

Charge and currents distribution in 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 such a network is connected to infinite leads. We study the correlations of the charge in such graphs out of equilibrium, as well as the distribution of the currents in the wires, inside the graph. These quantities are related to the scattering matrix of the graph. We discuss the case where the graph is weakly connected to the wires.

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1 Introduction

Within the field of mesoscopic physics, the interest in graphs is motivated by the fact that they provide simple models for networks of wires, which are most of the time sufficient to describe the effect of interest (such as Aharonov-Bohm oscillations of the conductance of a ring for example). Scattering theory plays a central role in mesoscopic physics : it provides a transparent formalism to study transport properties of phase coherent systems. Moreover, many other physical quantities can be related to scattering properties, like the current noise [1, 2], the density of states through the Friedel sum rule, mesoscopic capacitance, relaxation resistance [3, 4]. Scattering on graphs has attracted the attention of many authors among which we can quote [5, 6, 7, 8, 9, 10, 11, 12, 13, 14].

Despite the scattering matrix is a global quantity characterizing the full system, some local information can be extracted from it. This idea has been fruitfully exploited in many works of Büttiker *et al* (see review articles [15, 16] and references therein). To understand this point let us first consider the case of an isolated system (an isolated graph for example). In this case, the spectrum of the Schrödinger operator is discrete : $E_n, \varphi_n(x)$. Let us consider a physical quantity described by the operator $\hat{X}$, related to a conjugate variable f (that is $\hat{X} = \frac{\partial}{\partial f} \hat{H}$ where $\hat{H}$ is the Hamiltonian). Typical examples are provided by a magnetization $\mathcal{M}$, a persistent current

I , or the local density $\rho(x)$, which are conjugated to the magnetic field $-\mathcal{B}$, a flux¹ $-\phi$ and the potential $V(x)$, respectively. As it is well known, a simple way to obtain the expectation value of the physical quantity of interest is to compute the derivative of the eigenenergies with respect to f : $X_n = \langle \varphi_n | \hat{X} | \varphi_n \rangle = \frac{\partial E_n}{\partial f}$. This result is known as the Feynman-Hellmann theorem.

A natural question is to extend these relations to open systems that are connected to reservoirs possibly in an out of equilibrium situation. As it is well known, the scattering approach will prove to be relevant for this purpose. The open system of interest in the present article will be a graph connected to some infinite wires. In this case the spectrum is continuous. The stationary scattering states $\tilde{\psi}_E^{(\alpha)}(x)$ describing the injection of a plane wave at contact α provide the convenient basis of states for the discussion. Then we can relate the quantity of interest (that can give a local information) to the scattering matrix Σ through the relation: $\langle \tilde{\psi}_E^{(\alpha)} | \hat{X} | \tilde{\psi}_E^{(\beta)} \rangle = -\frac{1}{2i\pi} \left(\Sigma^\dagger \frac{\partial \Sigma}{\partial f} \right)_{\alpha\beta}$. In the case of graphs, this idea will be made explicit in three cases: (i) when $\hat{X} \rightarrow \hat{\rho}(x)$ is the local density of electrons² (then $f \rightarrow V(x)$ is the local potential), (ii) if $\hat{X} \rightarrow \hat{Q}$ is the charge of the graph ($f \rightarrow U$ is a potential constant inside the graph) and (iii) if $\hat{X} \rightarrow \hat{J}_{\mu\nu}$ is the current in an arc of the graph ($f \rightarrow \theta_{\mu\nu}$ is the flux along the arc).

The purpose of our article is to study the distribution of charge and current densities in a graph out of equilibrium. The out of equilibrium regime is obtained by imposing different potentials at the external leads. A motivation for this study comes from the recent interest in quantum coherent devices such as Cooper pair boxes used for building charge Qubits (see [20] for a review). The full spectrum of charge fluctuations is involved in the study of the dephasing in a Qubit perturbed by the charge fluctuations of another conductor capacitively coupled to the first one [15, 21, 22]. In the same way, current density fluctuations are a source of dephasing for Qubits based on flux states. Since the formalism developed in the present paper provides a systematic way for evaluating the charge and current density noise fluctuations in a mesoscopic circuit, it might be useful for estimating the dissipation and decoherence properties of some experimental systems of Qubits. More precisely, it was shown that transition rates of a two level system weakly coupled to a quantum environment are directly related to the unsymmetrized correlator : see for example [23] where the roles of the negative and the positive part of the spectrum of the unsymmetrized correlator are studied. On the other hand the relaxation and decoherence rates are related to a symmetrized correlator [20]. Correlators are more directly accessible in noise measurements : in a recent work, Gavish *et al.* [24, 25] proposed a description of the full measurement chain for the current noise of a mesoscopic sample. In this work, the unsymmetrized correlator is involved in excess noise measurement. Finally one should mention that experimentalists are now able, using photon assisted tunneling in a superconductor-insulator-superconductor tunnel junction, to measure the unsymmetrized current noise correlator in quantum mesoscopic devices [26]. The question of which correlator (symmetrized or not) to consider depends on the question of interest. Therefore we will consider in the following the unsymmetrized correlator as the fundamental object³.

In this paper, electron-electron interactions will not be taken into account. However, even if this limits the applicability of our results, we recall that they can be taken into account in a mean field Hartree approximation within the scattering approach, as it has been developed in several papers by Büttiker and collaborators [3, 4, 27] (see also [28] for a review). In this framework the charge (or the current) contains two contributions : a bare contribution (injected

¹The variable conjugate to a flux line threading a loop of a planar graph is the current flowing through the semi infinite line issuing from the flux [17] (see also [18]). This can also be easily understood in the 2-dimensional plane [19].

²In this case $\langle \tilde{\psi}_E^{(\alpha)} | \hat{\rho}(x) | \tilde{\psi}_E^{(\beta)} \rangle = \tilde{\psi}_E^{(\alpha)*}(x) \tilde{\psi}_E^{(\beta)}(x)$ is an off diagonal element of the local DoS [15, 13]

³There are indeed two unsymmetrized correlators depending on the order chosen. But for a system in a stationary regime, they can be simply related as shown in appendix A.

charge) and a contribution from screening. Screening affects ac transport or finite frequency noise. It is not the purpose of our article to consider such interaction effects; in other terms we will focus on the bare contribution of the charge and its relation to the scattering matrix of a graph.

This paper is organized as follows: first of all, the basic formalism [10] necessary for the discussion is recalled. Then the charge distribution inside the graph is analyzed in details. The first and second moments of the total charge are related to the scattering matrix. Finally analytic expressions for the full spectrum of charge fluctuations are provided.

In a second part we will show how currents inside the graph can be related to the scattering matrix. It was shown in [17] that the persistent current can be related to the derivative of the Friedel phase with respect to the magnetic flux. In this work the possible generalization to an out of equilibrium situation was not considered because the authors did not identify the different contributions of the various scattering states associated to the different leads. These contributions were identified later in [29]. Moreover, in Taniguchi's work, a formula relating the current-current correlations and the scattering matrix was proposed. Despite the contributions of the scattering states to the correlator were given, it is still not sufficient to study current-current correlations in an out-of-equilibrium situation (this point will be made clear later). Our results go beyond this limitation and provide the generalization of Taniguchi's result.

2 Basic formalism : scattering matrix

We consider the Schrödinger operator $-D_x^2 + V(x)$ on a graph, where $D_x = d_x - iA(x)$ is the covariant derivative (we choose units : $\hbar = 2m = e = 1$). The graph is made of B bonds $(\alpha\beta)$, each being identified with an interval $[0, l_{\alpha\beta}] \in \mathbb{R}$. We call $x_{\alpha\beta}$ the coordinate that measures the distance from the vertex α . The Schrödinger operator acts on a scalar function $\varphi(x)$ which is described by B components $\varphi_{(\alpha\beta)}(x_{\alpha\beta})$, one for each bond. The bonds are connected at V vertices. The adjacency matrix $a_{\alpha\beta}$ encodes the structure of the graph : $a_{\alpha\beta} = 1$ if $(\alpha\beta)$ is a bond and $a_{\alpha\beta} = 0$ otherwise.

Vertex formulation

Let us first assume that the wave function is continuous at each vertex. This allows to introduce vertex variables ; we denote $\varphi_\alpha \equiv \varphi(\alpha)$ the function at the vertex α . The continuity condition reads : $\varphi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = \varphi_\alpha$ for all vertices β neighbours of α . A second condition is added to ensure current conservation at the vertices : $\sum_\beta a_{\alpha\beta} D_x \varphi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = \lambda_\alpha \varphi_\alpha$ where the sum over β runs over all neighbouring vertices of α due to the presence of the adjacency matrix. λ_α is a real parameter. The requirement of continuity of the wave function imposes a special scattering at the vertices : in particular, the transmission amplitudes of a plane wave of energy $E = k^2$ between two leads issuing from the same vertex of coordinence $m_\alpha = \sum_\beta a_{\alpha\beta}$ are all equal to $2/(m_\alpha + i\lambda_\alpha/k)$.

The wave function on the bond $(\alpha\beta)$ is :

$$\varphi_{(\alpha\beta)}(x_{\alpha\beta}) = e^{ix_{\alpha\beta}\theta_{\alpha\beta}/l_{\alpha\beta}} \left(\varphi_\alpha f_{\alpha\beta}(x_{\alpha\beta}) + \varphi_\beta e^{-i\theta_{\alpha\beta}} f_{\beta\alpha}(x_{\alpha\beta}) \right) \quad (1)$$

where $\theta_{\alpha\beta}$ is the magnetic flux along the bond $(\alpha\beta)$ (the vector potential is $A_{\alpha\beta} = \theta_{\alpha\beta}/l_{\alpha\beta}$). The two real functions $f_{\alpha\beta}(x)$, $f_{\beta\alpha}(x)$ are the two linearly independent solutions of the Schrödinger equation $[E + d_x^2 - V_{(\alpha\beta)}(x)]f(x) = 0$ on the bond satisfying boundary conditions : $f_{\alpha\beta}(0) = 1$, $f_{\alpha\beta}(l_{\alpha\beta}) = 0$, $f_{\beta\alpha}(0) = 0$ and $f_{\beta\alpha}(l_{\alpha\beta}) = 1$. These two functions encode the information about the potential on the bond. For example, in the absence of potential, $V(x) = 0$, we have $f_{\alpha\beta}(x_{\alpha\beta}) = \frac{\sin k(l_{\alpha\beta} - x_{\alpha\beta})}{\sin kl_{\alpha\beta}}$.

The graph is connected to L leads. Each lead is a semi-infinite line plugged at a vertex of the graph, with a coupling parameter $w_\alpha \in \mathbb{R}$ (see figure 1). The introduction of these couplings allows to go continuously from an isolated graph to a connected one. The precise physical meaning of these parameters is given in [10]. In particular, the transmission amplitude through the box between the graph and the lead is $2w_\alpha/(1+w_\alpha^2)$. We introduce the $L \times V$ matrix W :

$$W_{\alpha\beta} = w_\alpha \delta_{\alpha\beta} \quad (2)$$

where α belongs to the set of vertices connected to leads and β to the set of all vertices of the graph. This matrix encodes the information about the way the graph is connected to the external leads.

The scattering matrix Σ is a $L \times L$ matrix describing how a plane wave of energy E entering from a lead is scattered into the other leads by the graph. It is given by

$$\Sigma = -1 + 2W \frac{1}{M + W^T W} W^T \quad (3)$$

where the matrix M is :

$$M_{\alpha\beta}(-E) = \frac{i}{\sqrt{E}} \left(\delta_{\alpha\beta} \left[\lambda_\alpha - \sum_\mu a_{\alpha\mu} \frac{df_{\alpha\mu}}{dx_{\alpha\mu}}(\alpha) \right] + a_{\alpha\beta} \frac{df_{\alpha\beta}}{dx_{\alpha\beta}}(\beta) e^{i\theta_{\alpha\beta}} \right). \quad (4)$$

Note that for $E > 0$, this matrix is antihermitian : $M^\dagger = -M$. It can also be related [10] to reflexion and transmission coefficients describing the potential on each bond :

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

The expressions (4,5), together with (3), generalize results known in the absence of the potential [6].

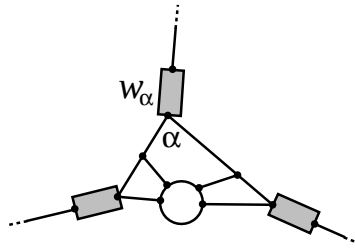


Figure 1: Example of graph. The boxes represent the couplings between the infinite leads and the graph.

