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Scattering theory on graphs: II. The Friedel sum rule

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Abstract

We consider the Friedel sum rule (FSR) in the context of the scattering theory for the Schrödinger operator $-\mathrm{D}_x^2 + V(x)$ on graphs made of one-dimensional wires connected to external leads. We generalize the Smith formula for graphs. We give several examples of graphs where the state counting method given by the FSR does not work. The reason for the failure of the FSR to count the states is the existence of states localized in the graph and not coupled to the leads, which occurs if the spectrum is degenerate and the number of leads too small.

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1. Introduction

This article follows [1], in which we considered the scattering problem for the Schrödinger operator on graphs. The graphs we are interested in are networks made of one-dimensional wires identified with finite intervals of $\mathbb{R}$ and connected at vertices. The study of such systems has been shown to be relevant in many contexts (for references see [1–7]). For example graphs have been often considered as simple modellizations for the mesoscopic networks realized experimentally. In this context scattering theory is a fundamental tool involved in the study of transport properties and many other questions. Several works have been devoted to the study of scattering theory on graphs, among which we can quote [1, 3, 8, 9]. In our work we examine an important aspect of scattering theory, namely the relation between the scattering and spectral properties that is established through the Friedel sum rule (FSR). The essence of the FSR is to count the number of states in the scattering region, that is related to the phases of the eigenvalues of the scattering matrix. The purpose of this article is to show that one must be careful when applying the FSR to graphs since this formula does not hold for any graph, one of the reasons for the breakdown being the occurrence of degeneracies in the spectrum of the graph (this is a necessary but not a sufficient condition as we shall see).

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Here we consider the Schrödinger operator

$$H = -\mathrm{D}_x^2 + V(x) \tag{1}$$

where $\mathrm{D}_x = \mathrm{d}_x - \mathrm{i}A(x)$ is the covariant derivative; the x coordinate lives on the graph $\mathcal{G}$. We briefly recall the notations adopted in previous works [1, 7, 10]. The graph $\mathcal{G}$ is made of B one-dimensional wires connected at V vertices. We shall denote the vertices with Greek letters $(\alpha, \beta, \mu, \ldots)$. The $V \times V$ adjacency matrix $a_{\alpha\beta}$ (or connectivity matrix) is defined as $a_{\alpha\beta} = 1$ if the vertices α and β are connected by a bond and $a_{\alpha\beta} = 0$ otherwise. The coordination of the vertex α (number of bonds issuing from the vertex) is therefore $m_\alpha = \sum_\beta a_{\alpha\beta}$. The bond between the vertices α and β will be designated with parentheses: $(\alpha\beta)$. We also introduce the notion of *arc*, which is an *oriented bond*. Each bond $(\alpha\beta)$ is associated with two arcs: $\alpha\beta$ and $\beta\alpha$. The arcs are labelled with Roman letters $(i, j, \ldots)$ and we denote the reversed arc of i with a bar: $\bar{i}$.

The coordinate $x_{\alpha\beta}$ on the bond $(\alpha\beta)$ of length $l_{\alpha\beta}$ belongs to the interval: $x_{\alpha\beta} \in [0, l_{\alpha\beta}]$ where $l_{\alpha\beta}$ is the length of the bond $(\alpha\beta)$ (note that by definition $x_{\beta\alpha} = l_{\alpha\beta} - x_{\alpha\beta}$).

The Schrödinger operator acts on scalar functions $\psi(x)$ living on $\mathcal{G}$ that are represented by a set of B components $\psi_{(\alpha\beta)}(x_{\alpha\beta})$ satisfying appropriate boundary conditions at the vertices [2, 11].

(i) Continuity

$$\psi_{(\alpha\beta_i)}(x_{\alpha\beta_i} = 0) = \psi_\alpha \qquad \text{for } i = 1, \ldots, m_\alpha \tag{2}$$

$\{\beta_i \,/\, i = 1, \ldots, m_\alpha\}$ is the set of vertices that are neighbours of the vertex α; the wavefunction at the vertex is ψ_α.

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

$$\sum_\beta a_{\alpha\beta}\, \mathrm{D}_{x_{\alpha\beta}} \psi_{(\alpha\beta)}(x_{\alpha\beta} = 0) = \lambda_\alpha \psi_\alpha, \tag{3}$$

where λ_α is a real parameter. Due to the presence of the connectivity matrix $a_{\alpha\beta}$, the sum runs over all neighbouring vertices linked with vertex α.

