sigma(k^2, \theta) = \mathrm{e}^{\mathrm{i}\delta_f} = \frac{2(\cos kl - \cos \theta) + \mathrm{i}w^2 \sin kl}{-2(\cos kl - \cos \theta) + \mathrm{i}w^2 \sin kl} . \tag{117}$$

At zero flux :

$$\Sigma(k^2, 0) = \frac{-2\sin(kl/2) + \mathrm{i}w^2\cos(kl/2)}{2\sin(kl/2) + \mathrm{i}w^2\cos(kl/2)} . \tag{118}$$

When we study the system through its scattering properties, there is no reason to introduce some arbitrary jumps of $\delta_f(k^2)$, and the only natural choice is to impose the continuity of $\delta_f(k^2)$ as a function of energy, by convention. Then, in the absence of localized states when the FSR holds, it is related to the integrated DoS (IDoS) $\mathcal{N}(E)$ of the graph by $\mathcal{N}(E) \simeq \frac{1}{2\pi}\delta_f(E)$ up to some oscillatory term inessential at the level of the Weyl term of the IDoS.

In the case of the ring we see that Σ is discontinuous as a function of θ. For example at the energies $kl = 2n\pi$:

$$\lim_{\theta \to 0} \lim_{kl \to 2n\pi} \Sigma(k^2, \theta) = -1 \tag{119}$$

whereas

$$\lim_{kl \to 2n\pi} \lim_{\theta \to 0} \Sigma(k^2, \theta) = +1 . \tag{120}$$

The discontinuous behaviour is even more stricking on the Friedel phase which is plotted for different values of θ. If $\theta \neq 0$ the Weyl term of the Friedel phase is $\delta_f \simeq 2kl$, but if $\theta = 0$ it only grows like $\delta_f \simeq kl$ [26] as illustrated on the figure.

B   Time reversal symmetry and some useful relations

Note that the unitarity of (12) is demonstrated by using the fact that the matrix M is anti-hermitian [25] $M^\dagger = -M$ and by using the obvious relation :

$$\frac{1}{M + W^{\mathrm{T}}W} + \frac{1}{-M + W^{\mathrm{T}}W} = \frac{1}{M + W^{\mathrm{T}}W} 2W^{\mathrm{T}}W \frac{1}{-M + W^{\mathrm{T}}W} . \tag{121}$$

With the help of this relation we can easily find the relation between the wave function and the one of the time-reversed graph. From (12,18,19) :

$$\Sigma^\dagger(\tilde{\Psi}^{t.r.})^{\mathrm{T}} = \tilde{\Psi}^\dagger \tag{122}$$

or

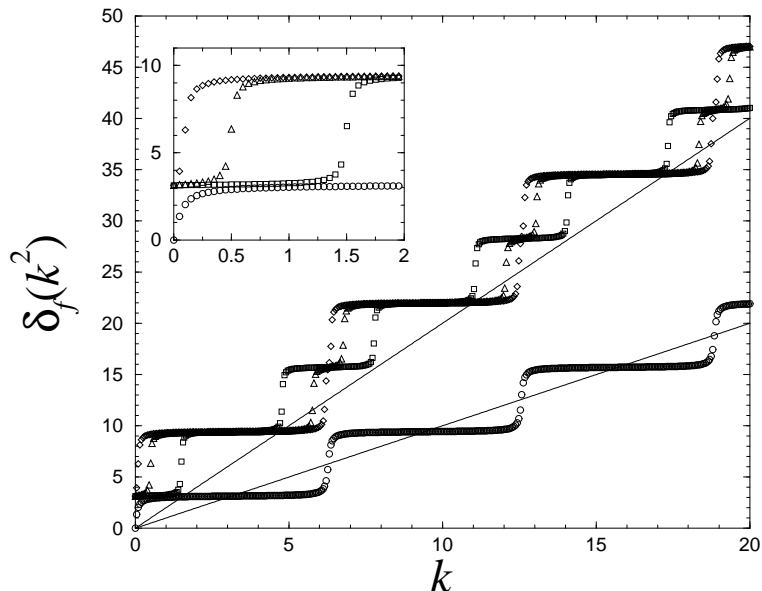$$\tilde{\Psi}^{t.r.} = \tilde{\Psi}^* \Sigma^{\mathrm{T}} . \tag{123}$$

Figure 8: Friedel phase $\delta_f(k^2)$. The coupling is $w = 0.25$ and the length $l = 1$. The four curves corresponds to $\theta = 1.5$ (squares), $\theta = 0.5$ (triangles), $\theta = 0.1$ (diamonds) and $\theta = 0$ (circles). The two lines are kl and $2kl$. If $\theta \neq 0$ there are two jumps of 2π per interval $[2n\pi, 2(n+1)\pi[$ at the energies of the two eigenstates of the isolated ring. If $\theta = 0$ there is only one jump of 2π at the degenerate energy. In the inset we clearly see the discontinuity of $\delta_f(k^2 = 0)$ which equals π for $\theta \neq 0$ and 0 for $\theta = 0$.