The vertex formulation that we have just recalled is rather efficient mainly because vertex matrices are rather compact. However, as we have noticed, it corresponds to a particular choice of vertex scattering which does not describe all allowed relevant physical situations. In the most general situation it is not anymore possible to introduce vertex variables and one has to use the arc formulation that will now be briefly described.

Arc formulation

An arc is an oriented bond. 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 2). Equivalently, 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. 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 : $A^{\text{int}} = R B^{\text{int}}$. The matrix element between arc i and j is given by :

$$R_{ij} = r_i \delta_{i,j} + t_i \delta_{\bar{i},j} \quad (6)$$

where $\bar{i}$ designate the reversed arc. r_i and t_i are the reflexion and transmission coefficients describing the scattering of a plane wave by the potential of the bond (i). 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 can be separated into blocks:

$$Q = \left(\begin{array}{c|c} Q^{\text{int}} & \tilde{Q}^{\text{T}} \\ \hline \tilde{Q} & Q^{\text{ext}} \end{array} \right) \quad (7)$$

The scattering matrix reads :

$$\Sigma = Q^{\text{ext}} + \tilde{Q} (R^\dagger - Q^{\text{int}})^{-1} \tilde{Q}^{\text{T}}. \quad (8)$$

For more details, see [10]. Historically, the arc approach has been followed in many works, like [30, 31, 32] since it is the most natural approach. It has been formalized more systematically in [33] without potential and in [10] in the most general case.

How can we express the wave function inside the graph within the arc formulation ? In this case, the appropriate basis of solutions of the Schrödinger equation on the bond $[E + d_x^2 - V_{(\alpha\beta)}(x)]f(x) = 0$ is not anymore the functions $f_{\alpha\beta}(x)$ and $f_{\beta\alpha}(x)$ introduced above, but the couple of stationary scattering states $\phi_{\alpha\beta}(x)$ and $\phi_{\beta\alpha}(x)$ associated to the potential $V_{(\alpha\beta)}(x)$ on the bond $(\alpha\beta)$. If we imagine that the potential $V_{(\alpha\beta)}(x)$ is embedded in $\mathbb{R}$, then the function $\phi_{\alpha\beta}(x)$ is the scattering state incoming on the potential from the vertex α and is matched out of the bond to : $\phi_{\alpha\beta}(x) = e^{ikx} + r_{\alpha\beta} e^{-ikx}$ for $x < 0$ and $\phi_{\alpha\beta}(x) = t_{\alpha\beta} e^{ik(x-l_{\alpha\beta})}$ for $x > l_{\alpha\beta}$ [10].

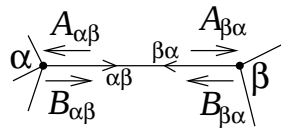


Figure 2: The internal amplitudes associated to the arcs $\alpha\beta$ and $\beta\alpha$.

Then the component of the wave function $\varphi(x)$ on the bond $(\alpha\beta)$ reads :

$$\varphi_{(\alpha\beta)}(x_{\alpha\beta}) = B_{\alpha\beta} \phi_{\alpha\beta}(x_{\alpha\beta}) + B_{\beta\alpha} \phi_{\beta\alpha}(x_{\alpha\beta}). \quad (9)$$

3 Charge of the graph

This section is devoted to the study of the charge distribution in the graph. Our discussion will focus on the average and correlation of the total charge of the graph. The average charge and the zero frequency charge noise can be related to the graph's scattering matrix. These relations provide an extension of the Feynman-Hellman theorem for open systems in an out of equilibrium situation. Then, we present a detailed study of the charge noise at finite frequency, emphasizing the effect of the non equilibrium regime. For simplicity, we shall work at vanishing temperature.

It is convenient to use the language of “second-quantization” and introduce the field operator :

$$\hat{\psi}(x, t) = \sum_{\alpha=1}^L \int_0^\infty dE \tilde{\psi}_E^{(\alpha)}(x) \hat{a}_\alpha(E) e^{-iEt}, \quad (10)$$

where $\hat{a}_\alpha(E)$ is the annihilation operator associated to the stationary scattering state $\tilde{\psi}_E^{(\alpha)}(x)$ corresponding to a plane wave of energy E injected from the lead α . Note that $\hat{\psi}(x, 0)|\tilde{\psi}_E^{(\alpha)}\rangle = \tilde{\psi}_E^{(\alpha)}(x)|\text{vacuum}\rangle$.

Studying the charge distribution for graphs with localized states [34, 11, 13] would require taking into account the contribution of the discrete spectrum in the field operator : $\sum_n \sum_{j=1}^{g_n} \varphi_{n,j}(x) \hat{a}_{n,j} e^{-iE_n t}$ (the function $\varphi_{n,j}(x)$ is an eigenstate of energy E_n localized in the graph and thus normalized to unity in the graph, and j denotes a degeneracy label). However, such a situation is not generic but arises from symmetries of the graph. For this reason, we shall not discuss it here.

In a non equilibrium situation, the quantum statistical average gives : $\langle \hat{a}_\alpha^\dagger(E) \hat{a}_\beta(E') \rangle = \delta_{\alpha\beta} \delta(E - E') f_\alpha(E)$ where $f_\alpha(E)$ is the Fermi-Dirac distribution function giving the occupation of the scattering states coming from the lead α .

Charge operator. The charge operator is :

$$\hat{Q}(t) = \int_{\text{Graph}} dx \hat{\psi}^\dagger(x, t) \hat{\psi}(x, t). \quad (11)$$

We introduce its matrix elements on the shell of energy E :

$$\rho^{(\alpha, \beta)}(E) = \langle \tilde{\psi}_E^{(\alpha)} | \hat{Q}(t) | \tilde{\psi}_E^{(\beta)} \rangle. \quad (12)$$

Since the spectrum is continuous, these matrix elements have the dimension of a density of states (DoS). They can be related to the scattering matrix :

$$\rho^{(\alpha, \beta)}(E) = -\frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{dU} \right)_{\alpha\beta}, \quad (13)$$

where U is a constant potential added inside the graph only (the variable conjugate to the charge of the graph). Instead of differentiating with respect to some additional background potential U , it is also possible to relate it to the derivative with respect to the energy :

$$\rho^{(\alpha, \beta)}(E) = \int_{\text{Graph}} dx \tilde{\psi}_E^{(\alpha)}(x)^* \tilde{\psi}_E^{(\beta)}(x) = \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{dE} + \frac{1}{4E} (\Sigma - \Sigma^\dagger) \right)_{\alpha\beta}. \quad (14)$$

Note that $\sum_\alpha \rho^{(\alpha, \alpha)}(E)$ is the DoS of the graph, *i.e.* the local DoS integrated inside the graph. These relations are proven in appendix C.

Average charge. The average charge :

$$\langle \hat{Q}(t) \rangle = \sum_\alpha \int_0^\infty dE f_\alpha(E) \int_{\text{Graph}} dx |\tilde{\psi}_E^{(\alpha)}(x)|^2 = \sum_\alpha \int_0^\infty dE f_\alpha(E) \rho^{(\alpha, \alpha)}(E) \quad (15)$$

involves the injectivities $\rho(x, \alpha; E) = |\tilde{\psi}_E^{(\alpha)}(x)|^2$, which are the contributions to the local density of states (LDoS) coming from the scattering state $\tilde{\psi}_E^{(\alpha)}(x)$. The contribution $\rho^{(\alpha, \alpha)}(E)$ of the scattering state $\tilde{\psi}_E^{(\alpha)}$ to the DoS of the graph is weighted by the occupation Fermi factor in the lead α . This illustrates the necessity of the concept of injectivities, emissivities, etc, in the context of out of equilibrium systems [3, 35] (see also [13] for a discussion in the context of graphs).

Charge correlation function. The charge correlation function is defined as :

$$S_{QQ}(\omega) = \int_{-\infty}^{+\infty} dt(t-t') \left(\langle \hat{Q}(t) \hat{Q}(t') \rangle - \langle \hat{Q}(t) \rangle \langle \hat{Q}(t') \rangle \right) e^{i\omega(t-t')}. \quad (16)$$

In appendix A, the relation between this unsymmetrized correlator and the other one ($Q(t)$ and $Q(t')$ in reverse order) is clarified. Definition (16) matches with the one used reference [23] which contains a detailed discussion of the relation between the unsymmetrized correlator and transition rates in a two level system linearly coupled to the charge operator.

Using the relation $\langle \hat{a}_\alpha^\dagger \hat{a}_\beta \hat{a}_\mu^\dagger \hat{a}_\nu \rangle - \langle \hat{a}_\alpha^\dagger \hat{a}_\beta \rangle \langle \hat{a}_\mu^\dagger \hat{a}_\nu \rangle = \delta_{\alpha\nu} \delta_{\beta\mu} f_\alpha (1 - f_\beta)$ we obtain :

$$S_{QQ}(\omega) = 2\pi \sum_{\alpha, \beta} \int_0^\infty dE f_\alpha(E) [1 - f_\beta(E + \omega)] \left| \int_{\text{Graph}} dx \tilde{\psi}_E^{(\alpha)}(x)^* \tilde{\psi}_{E+\omega}^{(\beta)}(x) \right|^2. \quad (17)$$

Only the zero frequency correlations involve the $\rho^{(\alpha, \beta)}(E)$:

$$S_{QQ}(\omega = 0) = 2\pi \sum_{\alpha, \beta} \int_0^\infty dE f_\alpha(E) [1 - f_\beta(E)] \rho^{(\alpha, \beta)}(E) \rho^{(\beta, \alpha)}(E). \quad (18)$$

Using equation (14) the zero frequency noise of the total charge is related to the scattering matrix of the graph.

Charge fluctuations. The charge fluctuations at a given time involve the integral of the full spectrum :

$$q_2 = \langle \hat{Q}(t)^2 \rangle - \langle \hat{Q}(t) \rangle^2 = \frac{1}{2\pi} \int d\omega S_{QQ}(\omega). \quad (19)$$

In terms of the stationary scattering states, we get :

$$q_2 = \sum_{\alpha, \beta} \int_0^\infty dE dE' f_\alpha(E) [1 - f_\beta(E')] \left| \int_{\text{Graph}} dx \tilde{\psi}_E^{(\alpha)}(x)^* \tilde{\psi}_{E'}^{(\beta)}(x) \right|^2. \quad (20)$$

Weakly connected graphs

To go further let us focus on the case of graphs weakly coupled to the leads ($w_\alpha \rightarrow 0$). Note that we do not consider charging effect in the following (Coulomb blockade) which is important if the capacitance describing the Coulomb interaction between the leads and the graph is small (see [36] for a review article). A description of such effects would require a different approach. However, in the neighbourhood of the Coulomb peak, a description within the scattering approach can be sufficient to describe transport, like it has been done very recently in [37] to analyze Fano profile measurements in a ring with a dot embedded in one of its arm.

If $w_\alpha \rightarrow 0$ the decomposition of the scattering states over the resonances (levels of the isolated graph), derived in appendix B, can be used

$$\tilde{\psi}_E^{(\alpha)}(x) \simeq \sum_n \frac{1}{\sqrt{\pi}} \frac{iE_n^{1/4} w_\alpha \varphi_n^*(\alpha)}{E - E_n + i\Gamma_n} \varphi_n(x). \quad (21)$$

Here $\varphi_n(x)$ denotes the wave function of the eigenstate of energy E_n of the isolated graph, normalized to unity in the graph. From this expression we get :

$$\rho^{(\alpha,\beta)}(E) \simeq \sum_n \frac{1}{\pi} \frac{\sqrt{\Gamma_{n,\alpha}\Gamma_{n,\beta}} e^{i\chi_{\alpha\beta}}}{(E - E_n)^2 + \Gamma_n^2}, \quad (22)$$

where $\Gamma_{n,\alpha} = \sqrt{E_n} w_\alpha^2 |\varphi_n(\alpha)|^2$ is the contribution of the contact α to the resonance width $\Gamma_n = \sum_\alpha \Gamma_{n,\alpha}$. The phase is given by $e^{i\chi_{\alpha\beta}} = \frac{\varphi_n(\alpha)^* \varphi_n(\beta)}{|\varphi_n(\alpha)\varphi_n(\beta)|}$.