Note that the conservation of the current alone leads to more general boundary conditions and does not require the continuity of the wavefunction at the nodes (see [5, 12] for example)

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

In a scattering situation the graph is connected to the exterior by leads plugged in on vertices (we designate by 'graph' the compact part that does not include the leads). We call L the number of leads through which some plane wave is injected. The quantity of interest is the on-shell scattering matrix Σ, which is an $L \times L$ matrix that relates the incoming amplitudes in the L channels to the outgoing ones. We denote by A_α^{ext} (B_α^{ext}) the incoming (outgoing) amplitude on the external lead connected at vertex α (i.e. A_α^{ext} is the coefficient of a plane wave $\mathrm{e}^{-\mathrm{i}kx}$ sent from the lead connected to vertex α). By definition

$$B^{\mathrm{ext}} = \Sigma\, A^{\mathrm{ext}}. \tag{4}$$

The purpose of [1] was to formulate in general terms the scattering theory for the Schrödinger operator, generalizing results known in the absence of potential $V(x)$ (Laplace operator) [2, 4, 13]. We have found various expressions of Σ for arbitrary graphs and related Σ to matrices encoding information about the topology of the graph, the potential on the bonds and the way the graph is connected to the leads. We recall here the main results of [1] that will be necessary in the following discussion.

1.1. The arc matrix formulation

We express here Σ on the energy shell $E = k^2$ in terms of matrices that couple arcs. The graph is described by $2B$ internal arcs. L external arcs are associated with the L leads. We introduce the matrix R that encodes the information about the potential on the graph and couples the $2B$ internal arcs of the graph:

$$R_{ij} = r_i\,\delta_{i,j} + t_{\bar{i}}\,\delta_{\bar{i},j} \tag{5}$$

is the matrix element between arcs i and j. The potential on each bond (i) is characterized by reflection and transmission coefficients: r_i, t_i for the injection of the wave in the direction of arc i and $r_{\bar{i}}$, $t_{\bar{i}}$ for the injection in the direction of the reversed arc $\bar{i}$. R is the bond scattering matrix. If the potential vanishes ($V(x) = 0$) we have $r_i = 0$ and $t_i = \exp(\mathrm{i}kl_i + \mathrm{i}\theta_i)$.

Next we introduce the vertex scattering matrix Q that encodes the information on the topology of the graph and the way it is connected to leads:

$$Q_{ij} = \frac{2}{m_\alpha + \mathrm{i}\lambda_\alpha/k} - 1 \qquad \text{if } i = j \ (i \text{ issues from the vertex } \alpha) \tag{6}$$

$$= \frac{2}{m_\alpha + \mathrm{i}\lambda_\alpha/k} \qquad \text{if } i \neq j \text{ both issuing from the vertex } \alpha \tag{7}$$

$$= 0 \qquad \text{otherwise.} \tag{8}$$

This expression of the vertex scattering matrix is a consequence of the conditions (2) and (3). We have also explained in [1] how this matrix is affected by the introduction of tunable couplings to the leads. The $(2B+L)\times(2B+L)$ matrix Q couples the $2B$ internal arcs together but also the latter to the L external arcs. If we separate Q into corresponding blocks:

$$Q = \left(\begin{array}{c|c} Q^{\mathrm{int}} & \tilde{Q}^{\mathrm{T}} \\ \hline \tilde{Q} & Q^{\mathrm{ext}} \end{array}\right) \tag{9}$$

then the scattering matrix is

$$\Sigma = Q^{\mathrm{ext}} + \tilde{Q}\,(R^\dagger - Q^{\mathrm{int}})^{-1}\,\tilde{Q}^{\mathrm{T}}. \tag{10}$$

The expression (10) generalizes the result known in the absence of potential [13].

1.2. The vertex matrix formulation

The previous approach is quite natural since we considered scattering matrices of the different parts of the system but it has the disadvantage of dealing with rather large matrices. It is more efficient to consider matrices that couple vertices. We define the $L \times V$-matrix W that encodes the information about the way the graph is connected to leads:

$$W_{\alpha\beta} = w_\alpha\,\delta_{\alpha\beta} \tag{11}$$

with $\alpha \in \mathcal{V}_{\mathrm{ext}}$ and $\beta \in \mathcal{V}$, where $\mathcal{V} = \{1, \ldots, V\}$ 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 physical meaning is discussed in [1]. In the arc matrix formulation these parameters are introduced in the matrix Q [1]. We just recall that $w_\alpha = 1$ corresponds to perfect coupling (the case considered above in section 1.1), whereas $w_\alpha = 0$ corresponds to disconnecting the lead. The limit $w_\alpha = \pm\infty$ also corresponds to disconnection of the lead; however, the current is not allowed to flow through the vertex in this case and this way to disconnect the lead is equivalent to imposing a Dirichlet boundary at the vertex ($\lambda_\alpha = \infty$).