These two last relations express how time reversal symmetry acts on the scattering states. Let us now discuss this point in more detail. If we consider a close graph $\mathcal{G}$ characterized by a matrix $M(\gamma)$, the graph $\mathcal{G}^{t.r.}$ obtained by reversing the magnetic fluxes is described by the matrix $M(\gamma)^{\mathrm{T}}$ [see eq. (4,5)]. If the original graph $\mathcal{G}$ has a spectrum $\{E_0, E_1, \cdots\}$, the time reversed graph $\mathcal{G}^{t.r.}$ has the same set of energies :

$$E_n(\{\theta_{\mu\nu}\}) = E_n(\{-\theta_{\mu\nu}\}) \,. \tag{124}$$

This very general feature is easily demonstrated for graphs since the spectrum is given by $\det M(-E_n) = 0$. Note that stricktly speaking the energies are not in general even functions of the magnetic field. It is only the full spectrum which is invariant under time reversal symmetry, however we do not change the labels on both sides of equation (124) to simplify the discussion.

If $\varphi_n(x)$ is an eigenstate of $\mathcal{G}$, then the basic fact that the corresponding eigenstate of $\mathcal{G}^{t.r.}$ is its complex conjugate,

$$\varphi_n^{t.r.}(x) = \varphi_n(x)^* \,, \tag{125}$$

can be also easily recovered. Indeed, if we call φ_n the V-column vector gathering the values of the wave function at the nodes, $\varphi_n^{\mathrm{T}} = (\varphi_{n,1}, \cdots, \varphi_{n,V})$, it is a solution of $M(-E_n)\varphi_n = 0$. Since $M(-E_n)^\dagger = -M(-E_n)$ we see that the eigenvector of $M(-E_n)^{\mathrm{T}}$ is φ_n^*.

Now we examine the connected graph and its stationary scattering states. What is the relation between the scattering states of $\mathcal{G}$ and $\mathcal{G}^{t.r.}$? Equation (122) relates the values of $\tilde{\psi}$ and $\tilde{\psi}^{t.r.}$ at all the vertices. Since we can always introduce an additional vertex on a bond, it can be written as :

$$\sum_\alpha \Sigma_{\alpha\beta}^* \, \tilde{\psi}^{t.r.\,(\alpha)}(x) = \tilde{\psi}^{(\beta)}(x)^* \,. \tag{126}$$

If the graph is weakly coupled, the scattering matrix has a resonant structure :

$$\Sigma_{\alpha\beta} \underset{E \sim E_n}{\simeq} - \delta_{\alpha\beta} + \frac{2\mathrm{i}\sqrt{E_n}\, w_\alpha \varphi_n(\alpha)\, w_\beta \varphi_n(\beta)^*}{E - E_n + \mathrm{i}\Gamma_n}\, , \tag{127}$$

where $\Gamma_n = \sum_\alpha \Gamma_{n,\alpha}$ with $\Gamma_{n,\alpha} = \sqrt{E_n} w_\alpha^2 |\varphi_n(\alpha)|^2$ [34]. The positions of the resonances and their widths remain unchanged by reversing the fluxes. The scattering states behave like [34] :

$$\tilde{\psi}^{(\alpha)}(x) \underset{E \sim E_n}{\simeq} \frac{1}{\sqrt{\pi}} \frac{\mathrm{i}E_n^{1/4} w_\alpha \varphi_n(\alpha)^*}{E - E_n + \mathrm{i}\Gamma_n}\, \varphi_n(x) \tag{128}$$

near a resonance E_n, and the scattering states of $\mathcal{G}^{t.r.}$ behave like :

$$\tilde{\psi}^{t.r.\,(\alpha)}(x) \underset{E \sim E_n}{\simeq} \frac{1}{\sqrt{\pi}} \frac{\mathrm{i}E_n^{1/4} w_\alpha \varphi_n(\alpha)}{E - E_n + \mathrm{i}\Gamma_n}\, \varphi_n(x)^*\, . \tag{129}$$

From the last equations we see that we must take care of the fact that $\tilde{\psi}^{t.r.\,(\alpha)}(x) \neq \tilde{\psi}^{(\alpha)}(x)^*$.

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