Average charge

Equation (15) gives :

$$\langle \hat{Q}(t) \rangle \simeq \sum_\alpha \int_0^\infty dE f_\alpha(E) \sum_n \frac{\Gamma_{n,\alpha}/\pi}{(E - E_n)^2 + \Gamma_n^2} = \sum_n \sum_\alpha \frac{\Gamma_{n,\alpha}}{\Gamma_n} \left(\frac{1}{\pi} \arctan \frac{V_\alpha - E_n}{\Gamma_n} + \frac{1}{2} \right) \quad (23)$$

where the sum over n runs over the energies of the resonances (energies of the isolated graph). V_α is the potential at contact α . This equation was derived in [38] by tracing out the lead's degrees of freedom. Since the average charge is the sum of contributions of the various levels, we can consider only one level E_n . If the level is below the potentials, $E_n < V_R < V_L$, the occupation of the level is 1. On the other hand, if the level E_n is between the potentials, $V_R < E_n < V_L$, and far enough from them (on the scale Γ_n), it gives a contribution $\Gamma_{n,L}/\Gamma_n$ to the average charge, which simply expresses that only the left scattering state is contributing to the occupation of the resonant level.

Charge noise at finite frequency

Let us now discuss the finite frequency structure of the charge noise for weakly connected graphs. Equation (17) requires evaluating

$$\left| \int_{\text{Graph}} dx \tilde{\psi}_E^{(\alpha)}(x)^* \tilde{\psi}_{E+\omega}^{(\beta)}(x) \right|^2 \simeq \left| \sum_n \frac{1}{\pi} \frac{\sqrt{E_n} w_\alpha w_\beta \varphi_n(\alpha) \varphi_n^*(\beta)}{(E - E_n - i\Gamma_n)(E + \omega - E_n + i\Gamma_n)} \right|^2. \quad (24)$$

Let us keep only the diagonal elements in the double sum. This diagonal approximation is valid in the limit of narrow resonances ($\Gamma_n \ll |E_{n+1} - E_n|$) since the energies E and $E + \omega$ are then compelled to be both in the neighbourhood of the level E_n . Then the correlation appears as a sum of contributions of the different energy levels :

$$S_{QQ}(\omega) \simeq \sum_n S_{QQ}^{(n)}(\omega). \quad (25)$$

The contribution of the level E_n reads :

$$S_{QQ}^{(n)}(\omega) = 2\pi \sum_{\alpha,\beta} \int dE f_\alpha(E) [1 - f_\beta(E + \omega)] \frac{\Gamma_{n,\alpha}/\pi}{(E - E_n)^2 + \Gamma_n^2} \frac{\Gamma_{n,\beta}/\pi}{(E + \omega - E_n)^2 + \Gamma_n^2}. \quad (26)$$

Performing the integrals leads to

$$S_{QQ}^{(n)}(\omega) = \frac{1}{2\pi} \frac{1}{1 + \omega^2/4\Gamma_n^2} \sum_{\alpha,\beta} \frac{\Gamma_{n,\alpha}\Gamma_{n,\beta}}{\Gamma_n^3} \theta(\omega + V_\alpha - V_\beta) A(V_\alpha, V_\beta; \omega) \quad (27)$$

where $\theta(\omega)$ is the Heaviside function and

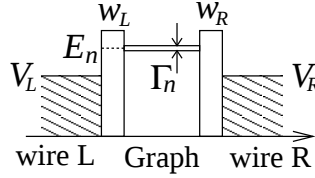
$$\begin{aligned}
A(V_\alpha, V_\beta; \omega) = & \arctan\left(\frac{V_\alpha - E_n}{\Gamma_n}\right) - \arctan\left(\frac{V_\beta - E_n}{\Gamma_n}\right) \\
& + \arctan\left(\frac{V_\alpha + \omega - E_n}{\Gamma_n}\right) - \arctan\left(\frac{V_\beta + \omega - E_n}{\Gamma_n}\right) \\
& + \frac{\Gamma_n}{\omega} \ln \frac{[(V_\alpha + \omega - E_n)^2 + \Gamma_n^2][(V_\beta - \omega - E_n)^2 + \Gamma_n^2]}{[(V_\alpha - E_n)^2 + \Gamma_n^2][(V_\beta - E_n)^2 + \Gamma_n^2]}.
\end{aligned} \tag{28}$$

For the particular case of a two terminal geometry the noise reads

$$\begin{aligned}
S_{QQ}^{(n)}(\omega) = & \frac{1}{2\pi\Gamma_n^3} \frac{1}{1 + \omega^2/4\Gamma_n^2} [\Gamma_{n,L}^2 \theta(\omega) A(V_L, V_L; \omega) + \Gamma_{n,R}^2 \theta(\omega) A(V_R, V_R; \omega) \\
& + \Gamma_{n,L}\Gamma_{n,R} \theta(\omega + V) A(V_L, V_R; \omega) + \Gamma_{n,R}\Gamma_{n,L} \theta(\omega - V) A(V_R, V_L; \omega)] ,
\end{aligned} \tag{29}$$

where $V = V_L - V_R > 0$ is the voltage drop.

• **Equilibrium case :** $V_L = V_R = 0$.



$$\begin{aligned}
S_{QQ}^{(n)}(\omega) = & \frac{1}{2\pi\Gamma_n} \frac{\theta(\omega)}{1 + \omega^2/4\Gamma_n^2} \left[\arctan\left(\frac{\omega - E_n}{\Gamma_n}\right) + \arctan\left(\frac{\omega + E_n}{\Gamma_n}\right) \right. \\
& \left. + \frac{\Gamma_n}{\omega} \ln \frac{[(\omega - E_n)^2 + \Gamma_n^2][(\omega + E_n)^2 + \Gamma_n^2]}{[E_n^2 + \Gamma_n^2]^2} \right].
\end{aligned} \tag{30}$$

We consider the case of narrow resonances where Γ_n is the smallest energy scale, then if the frequency is smaller than $|E_n|$, the contribution is zero, but if ω is sufficiently large to excite an energy level $\omega \gtrsim |E_n|$, we get a contribution :

$$S_{QQ}^{(n)}(\omega) \simeq \frac{1}{2\Gamma_n} \frac{\theta(\omega)}{1 + \omega^2/4\Gamma_n^2} \times \begin{cases} 0 & \text{if } \omega \lesssim |E_n| \\ 1 & \text{if } \omega \gtrsim |E_n|. \end{cases} \tag{31}$$

Obviously, the transition between the two results is not sharp but occurs on a scale Γ_n . Practically all the noise power is concentrated at low frequencies as shown on figure 3.

Note that this contribution is independent of the fact that the level is occupied ($E_n < 0$) or empty ($E_n > 0$) since it is an even function of E_n . At $V_L = V_R$, the low frequency charge noise can be understood using a classical stochastic model describing the relaxation process of an electron (or a hole) with lifetime $1/2\Gamma_n$.

• **Non equilibrium regime :** $V_L \neq V_R$.

Zero frequency limit. Then only the term with $A(V_L, V_R; 0)$ contributes :

$$\begin{aligned}
S_{QQ}^{(n)}(\omega = 0) \simeq & \frac{1}{\pi} \frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n^3} \left\{ \arctan\left(\frac{V_L - E_n}{\Gamma_n}\right) + \arctan\left(\frac{E_n - V_R}{\Gamma_n}\right) \right. \\
& \left. + \frac{\Gamma_n(V_L - E_n)}{(V_L - E_n)^2 + \Gamma_n^2} + \frac{\Gamma_n(E_n - V_R)}{(E_n - V_R)^2 + \Gamma_n^2} \right\}.
\end{aligned} \tag{32}$$

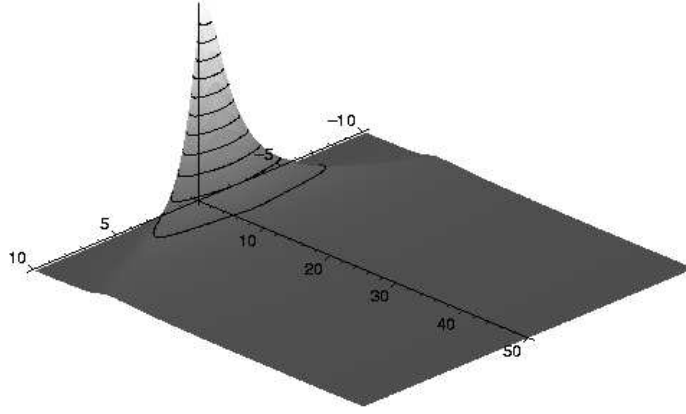


Figure 3: Equilibrium noise in terms of $-10 < \omega/\Gamma_n < 10$ and of the energy of the level $(-E_n)/\Gamma_n$ (this is equivalent to vary the energy or the chemical potential).

Each energy level brings a contribution only if it is between the potentials ($V_R < E_n < V_L$) and far enough from them (on the scale Γ_n). In this case, the zero frequency charge noise is given by :

$$S_{QQ}^{(n)}(\omega = 0) \simeq \frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n^3}. \quad (33)$$

We recognize the factor $\Gamma_{n,R}\Gamma_{n,L}$ characteristic of partition noise : if one of the couplings vanishes ($\Gamma_{n,R} = 0$ or $\Gamma_{n,L} = 0$) the occupation of the level is either 0 or 1 and does not fluctuate. These fluctuations are a signature of the non equilibrium regime of the mesoscopic circuit. The charge fluctuations at fixed time can be obtained by integrating the noise spectrum (19). Using the approximate expression (21) in (20) we obtain

$$q_2 \simeq \sum_n \sum_{\alpha,\beta} \frac{\Gamma_{n,\alpha}\Gamma_{n,\beta}}{\Gamma_n^2} \left(\frac{1}{\pi} \arctan \frac{V_\alpha - E_n}{\Gamma_n} + \frac{1}{2} \right) \left(\frac{1}{\pi} \arctan \frac{E_n - V_\beta}{\Gamma_n} + \frac{1}{2} \right) \quad (34)$$

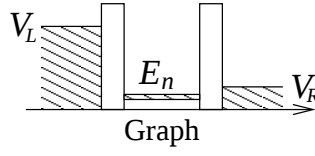
In the two leads case, only the levels between the two potentials bring the contribution :

$$q_2 \simeq \frac{\Gamma_{n,L}\Gamma_{n,R}}{\Gamma_n^2}. \quad (35)$$

Note that this result cannot be simply inferred from the current shot noise. Near a resonance, the transmission probability through the graph is $T(E) \simeq \frac{4\Gamma_{n,L}\Gamma_{n,R}}{(E-E_n)^2 + \Gamma_n^2}$. The average current in the lead is given by the Landauer formula $\langle I \rangle = \frac{1}{2\pi} \int_{V_R}^{V_L} dE T(E)$ whereas the current and the shot noise by $S_{II}(\omega = 0) = \frac{1}{2\pi} \int_{V_R}^{V_L} dE T(E)(1 - T(E))$ [1, 2, 39]. If only one level E_n lies between the two potentials, we obtain in this non linear regime [40] : $\langle I \rangle \simeq 2 \frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n}$ and $S_{II}(\omega = 0) \simeq 2 \frac{\Gamma_{n,R}\Gamma_{n,L}}{\Gamma_n^3} (\Gamma_{n,R}^2 + \Gamma_{n,L}^2)$.

Finite frequency noise. Let us choose the origin of the energies in such a way that : $V_R = 0$, $V_L = V > 0$. Four energy scales must be considered : E_n , Γ_n , V and ω . Several regimes can be observed according to the frequency. To help the discussion we neglect the smallest scale, supposed to be Γ_n , as we did above.

(i) Let us first discuss the case of a fully occupied level : $E_n < V_R = 0$.



At small frequencies, correlations are roughly zero. When ω reaches $V_R - E_n$, contributions from the second and third terms appear, while all terms contribute for ω larger than $V_L - E_n$. To summarize these three regimes :

$$S_{QQ}^{(n)}(\omega) \simeq \frac{1}{2\Gamma_n} \frac{1}{1 + \omega^2/4\Gamma_n^2} \times \begin{cases} 0 & \text{if } \omega \lesssim V_R - E_n \\ \frac{\Gamma_{n,R}}{\Gamma_n} & \text{if } V_R - E_n \lesssim \omega \lesssim V_L - E_n \\ 1 & \text{if } V_L - E_n \lesssim \omega, \end{cases} \quad (36)$$

where we have factorized the equilibrium result.

In the second regime $V_R - E_n \lesssim \omega \lesssim V_L - E_n$, the energy ω is sufficient to excite the state originating from the right reservoir but not from the left reservoir. This is the origin of the ratio $\Gamma_{n,R}/\Gamma_n$. In the third regime, both reservoirs contribute to the noise. At fixed non zero bias voltage, this leads to a double peak structure in terms of the ω which corresponds to the threshold for creating electron-holes pairs involving the left and right leads (see figure 4). At small V these two peaks tend to merge into a single more pronounced one. At large V the second peak occurs at a larger frequency and is less pronounced because of the Lorentzian factor.

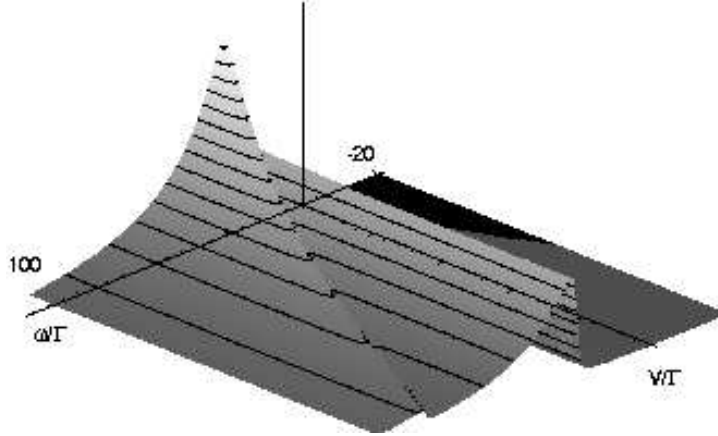
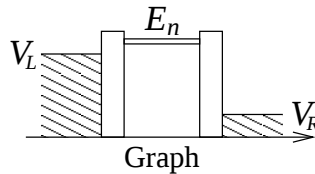


Figure 4: Non equilibrium noise in terms of $-20 < \omega/\Gamma_n < 100$ and of the voltage drop V/Γ_n for a fully populated level ($V_R = E_n + 50\Gamma_n$).

(ii) Let us now discuss the case of an empty level : $E_n > V_L$.

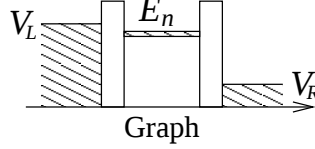


The physical picture can be obtained using a hole picture. Three different regimes can also be

distinguished :

$$S_{QQ}^{(n)}(\omega) \simeq \frac{1}{2\Gamma_n} \frac{1}{1 + \omega^2/4\Gamma_n^2} \times \begin{cases} 0 & \text{if } \omega \lesssim E_n - V_L \\ \frac{\Gamma_{n,L}}{\Gamma_n} & \text{if } E_n - V_L \lesssim \omega \lesssim E_n - V_R \\ 1 & \text{if } E_n - V_R \lesssim \omega \end{cases} \quad (37)$$

(iii) Finally we consider the case of a level between the two potentials $V_R < E_n < V_L$.



Considering the case where the level is closer to V_L than to V_R , we obtain

$$S_{QQ}^{(n)}(\omega) \simeq \frac{1}{2\Gamma_n} \frac{1}{1 + \omega^2/4\Gamma_n^2} \times \begin{cases} 0 & \text{if } \omega \lesssim -E_n + V_R \\ \frac{\Gamma_{n,L}\Gamma_{n,R}}{\Gamma_n^2} & \text{if } -E_n + V_R \lesssim \omega \lesssim -V_L + E_n \\ \frac{2\Gamma_{n,L}\Gamma_{n,R}}{\Gamma_n^2} & \text{if } -V_L + E_n \lesssim \omega \lesssim V_L - E_n \\ \frac{2\Gamma_{n,L}\Gamma_{n,R} + \Gamma_{n,L}^2}{\Gamma_n^2} & \text{if } V_L - E_n \lesssim \omega \lesssim E_n - V_R \\ 1 & \text{if } E_n - V_R \lesssim \omega \end{cases} \quad (38)$$

The fluctuation spectrum is symmetric in the interval centered around $\omega = 0$ with width of order V . The main contribution to the noise appears at low frequency as can be seen from figure 5. The multiple plot (figure 6) shows how the low frequency peak develops when V_L crosses the energy level.

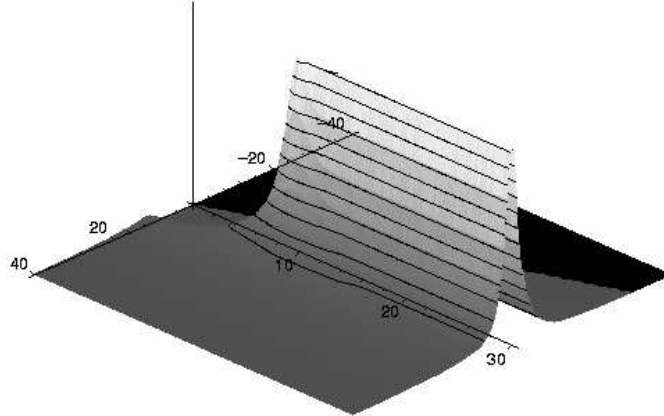


Figure 5: Non equilibrium noise in terms of $-40 < \omega/\Gamma_n < 40$ and of V/Γ_n . The right lead chemical potential is fixed to $-10\Gamma_n$. Case (iii) corresponds to $V > 10\Gamma_n$ and exhibits an important low frequency noise whereas $V < 10\Gamma_n$ corresponds to case (ii).

Interestingly, correlations are proportional to the partition factor $\Gamma_{n,R}\Gamma_{n,L}$ only for small frequencies $|\omega| \ll V$ (or large time scales $t \gg 1/V$). For large frequencies $|\omega| \gg V$, the partition factor does not appear. The high frequency part of the charge fluctuation spectrum is insensitive to the fact that the system is out of equilibrium. In this limit, the equilibrium result (31) is recovered.

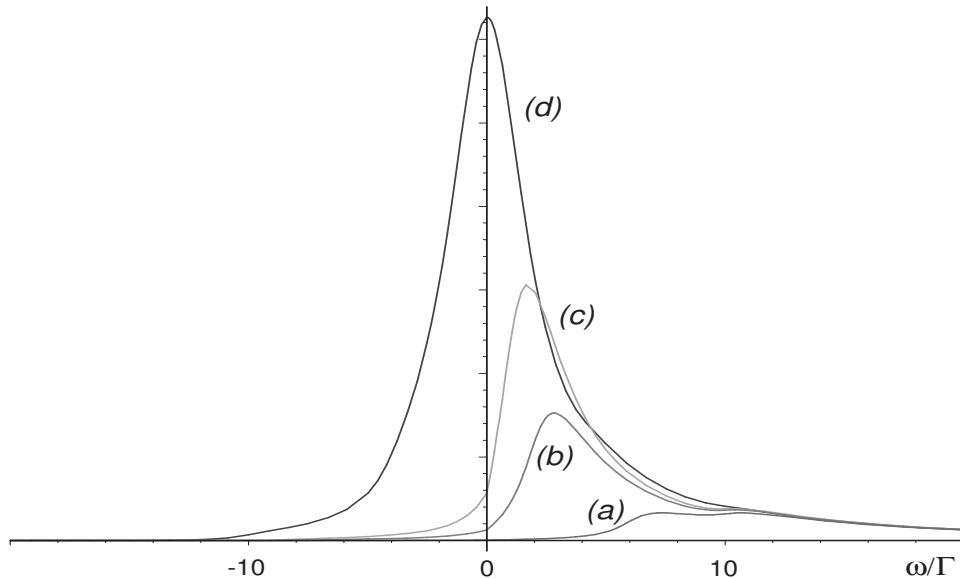


Figure 6: Multiple plots of non equilibrium charge noise in terms of $-20 < \omega/\Gamma_n < 20$ for different values of V/Γ_n . The right lead chemical potential is fixed as on figure 5. (a) $V/\Gamma_n = 4$, (b) $V/\Gamma_n = 8$, (c) $V/\Gamma_n = 9$ and (d) $V/\Gamma_n = 14$.

4 Currents inside the graph

A possible way to probe a mesoscopic device is to attach some leads to it, through which some currents are injected. Some information can be extracted from transport or noise properties : average values and correlations of currents in the *external* leads. All these properties can be related to the scattering matrix (see [40] for a review). If one is now interested in local information on the system, like the measurement of a persistent current, a natural way would be to introduce some local probe. However, as we have recalled in the introduction, local information can also be extracted from scattering properties. Here, we investigate the currents in the *internal* wires, and show the relation to the scattering properties. The starting point, exposed in the introduction, is the relation between the current in a wire and the derivative of the scattering matrix with respect to its conjugate variable, the flux in the wire. This idea comes from [17] and has been elaborated further in [29] to include derivation of correlations of the current density. Here, we focus on the case of graphs in the context of which we will generalize these previous results to the non equilibrium situation.

4.1 Current in a closed graph

First we derive an expression for the current density in a closed graph. It is convenient to introduce the spectral determinant of the Schrödinger operator

$$S(\gamma) = \det(-\Delta + V(x) + \gamma) = \prod_n (E_n + \gamma) \quad (39)$$

where γ is a spectral parameter. The set of E_n 's is the spectrum of the Schrödinger operator on the graph. It was shown in [41, 42, 43, 44] that the spectral determinant, which is the determinant of an unbounded operator, can be related to the determinant of a finite size matrix. In the vertex approach, the formula (100) involves a $V \times V$ matrix, whereas in the arc language the spectral determinant involves a $2B \times 2B$ matrix : $S(-E) \propto \det(1 - QR)$ [42, 44]. Note

that for a closed graph, the vertex scattering matrix Q has the same dimension as the bond scattering matrix. We introduce the current density $j(E)$ associated to the states in the interval $[E, E + dE]$. The current density in the arc a is :

$$j_a(E) = - \sum_n \delta(E - E_n) \frac{\partial E_n}{\partial \theta_a} = \frac{1}{\pi} \text{Im} \frac{\partial}{\partial \theta_a} \ln S(-E + i0^+) , \quad (40)$$

where θ_a is the magnetic flux along this arc.

Example : Consider a closed ring of perimeter l threaded by a flux θ . Its spectral determinant is $S(\gamma) = \text{ch}(\sqrt{\gamma}l) - \cos(\theta)$ [42]. We write : $\gamma = -k^2 + i0^+$, then $\text{ch}(\sqrt{\gamma}l) = \cos(kl) + i0^+ \sin(kl)$ and we get for the current density in the ring :

$$j(E) = - \sin \theta \text{sign}(\sin kl) \delta(\cos kl - \cos \theta) = \sum_n \delta(E - E_n) I_n , \quad (41)$$

with $I_n = -\partial_\theta E_n$ where $E_n = (2n\pi - \theta)^2/l^2$.

4.2 Current in open graphs

Now we consider a graph connected to infinite leads.

The current operator is

$$\hat{J}(x, t) = \frac{1}{i} \left[\hat{\psi}^\dagger(x, t) D_x \hat{\psi}(x, t) - D_x^* \hat{\psi}^\dagger(x, t) \hat{\psi}(x, t) \right] \quad (42)$$

where $D_x = d_x - iA(x)$ is the covariant derivative.

We introduce the current matrix elements

$$j_{\mu\nu}^{(\alpha, \beta)}(E) = \langle \tilde{\psi}_E^{(\alpha)} | \hat{J}(x, t) | \tilde{\psi}_E^{(\beta)} \rangle \quad \text{for } x \in \mu\nu \quad (43)$$

which can be shown to be independent of the coordinate x along the arc (only if the two states have the same energy). This matrix element can then be computed at the vertex μ ($x = 0$) :

$$j_{\mu\nu}^{(\alpha, \beta)}(E) = \frac{1}{i} \left(\tilde{\psi}_\mu^{(\alpha)*} D_x \tilde{\psi}_{(\mu\nu)}^{(\beta)}(\mu) - D_x^* \tilde{\psi}_{(\mu\nu)}^{(\alpha)*}(\mu) \tilde{\psi}_\mu^{(\beta)} \right) . \quad (44)$$

The quantum and statistical average of the current operator in the arc $\mu\nu$ gives :

$$J_{\mu\nu} = \langle \hat{J}(x \in \mu\nu, t) \rangle = \sum_\alpha \int dE f_\alpha(E) j_{\mu\nu}^{(\alpha, \alpha)}(E) . \quad (45)$$

The correlations (unsymmetrized in time or frequency) between the currents in the arcs $\mu\nu$ and $\mu'\nu'$, defined as

$$S_{J_{\mu\nu} J_{\mu'\nu'}}(\omega) = \int_{-\infty}^{+\infty} d(t - t') \left(\langle \hat{J}(x, t) \hat{J}(x', t') \rangle - \langle \hat{J}(x, t) \rangle \langle \hat{J}(x', t') \rangle \right) e^{i\omega(t-t')} , \quad (46)$$

for $x \in \mu\nu$ and $x' \in \mu'\nu'$. They can be rewritten at zero frequency as :

$$S_{J_{\mu\nu} J_{\mu'\nu'}}(\omega = 0) = 2\pi \sum_{\alpha, \beta} \int dE f_\alpha(E) [1 - f_\beta(E)] j_{\mu\nu}^{(\alpha, \beta)}(E) j_{\mu'\nu'}^{(\beta, \alpha)}(E) . \quad (47)$$

Vertex formulation

Now we look for a relation between the current density and the scattering matrix. We start from the expression of the scattering state in the arc $\mu\nu$:

$$\psi_{(\mu\nu)}(x) = e^{i\theta_{\mu\nu}x/l_{\mu\nu}} \left(\psi_\mu f_{\mu\nu}(x) + \psi_\nu e^{-i\theta_{\mu\nu}} f_{\nu\mu}(x) \right). \quad (48)$$

Then :

$$j_{\mu\nu}^{(\alpha,\beta)} = \frac{1}{i} \left(-\tilde{\psi}_\mu^{(\alpha)*} \frac{df_{\mu\nu}}{dx_{\mu\nu}}(\nu) e^{-i\theta_{\mu\nu}} \tilde{\psi}_\nu^{(\beta)} + \tilde{\psi}_\nu^{(\alpha)*} \frac{df_{\nu\mu}}{dx_{\nu\mu}}(\mu) e^{i\theta_{\mu\nu}} \tilde{\psi}_\mu^{(\beta)} \right) \quad (49)$$

where we have used the fact that the Wronskian of $f_{\mu\nu}(x)$ and $f_{\nu\mu}(x)$ reads : $\frac{df_{\nu\mu}}{dx_{\mu\nu}}(\mu) = -\frac{df_{\mu\nu}}{dx_{\mu\nu}}(\nu)$. From the definition of the matrix M , we see that :

$$j_{\mu\nu}^{(\alpha,\beta)} = -\frac{k}{i} \left(\tilde{\psi}_\mu^{(\alpha)*} \frac{dM_{\mu\nu}}{d\theta_{\mu\nu}} \tilde{\psi}_\nu^{(\beta)} + \tilde{\psi}_\nu^{(\alpha)*} \frac{dM_{\nu\mu}}{d\theta_{\mu\nu}} \tilde{\psi}_\mu^{(\beta)} \right) \quad (50)$$

Only the two elements $M_{\mu\nu}$ and $M_{\nu\mu}$ depend on the flux $\theta_{\mu\nu}$, then :

$$j_{\mu\nu}^{(\alpha,\beta)} = -\frac{k}{i} \left(\tilde{\Psi}^\dagger \frac{dM}{d\theta_{\mu\nu}} \tilde{\Psi} \right)_{\alpha\beta}, \quad (51)$$

where $\tilde{\Psi}$ is the $V \times L$ -matrix that gathers the values of the L stationary states at the V vertices : $\tilde{\Psi}_{\mu\alpha} \equiv \tilde{\psi}_\mu^{(\alpha)}$. This matrix is [10, 13] :

$$\tilde{\Psi} = \frac{1}{\sqrt{\pi k}} \frac{1}{M + W^T W} W^T. \quad (52)$$

We can rewrite the current density in terms of matrices M and W :

$$j_{\mu\nu}^{(\alpha,\beta)} = -\frac{1}{i\pi} \left(W \frac{1}{-M + W^T W} \frac{dM}{d\theta_{\mu\nu}} \frac{1}{M + W^T W} W^T \right)_{\alpha\beta}. \quad (53)$$

Our aim is now to find the relation of this expression with the scattering matrix. We use the relation $\frac{d}{d\eta} A(\eta)^{-1} = -A(\eta)^{-1} \frac{dA(\eta)}{d\eta} A(\eta)^{-1}$ that gives the derivative of the inverse of a square matrix $A(\eta)$ depending on a parameter η . In the expression (3) only M depends on the fluxes, it follows that :

$$\frac{d\Sigma}{d\theta_{\mu\nu}} = -2W \frac{1}{M + W^T W} \frac{dM}{d\theta_{\mu\nu}} \frac{1}{M + W^T W} W^T. \quad (54)$$

If we multiply this expression by $\Sigma^\dagger$ from the left, it replaces the M in the left fraction by $-M$. We conclude that the off-diagonal elements of the current density reads :

$$j_{\mu\nu}^{(\alpha,\beta)}(E) = \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{d\theta_{\mu\nu}} \right)_{\alpha\beta}. \quad (55)$$

Note that this result is reminiscent to the one obtained by Taniguchi in [29] who derived some relation between the scattering matrix and the “current density”, *i.e.* the diagonal elements ($\alpha = \beta$) of (55).

Arc formulation

Let us now reformulate the previous demonstration in the arc language which allows to consider the most general case.

As explained in the introduction, the wave function on the bond $(\mu\nu)$ can be expressed as :

$$\psi_{(\mu\nu)}(x_{\mu\nu}) = B_{\mu\nu} \phi_{\mu\nu}(x_{\mu\nu}) + B_{\nu\mu} \phi_{\nu\mu}(x_{\mu\nu}) \quad (56)$$

where $\phi_{\mu\nu}(x_{\mu\nu})$ and $\phi_{\nu\mu}(x_{\mu\nu})$ are the left and right stationary scattering states for the bond potential $V_{(\mu\nu)}(x_{\mu\nu})$. Using the expressions of these functions at the extremities of the bond given in the introduction, we get the derivative of the wave function at the vertex μ :

$$D_x \psi_{(\mu\nu)}(\mu) = ik [B_{\mu\nu}(1 - r_{\mu\nu}) - B_{\nu\mu} t_{\nu\mu}] . \quad (57)$$

We call $\tilde{B}_{\mu\nu}^{(\alpha)}$ the internal amplitude corresponding to the stationary scattering state $\tilde{\psi}_E^{(\alpha)}(x)$. These amplitudes are obtained by solving the equations $B = QA$ and $A^{\text{int}} = RB^{\text{int}}$ with external amplitudes A^{ext} describing the injection of a plane wave on the lead arriving at vertex α : its components are $\tilde{A}_i^{(\alpha)\text{ext}} = \frac{1}{\sqrt{4\pi k}} \delta_{i,\text{arc } \alpha}$ where “arc α ” designates the arc related to the lead issuing from α . Then the amplitude

$$\tilde{B}_{\mu\nu}^{(\alpha)} = \frac{1}{\sqrt{4\pi k}} \left[(1 - Q^{\text{int}} R)^{-1} \tilde{Q}^T \right]_{\mu\nu, \text{arc } \alpha} \quad (58)$$

is related to the matrix element between the internal arc $\mu\nu$ and the external arc “arc α ”.

After a little bit of algebra, we get for the current density on the arc $\mu\nu$:

$$j_{\mu\nu}^{(\alpha,\beta)} = 2k \left[\tilde{B}_{\mu\nu}^{(\alpha)*} |t_{\mu\nu}|^2 \tilde{B}_{\mu\nu}^{(\beta)} + \tilde{B}_{\mu\nu}^{(\alpha)*} t_{\mu\nu}^* r_{\nu\mu} \tilde{B}_{\nu\mu}^{(\beta)} - \tilde{B}_{\nu\mu}^{(\alpha)*} t_{\nu\mu}^* r_{\mu\nu} \tilde{B}_{\mu\nu}^{(\beta)} - \tilde{B}_{\nu\mu}^{(\alpha)*} |t_{\nu\mu}|^2 \tilde{B}_{\nu\mu}^{(\beta)} \right] . \quad (59)$$

We have used $t_{\mu\nu}^* r_{\nu\mu} = -r_{\mu\nu}^* t_{\nu\mu}$ coming from the unitarity of R . In the bond scattering matrix R , only the transmissions depend on the magnetic fluxes : $t_{\mu\nu} \propto e^{i\theta_{\mu\nu}}$. It follows that, in the matrix $\frac{dR^\dagger}{d\theta_{\mu\nu}} R$, only the 2×2 block related to the arcs $\mu\nu$ and $\nu\mu$ is different from zero. It is given by :

$$i \begin{pmatrix} -|t_{\mu\nu}|^2 & -t_{\mu\nu}^* r_{\nu\mu} \\ t_{\nu\mu}^* r_{\mu\nu} & |t_{\nu\mu}|^2 \end{pmatrix} \quad (60)$$

Then it is straightforward to see that :

$$j_{\mu\nu}^{(\alpha,\beta)} = -2ik \sum_{i,j} \tilde{B}_i^{(\alpha)*} \left(\frac{dR^\dagger}{d\theta_{\mu\nu}} R \right)_{i,j} \tilde{B}_j^{(\beta)} \quad (61)$$

where the sum over i, j runs over the $2B$ internal arcs. Using the expression (58) for the amplitudes, we obtain :

$$j_{\mu\nu}^{(\alpha,\beta)} = -\frac{1}{2i\pi} \left(\tilde{Q}^* (1 - R^\dagger Q^{\text{int}})^{-1} \frac{dR^\dagger}{d\theta_{\mu\nu}} R (1 - Q^{\text{int}} R)^{-1} \tilde{Q}^T \right)_{\alpha,\beta} \quad (62)$$

$$= -\frac{1}{2i\pi} \left(\Sigma^\dagger \tilde{Q} (R^\dagger - Q^{\text{int}})^{-1} \frac{dR^\dagger}{d\theta_{\mu\nu}} (R^\dagger - Q^{\text{int}})^{-1} \tilde{Q}^T \right)_{\alpha,\beta} \quad (63)$$

$$= \frac{1}{2i\pi} \left(\Sigma^\dagger \tilde{Q} \frac{d}{d\theta_{\mu\nu}} (R^\dagger - Q^{\text{int}})^{-1} \tilde{Q}^T \right)_{\alpha,\beta} = \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{d\theta_{\mu\nu}} \right)_{\alpha,\beta} . \quad (64)$$

We have recovered the formula (55) within the arc language⁴. This demonstrates that equation (55) applies to the most general situation, as expected.

⁴We have used the relation $\Sigma^\dagger \tilde{Q} (R^\dagger - Q^{\text{int}})^{-1} = \tilde{Q}^* (1 - R^\dagger Q^{\text{int}})^{-1}$, coming from the unitarity of the scattering matrices [13].

Average current and current correlations in terms of the scattering matrix

The average current can be written, as could have been guessed from the general discussion of the introduction :

$$J_{\mu\nu} = \sum_{\alpha} \int dE f_{\alpha}(E) \frac{1}{2i\pi} \left(\Sigma^{\dagger} \frac{d\Sigma}{d\theta_{\mu\nu}} \right)_{\alpha\alpha} . \quad (65)$$

The correlations of currents at zero frequency rewrite in terms of scattering matrix :

$$S_{J_{\mu\nu}J_{\mu'\nu'}}(\omega = 0) = -\frac{1}{2\pi} \sum_{\alpha,\beta} \int dE f_{\alpha}[1 - f_{\beta}] \left(\Sigma^{\dagger} \frac{d\Sigma}{d\theta_{\mu\nu}} \right)_{\alpha\beta} \left(\Sigma^{\dagger} \frac{d\Sigma}{d\theta_{\mu'\nu'}} \right)_{\beta\alpha} . \quad (66)$$

If $\mu\nu = \mu'\nu'$ this gives the noise of the persistent current. At equilibrium, all potentials are equal $f_{\alpha}(E) = f(E) \forall \alpha$, and we recover an expression reminiscent of the one given in [29] :

$$S_{J_{\mu\nu}J_{\mu'\nu'}}(\omega = 0) = \frac{1}{2\pi} \int dE f(E)[1 - f(E)] \text{Tr} \left\{ \frac{d\Sigma}{d\theta_{\mu\nu}} \frac{d\Sigma^{\dagger}}{d\theta_{\mu'\nu'}} \right\} . \quad (67)$$

In his work, Taniguchi identifies the contribution $\left(\frac{d\Sigma}{d\theta_{\mu\nu}} \frac{d\Sigma^{\dagger}}{d\theta_{\mu'\nu'}} \right)_{\alpha\alpha}$ of a given scattering state to this trace. However we see that it is not sufficient to go back to the expression (66) describing the non equilibrium situation.

4.3 Gauge invariance

Since many formulae involve the fluxes along the wires, it is important to discuss how a gauge transformation would affect them and to check that all the measurable quantities are indeed gauge invariant. A gauge transformation changes the vector potential according to $A(x) \rightarrow A(x) + \partial_x \chi(x)$, where $\chi(x)$ is a scalar function. The magnetic flux $\theta_{\mu\nu}$ along the arc $\mu\nu$ is then modified according to :

$$\theta_{\mu\nu} \longrightarrow \theta'_{\mu\nu} = \theta_{\mu\nu} + \chi_{\mu} - \chi_{\nu} \quad (68)$$

where $\chi_{\mu} \equiv \chi(\mu)$ is the value taken by the function at the vertex μ . In the vertex approach, we immediately see from its definition that the matrix M is changed as :

$$M_{\mu\nu} \longrightarrow M'_{\mu\nu} = M_{\mu\nu} e^{i\chi_{\mu} - i\chi_{\nu}} . \quad (69)$$

We can write $M' = \mathcal{U} M \mathcal{U}^{\dagger}$ where the diagonal unitary matrix reads : $\mathcal{U}_{\alpha\beta} = \delta_{\alpha\beta} e^{i\chi_{\alpha}}$. Since $W^{\text{T}} W$ is also diagonal it is clear that $(\pm M' + W^{\text{T}} W)^{-1} = \mathcal{U} (\pm M + W^{\text{T}} W)^{-1} \mathcal{U}^{\dagger}$. The scattering matrix changes in the same way :

$$\Sigma_{\alpha\beta} \longrightarrow \Sigma'_{\alpha\beta} = \Sigma_{\alpha\beta} e^{i\chi_{\alpha} - i\chi_{\beta}} . \quad (70)$$

From (53) or (55) we see that the matrix elements of the current operator pick up a phase through a gauge transformation

$$j_{\mu\nu}^{(\alpha,\beta)} \longrightarrow j_{\mu\nu}^{(\alpha,\beta)} e^{i\chi_{\alpha} - i\chi_{\beta}} . \quad (71)$$

Nevertheless, the average current (45) and the correlations (47) are gauge invariant, as they should.

4.4 Weakly connected graphs

As we did for the charge distribution, it is interesting to consider the case of graphs weakly connected to the leads ($w_\alpha \rightarrow 0$) for which interesting results can be derived. The starting point is again the expression (21) of the scattering state near a resonance (when E is close to an eigenenergy of the isolated graph). Using this relation, the current density matrix element can be expressed as

$$j_{\mu\nu}^{(\alpha,\beta)}(E, E') = \langle \tilde{\psi}_E^{(\alpha)} | \hat{J}(x \in \mu\nu, t=0) | \tilde{\psi}_{E'}^{(\beta)} \rangle \quad (72)$$

$$\underset{E, E' \sim E_n}{\simeq} \frac{\sqrt{E_n}}{\pi} \frac{w_\alpha \varphi_n(\alpha)}{E - E_n - i\Gamma_n} \frac{w_\beta \varphi_n^*(\beta)}{E' - E_n + i\Gamma_n} I_{\mu\nu}^n, \quad (73)$$

where $I_{\mu\nu}^n$ is the current in the arc $\mu\nu$ associated to the eigenstate $\varphi_n(x)$ of the isolated graph :

$$I_{\mu\nu}^n = -i\varphi_n^*(x) D_x \varphi_n(x) + \text{c.c.} \quad \text{for } x \in \mu\nu. \quad (74)$$

Note that in principle the current matrix element (72) between scattering states of different energies depends on the coordinate x , however in the weak coupling limit, since the two scattering states are proportional to the same eigenstate $\varphi_n(x)$, the matrix element becomes x independent.

Equation (72) shows that the calculation of the average current is very similar to the calculation of the charge (23) :

$$J_{\mu\nu} \simeq \sum_\alpha \int_0^\infty dE f_\alpha \sum_n \frac{I_{\mu\nu}^n \Gamma_{n,\alpha}/\pi}{(E - E_n)^2 + \Gamma_n^2} = \sum_n I_{\mu\nu}^n \sum_\alpha \frac{\Gamma_{n,\alpha}}{\Gamma_n} \left(\frac{1}{\pi} \arctan \frac{V_\alpha - E_n}{\Gamma_n} + \frac{1}{2} \right). \quad (75)$$

The contribution of the resonant level can be written :

$$J_{\mu\nu}^{(n)} \simeq I_{\mu\nu}^n \langle \hat{Q}(t) \rangle^{(n)} \quad (76)$$

where $\langle \dots \rangle^{(n)}$ designates the contribution of the resonant level n .

Similarly we obtain for the correlations :

$$S_{J_{\mu\nu} J_{\mu'\nu'}}^{(n)}(\omega) \simeq I_{\mu\nu}^n I_{\mu'\nu'}^n S_{QQ}^{(n)}(\omega). \quad (77)$$

For example, for a situation with two contacts with a potential drop V and only one resonant level contributing we get :

$$J_{\mu\nu} \simeq I_{\mu\nu}^n \frac{\Gamma_{n,L}}{\Gamma_n} \quad (78)$$

and

$$S_{J_{\mu\nu} J_{\mu'\nu'}}(0) \simeq I_{\mu\nu}^n I_{\mu'\nu'}^n \frac{\Gamma_{n,L} \Gamma_{n,R}}{\Gamma_n^3} \quad (79)$$

4.5 Example

Let us focus on the simple example of a ring with two leads (see figure 7).

The scattering matrix of the ring reads :

$$\Sigma = -1 + \frac{2}{\tilde{S}} \begin{pmatrix} iw_1^2 \sin kl + w_1^2 w_2^2 s_a s_b & iw_1 w_2 (s_b e^{-i\theta_a} + s_a e^{i\theta_b}) \\ iw_2 w_1 (s_b e^{i\theta_a} + s_a e^{-i\theta_b}) & iw_2^2 \sin kl + w_1^2 w_2^2 s_a s_b \end{pmatrix} \quad (80)$$

where θ_a and θ_b are the fluxes of the two arcs and $\theta = \theta_a + \theta_b$ the total flux threadening the ring. We have denoted $s_{a,b} \equiv \sin kl_{a,b}$.

$$\tilde{S} = s_a s_b \det(M + W^T W) = 2(\cos \theta - \cos kl) + i(w_1^2 + w_2^2) \sin kl + w_1^2 w_2^2 s_a s_b \quad (81)$$

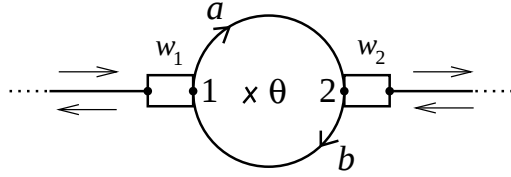


Figure 7: A ring with two arms of lengths l_a and l_b , threaded by a flux θ and coupled with two leads, with coupling parameters $w_{1,2}$. The boxes represent the tunable couplings, with transmission amplitudes $2w_{1,2}/(1 + w_{1,2}^2)$ (see [10]).

is the modified spectral determinant. The matrix involved in the current density in the arc a is :

$$\Sigma^\dagger \frac{d\Sigma}{d\theta_a} = \frac{2 \sin \theta}{\tilde{S}} (1 + \Sigma^\dagger) + \frac{2w_1 w_2 s_b}{\tilde{S}} \begin{pmatrix} -\Sigma_{21}^* e^{i\theta_a} & \Sigma_{11}^* e^{-i\theta_a} \\ -\Sigma_{22}^* e^{i\theta_a} & \Sigma_{12}^* e^{-i\theta_a} \end{pmatrix} \quad (82)$$

from which we get the contribution of the scattering state $\tilde{\psi}^{(1)}(x)$ to the current density in the arc a :

$$j_a^{(1,1)} = \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{d\theta_a} \right)_{11} = \frac{2}{\pi |\tilde{S}|^2} [-w_1^2 \sin \theta \sin kl + w_1^2 w_2^2 (s_b^2 + s_a s_b \cos \theta)] . \quad (83)$$

Let us now study the weak coupling limit $w_{1,2} \rightarrow 0$. Close to a resonance, we obtain :

$$j_a^{(1,1)}(k^2) \underset{k \sim k_n^\pm}{\simeq} \mp \frac{1}{l} \frac{w_1^2}{w_1^2 + w_2^2} \frac{\gamma/\pi}{(k - k_n^\pm)^2 + \gamma^2} \quad (84)$$

where $\gamma = \frac{w_1^2 + w_2^2}{2l}$. Integrating the contribution of the resonance peak, we get :

$$\int_{k_n^\pm - \delta K}^{k_n^\pm + \delta K} dk \, 2k \, j_a^{(1,1)}(k^2) \simeq \frac{w_1^2}{w_1^2 + w_2^2} \frac{4\pi}{l^2} \left(\mp n - \frac{\theta}{2\pi} \right) . \quad (85)$$

In the r.h.s we recognize the persistent current of the level of the isolated ring $-\frac{\partial}{\partial \theta} (k_n^\pm)^2 = -\frac{\partial}{\partial \theta} \left(\frac{2\pi n \pm \theta}{l} \right)^2$, multiplied by the “relative weight” $\frac{w_1^2}{w_1^2 + w_2^2}$ of the scattering state $\tilde{\psi}^{(1)}(x)$, as expected from (76).

4.6 Graphs with localized states

In this section we discuss the consequence of the possible existence of localized states in certain graphs. These states are not probed by scattering, consequently their contributions to the current is not given by the expressions derived above.

For the sake of simplicity our discussion will be focused on the example of a ring in the regime of the integer quantum Hall effect, with one edge state. The potential hill at the middle is called an antidot (figure 8, left). This example must be thought more as a toy model to understand the idea of localized states in graphs, than as a realistic model to describe current distribution in a quantum Hall device where the effect of screening is important (the interested reader will find some discussion on the nature of edge currents and the role of screening in [45, 46]). The system can be modeled by a ring with chiral scattering at the vertices (figure 8, right). The ring has two bonds, *i.e.* four internal arcs : two arcs a and b carrying fluxes θ_a and θ_b and the two reversed arcs denoted with a bar : $\bar{a}$ and $\bar{b}$. The two leads are described by arcs 1 and 2.

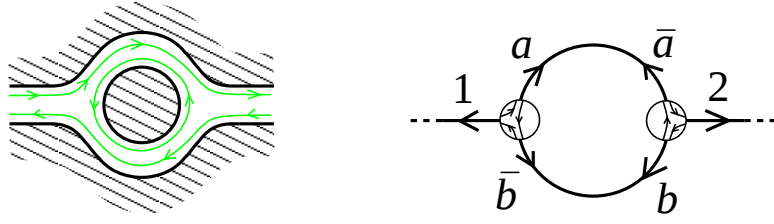


Figure 8: *Left* : A mesoscopic device in the regime of the IQHE with an antidot at the middle. One edge state is open. *Right* : The graph that models this arrangement. The scattering at the vertices is chiral.

In the basis of arcs $\{a, \bar{a}, b, \bar{b} | 1, 2\}$, its vertex scattering matrix and bond scattering matrix are :

$$Q = \left(\begin{array}{cccc|cc} 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{array} \right) = \left(\begin{array}{c|c} \frac{Q^{\text{int}}}{Q} & \tilde{Q}^{\text{T}} \\ \hline & Q^{\text{ext}} \end{array} \right) \quad (86)$$

The off diagonal blocks are not anymore transposed due to the breaking of the time reversal symmetry at the vertices (chiral scattering), however we keep the same notation as above for simplicity since there is no possible confusion. On the other hand

$$R = \left(\begin{array}{cc|cc} 0 & 0 & e^{ikl_a - i\theta_a} & 0 \\ 0 & 0 & 0 & e^{ikl_b + i\theta_b} \\ \hline e^{ikl_a + i\theta_a} & 0 & 0 & 0 \\ 0 & e^{ikl_b - i\theta_b} & 0 & 0 \end{array} \right). \quad (87)$$

We recall that Q_{ij} is the transmission amplitude from arc j to arc i due to vertex scattering, and R_{ij} describes bond scattering due to the potential.

Scattering. The scattering matrix can be computed from Q and R with equation (8), however the result is obvious here, due to the absence of multiple scattering :

$$\Sigma = \left(\begin{array}{cc} 0 & e^{ikl_b + i\theta_b} \\ e^{ikl_a + i\theta_a} & 0 \end{array} \right) \quad (88)$$

The current density in the arc a is given by the matrix :

$$\Sigma^\dagger \frac{d\Sigma}{d\theta_a} = \left(\begin{array}{cc} i & 0 \\ 0 & 0 \end{array} \right) \quad (89)$$

From (55) we get the contribution of the scattering state $\tilde{\psi}^{(1)}(x)$ to the current density in the arm a : $j_a^{(1,1)} = \frac{1}{2\pi}$, whereas the contribution of $\tilde{\psi}^{(2)}(x)$ obviously vanishes $j_a^{(2,2)} = 0$, since this latter scattering state does not send current into the arc a .

Localized states. We follow the discussion of [11, 13] : if localized states are present, their discrete spectrum is given by solving $\det(R^\dagger - Q^{\text{int}}) = 0$. Here, we see that the equation indeed possesses a set of solutions since $\det(R^\dagger - Q^{\text{int}}) = e^{-ikl}(e^{-ikl} - e^{-i\theta})$ where $\theta = \theta_a + \theta_b$. The spectrum of localized states is $k_n = (2\pi n + \theta)/l$ for $n \in \mathbb{N}$ if $\theta \in [0, 2\pi[$, since $k \geq 0$ by convention. These states describe a clockwise motion of the electron in the loop of the graph (right part of

figure 8). In the quantum Hall ring picture, they correspond to states whose wave functions are localized on the edge of the antidot (left part of figure 8). The current associated to the state of energy k_n^2 in the arc a is $-\frac{\partial}{\partial\theta}k_n^2 = -2(2n\pi + \theta)/l^2$. Note that if one introduces some scattering on the bonds, the localized states are hybridized with the states of the continuum and the discrete part of the spectrum disappears.

The discrete spectrum also brings some contribution to the current in the arms of the ring, which cannot be obtained from the scattering properties. Since the state $\tilde{\psi}^{(2)}$ does not contribute, the total average current in arm a finally reads :

$$J_a = \int_0^\infty dE f_1(E) j_a^{(1,1)}(E) - \sum_{n=0}^\infty f_{\text{int}}(k_n^2) \frac{2}{l^2} (2n\pi + \theta) \quad (90)$$

where $f_1(E)$ is the Fermi distribution for the lead 1 and $f_{\text{int}}(E)$ the Fermi distribution for the localized states inside the graph.

Now we can give the general expression for the current in the arc a for a graph with localized states. Since the discrete spectrum of localized states $\{E_n\}$ is given by the equation

$$0 = \det(R^\dagger - Q^{\text{int}}) \propto \prod_n (E - E_n) \quad (91)$$

we have

$$J_a = \sum_\beta \int dE f_\beta(E) \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{\partial \Sigma}{\partial \theta_a} \right)_{\beta\beta} + \int dE f_{\text{int}}(E) \frac{1}{\pi} \text{Im} \frac{\partial}{\partial \theta_a} \ln \left(\det(R^\dagger - Q^{\text{int}}) \Big|_{E \rightarrow E+i0^+} \right), \quad (92)$$

where $f_{\text{int}}(E)$ is the Fermi distribution associated to localized states. The first term is the contribution of the scattering states whereas the second is the contribution of the localized states.

5 Summary

In this paper we have studied the two first cumulants of the charge of a graph connected to infinite wires, as well as the distribution of currents in the wires inside the graph. In particular, we have shown the relation with the scattering matrix, allowing to study these quantities in an out of equilibrium situation, when the graph is connected to wires put at different potentials. We have obtained a formula for the average current and the current correlations that generalizes previous results known for the equilibrium situation [17, 29].

We have also emphasized that the scattering matrix contains information only on the continuous part of the spectrum related to scattering states. If some states remain localized in the graph, they give an additional contribution to the current not taken into account by the scattering approach.

We have considered the case of graphs weakly coupled to the leads. It is interesting to remark that the results obtained in this context are expected to be of much more generality than graphs, since the starting point was to use an approximation of the scattering state near a resonant level (21), a form of great generality. In particular, the contribution of the resonant level n to the average of some quantity X defined inside the graph reads

$$\langle \hat{X}(t) \rangle^{(n)} \simeq X_n \langle \hat{Q}(t) \rangle^{(n)}, \quad (93)$$

where $X_n = \langle \varphi_n | \hat{X} | \varphi_n \rangle$ is the expectation of X in the eigenstate $|\varphi_n\rangle$ of the isolated system. Similarly the contribution of the n -th resonant level to the correlations of two observables X and Y reads :

$$S_{XY}^{(n)}(\omega) \simeq X_n Y_n S_{QQ}^{(n)}(\omega) . \quad (94)$$

These results apply to a situation with narrow resonances ($\Gamma_n \ll |E_{n+1} - E_n|$). We repeat that we have not considered the effect of electron electron interactions in this article (weakly connected devices with resonant tunneling present in principle Coulomb blockade). It would be interesting to incorporate some effects of interaction. This could be already done in a mean field approximation to describe the effect of screening in the charge and current distribution following Büttiker's approach [3, 4, 27].

Acknowledgements

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A Relation between the different unsymmetrized correlators

Let us consider A and B two hermitian operators associated to physical quantities in our system. There are two unsymmetrized correlation functions:

$$S_{A,B}(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} (\langle A(t+\tau) B(t) \rangle - \langle A(t+\tau) \rangle \langle B(t) \rangle) \quad (95)$$

$$\tilde{S}_{A,B}(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} (\langle B(t) A(t+\tau) \rangle - \langle B(t) \rangle \langle A(t+\tau) \rangle) . \quad (96)$$

These correlators do not depend on t for a system in a stationary state⁵. Note that, even if we consider out of equilibrium situations, only stationary states are considered in the present paper.

In this case, using time translation invariance of one and two point correlation functions, we have :

$$\tilde{S}_{A,B}(\omega) = \int_{-\infty}^{+\infty} d\tau e^{i\omega\tau} (\langle B(t-\tau) A(t) \rangle - \langle B(t-\tau) \rangle \langle A(t) \rangle) \quad (97)$$

and this gives:

$$\tilde{S}_{A,B}(\omega) = S_{B,A}(-\omega) . \quad (98)$$

When $A = B$, it shows that one unsymmetrized correlator determines the other one:

$$\tilde{S}_{A,A}(\omega) = S_{A,A}(-\omega) . \quad (99)$$

Finally, note that the correlator $S_{A,A}(\omega)$ is real since the correlator in time obeys $S_{A,A}(\tau)^* = S_{A,A}(-\tau)$.

B Structure of the stationary states near a resonance

If we consider a graph weakly coupled to the leads, we expect the stationary scattering states to be closely related to the eigenstates of the isolated graph. The purpose of the appendix is to demonstrate the precise relation. The relations we will obtain are very reminiscent of the

⁵Glassy systems are an example for which this is not possible since the system never reaches a stationary state (weak ergodicity breaking).

Hamiltonian approach of chaotic scattering [47] (see also [48]). In this latter case some small couplings are introduced between an isolated system and the leads, whereas we rather start from a situation where the coupling can be arbitrary large and study the weak coupling limit to see how the properties of the isolated graph emerges from its scattering properties.

Let us consider a graph $\mathcal{G}$, whose spectrum is supposed to be non degenerate for simplicity (the occurrence of degeneracies leads to complications related to possible existence of localized states in the graph non probed by scattering [11, 13]). In a first step we describe how the eigenstates of the Schrödinger operator in the graph are constructed and in a second step we will establish the relation with stationary states in the weak coupling limit.

Isolated graph. The spectrum of the Schrödinger operator in the graph is given by the equation : $S(\gamma) = 0$, where $S(\gamma) = \prod_n(\gamma + E_n)$ is the spectral determinant, whose construction is explained in [41, 42] for the case of free graphs, in [43, 49] for graphs with potential and in [44] for graphs with general boundary conditions (more general than the continuity of the wave function at vertices). If the wave function is continuous at vertices :

$$S(\gamma) = \gamma^{V/2} \prod_{(\alpha\beta)} \left(\frac{df_{\beta\alpha}}{dx_{\alpha\beta}}(\alpha) \right)^{-1} \det M(\gamma) . \quad (100)$$

The product runs over all the bonds of the graph. We recall that the functions $f_{\alpha\beta}(x)$ involved in $M(\gamma)$ are the solutions of the Schrödinger equation on the bond $[\gamma - d_x^2 + V_{(\alpha\beta)}(x)]f(x) = 0$ for an energy $E = -\gamma$. In general $S(\gamma) = 0$ possesses the same set of solutions as

$$\det M(\gamma) = 0 . \quad (101)$$

We do not discuss here the case where the sets of zeros of both equations do not coincide, which is a little bit pathological and would require to refine the following arguments. Let us however quote few examples of free graphs ($V(x) = 0$) for which it is the case : the graph made of one line (in this case $\det M = 1$ is independent of γ), the complete graph [42, 11],...

The component of the wave function $\varphi_n(x)$ on the bond $(\alpha\beta)$ is :

$$\varphi_{n(\alpha\beta)}(x) = e^{iA_{\alpha\beta}x} \left(\varphi_{n,\alpha} f_{\alpha\beta}(x) + \varphi_{n,\beta} e^{-i\theta_{\alpha\beta}} f_{\beta\alpha}(x) \right) \quad (102)$$

where $\varphi_{n,\alpha}$ is the wave function at the vertex α and $A_{\alpha\beta} = \theta_{\alpha\beta}/l_{\alpha\beta}$ the vector potential. (Do not confuse the label n of the eigenstate with the greek labels that designate vertices). If we gather the wave function at the nodes in the V -dimensional column vector φ_n , the eigenstate of energy E_n is solution of

$$M(-E_n)\varphi_n = 0 . \quad (103)$$

Normalization. The normalization condition for the eigenstate reads :

$$\int_{\text{Graph}} dx |\varphi_n(x)|^2 = \sum_{(\alpha\beta)} \int_0^{l_{\alpha\beta}} dx |\varphi_{n(\alpha\beta)}(x)|^2 = 1 . \quad (104)$$

If we use the following relations [43] :

$$\int_0^{l_{\alpha\beta}} dx_{\alpha\beta} f_{\alpha\beta}(x_{\alpha\beta})^2 = -\partial_\gamma \frac{df_{\alpha\beta}}{dx_{\alpha\beta}}(\alpha) \quad (105)$$

$$\int_0^{l_{\alpha\beta}} dx_{\alpha\beta} f_{\alpha\beta}(x_{\alpha\beta}) f_{\beta\alpha}(x_{\alpha\beta}) = \partial_\gamma \frac{df_{\alpha\beta}}{dx_{\alpha\beta}}(\beta) \quad (106)$$

we obtain

$$\int_{\text{Graph}} dx |\varphi_n(x)|^2 = \sum_{(\alpha\beta)} \left[\varphi_{n,\alpha}^* \partial_\gamma \left(-\frac{df_{\alpha\beta}}{dx_{\alpha\beta}}(\alpha) \right) \varphi_{n,\alpha} + \varphi_{n,\alpha}^* \partial_\gamma \left(\frac{df_{\alpha\beta}}{dx_{\alpha\beta}}(\beta) e^{-i\theta_{\alpha\beta}} \right) \varphi_{n,\beta} \right. \\ \left. + \varphi_{n,\beta}^* \partial_\gamma \left(\frac{df_{\beta\alpha}}{dx_{\beta\alpha}}(\alpha) e^{i\theta_{\alpha\beta}} \right) \varphi_{n,\alpha} + \varphi_{n,\beta}^* \partial_\gamma \left(-\frac{df_{\beta\alpha}}{dx_{\beta\alpha}}(\beta) \right) \varphi_{n,\beta} \right] \quad (107)$$

If we replace the sum over bonds by a sum over vertices, the matrix M appears. Finally, the normalization condition reads for the V -vector φ_n :

$$\varphi_n^\dagger \partial_\gamma [\sqrt{\gamma} M(\gamma)] \varphi_n = 1, \quad (108)$$

where the spectral parameter is taken, after derivation, equal to the eigenenergy $\gamma = -E_n - i0^+$.

Graph weakly connected to leads. When the graph is weakly coupled to leads ($w_\alpha \rightarrow 0$) we expect that the stationary state $\tilde{\psi}_E^{(\alpha)}(x)$ is proportional to the wave function of the isolated graph near the resonance $E \simeq E_n$: $\tilde{\psi}_E^{(\alpha)}(x) \propto \varphi_n(x)$ for $x \in \mathcal{G}$. The question is how to recover precisely this relation from our formalism ?

The resonance width. As a preliminary question, it is instructive to find an expression for the resonance widths. For this purpose, let us consider the determinant of the scattering matrix [11] :

$$\det \Sigma = (-1)^L \frac{\det(M - W^T W)}{\det(M + W^T W)} \quad (109)$$

and find an approximation near a resonance E_n .

For any fixed energy $E > 0$, M is an antihermitian matrix and can be written in terms of its purely imaginary eigenvalues $i\lambda_\alpha(E)$ and its associate eigenvectors $v_\alpha(E)$:

$$M(-E) = i \sum_{\alpha=1}^V \lambda_\alpha(E) v_\alpha(E) v_\alpha^\dagger(E). \quad (110)$$

The eigenvectors are normalized as $v_\alpha^\dagger v_\alpha = 1$. If the energy E is equal to the energy E_n of an eigenstate of the isolated graph, one of the eigenvalues of M is vanishing : $\lambda_1(E_n) = 0$. We suppose the spectrum of the isolated graph to be non degenerate. The eigenvector $v_1(E_n)$ coincides with the eigenstate : $v_1(E_n) = \nu_n^{-1} \varphi_n$; however these vectors are not normalized in the same way and differ in the multiplicative factor ν_n .

Since $\det M(-E)$ is proportional to the spectral determinant and the spectrum supposed to be non degenerate, the eigenvalue $\lambda_1(E)$ behaves linearly near the energy E_n : $\lambda_1(E) \simeq (E - E_n)\beta_n$. The normalization condition (108) reads :

$$-\varphi_n^\dagger \partial_E \left(-i\sqrt{E} \sum_{\alpha=1}^V i\lambda_\alpha(E) v_\alpha(E) v_\alpha^\dagger(E) \right) \Big|_{E=E_n} \varphi_n = 1 \quad (111)$$

then

$$-\beta_n \sqrt{E_n} \varphi_n^\dagger v_1(E_n) v_1^\dagger(E_n) \varphi_n = 1 \quad (112)$$

We obtain the normalization constant : $\nu_n = 1/\sqrt{-k_n \beta_n}$ where $E_n = k_n^2$.

We now come back to $\det \Sigma$. In the weak coupling limit $w_\alpha \rightarrow 0$ we can compute perturbatively the eigenvalues of $M \pm W^T W$ to express the determinant :

$$\det(M(-E) \pm W^T W) \underset{E \sim E_n}{\simeq} \prod_{\alpha=1}^V \left(i\lambda_\alpha(E) \pm v_\alpha^\dagger(E) W^T W v_\alpha(E) \right) \quad (113)$$

$$\simeq \left(i\beta_n (E - E_n) \pm v_1^\dagger(E_n) W^T W v_1(E_n) \right) \prod_{\alpha=2}^V i\lambda_\alpha(E_n) \quad (114)$$

We can use the relation $v_1(E_n) = \sqrt{-k_n \beta_n} \varphi_n$ to get :

$$\det(M(-k^2) \pm W^T W) \underset{k \sim k_n}{\simeq} \left(k - k_n \pm \frac{i}{2} \varphi_n^\dagger W^T W \varphi_n \right) 2i\beta_n k_n \prod_{\alpha=2}^V i\lambda_\alpha(k_n^2). \quad (115)$$

Then :

$$\det \Sigma \propto \frac{k - k_n - i\gamma_n}{k - k_n + i\gamma_n} \quad (116)$$

where the resonance width in k -scale is : $\gamma_n = \frac{1}{2} \varphi_n^\dagger W^T W \varphi_n = \frac{1}{2} \sum_{\alpha=1}^L w_\alpha^2 |\varphi_{n,\alpha}|^2$. This result is very satisfactory since it shows that the lead α brings a contribution to the resonance width proportional to the transmission probability w_α^2 between the graph and the lead⁶ and to the probability density $|\varphi_{n,\alpha}|^2 \equiv |\varphi_n(\alpha)|^2$ associated to the eigenstate of the isolated graph, taken at the vertex α where the graph is connected. In energy scale the resonance width reads :

$$\Gamma_n = 2k_n \gamma_n = \sqrt{E_n} \varphi_n^\dagger W^T W \varphi_n = \sum_{\alpha=1}^L \Gamma_{n,\alpha} \quad (117)$$

where

$$\Gamma_{n,\alpha} = \sqrt{E_n} w_\alpha^2 |\varphi_n(\alpha)|^2 \quad (118)$$

is the contribution of the lead α .

The wave function. We recall that the $V \times L$ -matrix $\tilde{\Psi}$ that gathers the values of the L scattering states at the V vertices is [10] :

$$\tilde{\Psi} = \frac{1}{\sqrt{\pi k}} \frac{1}{M + W^T W} W^T. \quad (119)$$

We call $\psi^{(\alpha)}$ the V -column vector gathering the values of $\psi^{(\alpha)}(x)$ at the V vertices : $\psi^{(\alpha)} = (\psi_1^{(\alpha)}, \dots, \psi_V^{(\alpha)})^T$. The matrix Ψ is obtained by gathering these L column vectors : $\Psi = (\psi^{(1)}, \dots, \psi^{(L)})$. In the weak coupling limit ($w_\alpha \rightarrow 0$) and near the resonance E_n we can keep only the contribution of the vanishing eigenvalue $i\lambda_1(E)$ of M to compute :

$$\frac{1}{M + W^T W} \simeq \frac{1}{i\beta_n(E - E_n) + v_1^\dagger(E_n) W^T W v_1(E_n)} v_1(E_n) v_1^\dagger(E_n). \quad (120)$$

It follows that the scattering state at the vertex μ is :

$$\tilde{\psi}_\mu^{(\alpha)} = \tilde{\Psi}_{\mu\alpha} \simeq \frac{1}{\sqrt{\pi k}} \frac{i/2}{k - k_n + i\gamma_n} \varphi_{n,\mu} (\varphi_n^\dagger W^T)_\alpha = \frac{1}{\sqrt{4\pi k}} \frac{i w_\alpha \varphi_{n,\alpha}^*}{k - k_n + i\gamma_n} \varphi_{n,\mu}. \quad (121)$$

Since the vertex μ could be any point of the graph because we have always the freedom to introduce an additional vertex of weight $\lambda = 0$ on any bond without changing the properties of the graph, we can rewrite more elegantly :

$$\tilde{\psi}_{k^2}^{(\alpha)}(x) \underset{k \sim k_n}{\simeq} \frac{1}{\sqrt{4\pi k_n}} \frac{i w_\alpha \varphi_n^*(\alpha)}{k - k_n + i\gamma_n} \varphi_n(x) \quad (122)$$

Or using energy scale :

$$\tilde{\psi}_E^{(\alpha)}(x) \underset{E \sim E_n}{\simeq} \frac{1}{\sqrt{\pi}} \frac{i E_n^{1/4} w_\alpha \varphi_n^*(\alpha)}{E - E_n + i\Gamma_n} \varphi_n(x). \quad (123)$$

⁶the transmission amplitude is $\frac{2w_\alpha}{1+w_\alpha^2}$ for finite w_α [10].

The local density of states. The contribution of the scattering state $\tilde{\psi}_E^{(\alpha)}(x)$ to the off-diagonal LDoS $\langle x | \delta(E - H) | x' \rangle$ is :

$$\tilde{\psi}_E^{(\alpha)}(x) \tilde{\psi}_E^{(\alpha)*}(x') \underset{E \sim E_n}{\simeq} \frac{\Gamma_{n,\alpha}/\pi}{(E - E_n)^2 + \Gamma_n^2} \varphi_n(x) \varphi_n^*(x'). \quad (124)$$

The LDoS is obtained by summing these contributions over α .

The scattering matrix. The same discussion can be done to find an approximation for the scattering matrix. We obtain the well-known Breit-Wigner structure :

$$\Sigma_{\alpha\beta}(E) \underset{E \sim E_n}{\simeq} -\delta_{\alpha\beta} + \frac{2i\sqrt{E_n} w_\alpha \varphi_n(\alpha) w_\beta \varphi_n^*(\beta)}{E - E_n + i\Gamma_n}. \quad (125)$$

C Matrix elements of the charge operator

Our aim is to relate

$$\rho^{(\alpha,\beta)}(E) = \int_{\text{Graph}} dx \tilde{\psi}_E^{(\alpha)}(x)^* \tilde{\psi}_E^{(\beta)}(x) = \sum_{(\mu\nu)} \int_0^{l_{\mu\nu}} dx \tilde{\psi}_{(\mu\nu)}^{(\alpha)*}(x) \tilde{\psi}_{(\mu\nu)}^{(\beta)}(x) \quad (126)$$

to the scattering matrix. The sum runs over the B bonds. The relation (14) was proven for $\alpha = \beta$ in [11] using a different method.

The computation of this integral follows exactly the lines of the one done discussing the normalization of the states in the isolated graph. Then we obtain :

$$\rho^{(\alpha,\beta)}(E) = \sum_{\mu,\nu} \tilde{\psi}_\mu^{(\alpha)*} \partial_E \left(i\sqrt{E} M_{\mu\nu} \right) \tilde{\psi}_\nu^{(\beta)}, \quad (127)$$

that is :

$$\rho^{(\alpha,\beta)}(E) = \left(\tilde{\Psi}^\dagger \frac{d}{dE} \left(i\sqrt{E} M \right) \tilde{\Psi} \right)_{\alpha\beta} \quad (128)$$

$$= -\frac{1}{2i\pi} \left(W \frac{1}{-M + W^T W} \left[2 \frac{dM}{dE} + \frac{1}{E} M \right] \frac{1}{M + W^T W} W^T \right)_{\alpha\beta} \quad (129)$$

where we have used (119). From (3) and

$$\frac{d\Sigma}{dE} = -2W \frac{1}{M + W^T W} \frac{dM}{dE} \frac{1}{M + W^T W} W^T \quad (130)$$

we finally obtain the desired relation :

$$\rho^{(\alpha,\beta)}(E) = \frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{dE} + \frac{1}{4E} (\Sigma - \Sigma^\dagger) \right)_{\alpha\beta}. \quad (131)$$

An alternative way to relate $\rho^{(\alpha,\beta)}(E)$ to derivative of the scattering matrix is to introduce the variable conjugate to the charge : a constant potential U in the graph. The total potential now reads $V(x) + U \theta_{\mathcal{G}}(x)$ where $\theta_{\mathcal{G}}(x) = 1$ if $x \in \mathcal{G}$ and $\theta_{\mathcal{G}}(x) = 0$ if x belongs to the leads. In the presence of U , the function $f_{\alpha\beta}(x)$ involved in M is solution of $[E + d_x^2 - V_{(\alpha\beta)}(x) - U] f_{\alpha\beta}(x) = 0$. These functions are obtained by a shift of the spectral parameter : $f_{\alpha\beta}^U(x; E) = f_{\alpha\beta}^0(x; E - U)$. It immediately follows that :

$$\rho^{(\alpha,\beta)}(E) = - \left(\tilde{\Psi}^\dagger \frac{d}{dU} \left(i\sqrt{E} M \right) \tilde{\Psi} \right)_{\alpha\beta}. \quad (132)$$

Using the same arguments as above we get :

$$\rho^{(\alpha,\beta)}(E) = -\frac{1}{2i\pi} \left(\Sigma^\dagger \frac{d\Sigma}{dU} \right)_{\alpha\beta} . \quad (133)$$

It is interesting to compare this relation with (131) : it shows that it is not similar to differentiate with respect to a constant potential U or with respect to the energy since the potential does not live in the wires. The difference however vanishes at high energy (WKB limit).

A relation between the stationary states and the functional derivative of the scattering matrix [15]

$$-\frac{1}{2i\pi} \left(\Sigma^\dagger \frac{\delta \Sigma}{\delta V(x)} \right)_{\alpha\beta} = \tilde{\psi}_E^{(\alpha)*}(x) \tilde{\psi}_E^{(\beta)}(x) \quad (134)$$

was proven for graphs [13] where it is explained how it can be computed with algebraic calculations only. It follows that we can rewrite the equation (131) :

$$-\int_{\text{Graph}} dx \frac{\delta \Sigma}{\delta V(x)} = -\frac{d\Sigma}{dU} = \frac{d\Sigma}{dE} + \frac{1}{4E} (\Sigma^2 - 1) . \quad (135)$$

The first equality, which is obtained by identification of (126,134) with (133), is also a consequence of the definition of the functional derivative.

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