We also introduce the matrix M that contains all the information on the isolated graph (potential on the bond and topology):

$$M_{\alpha\beta} = \delta_{\alpha\beta}\left(\mathrm{i}\frac{\lambda_\alpha}{k} + \sum_\mu a_{\alpha\mu}\frac{(1-r_{\alpha\mu})(1+r_{\mu\alpha}) + t_{\alpha\mu}\,t_{\mu\alpha}}{(1+r_{\alpha\mu})(1+r_{\mu\alpha}) - t_{\alpha\mu}\,t_{\mu\alpha}}\right) - a_{\alpha\beta}\frac{2\,t_{\alpha\beta}}{(1+r_{\alpha\beta})(1+r_{\beta\alpha}) - t_{\alpha\beta}\,t_{\beta\alpha}}. \tag{12}$$

Then, the scattering matrix reads

$$\Sigma = -1 + 2\,W(M + W^{\mathrm{T}}W)^{-1}W^{\mathrm{T}}. \tag{13}$$

These equations generalize the result known in the absence of potential [2, 4]. In this latter case we recover from (12) the well known matrix

$$M_{\alpha\beta} = \mathrm{i}\,\delta_{\alpha\beta}\sum_\mu a_{\alpha\mu}\mathrm{cotg}\,kl_{\alpha\mu} - a_{\alpha\beta}\frac{\mathrm{i}\,\mathrm{e}^{\mathrm{i}\theta_{\alpha\beta}}}{\sin kl_{\alpha\beta}}. \tag{14}$$

Some examples of application of these formulae are given in [1].

We describe the organization of this paper. Since there has recently been some confusion in the literature about the content of the FSR, we think it is useful to spend some time by reviewing some aspects around this relation, which will also be necessary for the following. In section 3 we generalize the Smith formula for graphs. Then we provide in section 4 several examples of violation of the FSR and explain the origin of this failure.

2. The Friedel sum rule

To be precise we consider the scattering theory for the Schrödinger equation on a three-dimensional Euclidean manifold and restrict ourselves to the case of a rotational invariant potential supposed to be concentrated in a sphere of radius R. A basis of eigenstates is given by the partial waves $\psi_l(r)\,Y_l^m(\theta,\varphi)$ (where $Y_l^m(\theta,\varphi)$ are the spherical harmonics) whose radial parts involve the phase shifts $\eta_l(E)$: $\psi_l(r) = (1/\sqrt{\pi k})(1/r)\sin(kr - l\pi/2 + \eta_l)$ for $r \geqslant R$. The energy of this eigenstate is $E = k^2$. The Krein–Friedel relation relates the variation of the density of states (DoS) to scattering properties. We introduce the local density of states (LDoS) $\rho(\vec{r};E) = \langle\,\vec{r}\,|\delta(E-H)|\,\vec{r}\,\rangle$. We denote by $\rho_0(\vec{r};E)$ the LDoS in the absence of the potential. The relation reads

$$\int \mathrm{d}\vec{r}\,[\rho(\vec{r};E) - \rho_0(\vec{r};E)] = \frac{1}{\pi}\sum_{l=0}^{\infty}(2l+1)\frac{\mathrm{d}\eta_l}{\mathrm{d}E}. \tag{15}$$

Since the integral in the lhs runs over the whole space, the total DoS is diverging like the volume of integration; however, the difference of the lhs is a finite quantity. The demonstration of (15) in the one-dimensional case is recalled in appendix B.

Using the fact that $\mathrm{e}^{2\mathrm{i}\eta_l}$ are the eigenvalues of the on-shell scattering matrix $\tilde{\Sigma}$ we can write[1]

$$\int \mathrm{d}\vec{r}\,[\rho(\vec{r};E) - \rho_0(\vec{r};E)] = \frac{1}{2\mathrm{i}\pi}\frac{\mathrm{d}}{\mathrm{d}E}\,\mathrm{Tr}\{\ln\tilde{\Sigma}(E)\} = \frac{1}{2\mathrm{i}\pi}\frac{\mathrm{d}}{\mathrm{d}E}\ln\det\tilde{\Sigma}(E), \tag{16}$$

where the trace is computed on the energy shell E over channel indices.

[1] The scattering matrix $\tilde{\Sigma}$ entering (16) is slightly different from the scattering matrix Σ we have introduced, the two being related through a simple transformation. The phase shifts $\eta_l(E)$ (phases of the eigenvalues $\mathrm{e}^{2\mathrm{i}\eta_l}$ of $\tilde{\Sigma}$) encode the effect of the scattering potential compared with the free case: in the absence of the potential, the phase shifts η_l vanish. On the other hand the phases $\delta_l(E)$ of the eigenvalues $\mathrm{e}^{\mathrm{i}\delta_l}$ of Σ are measured from the edge of the scattering region: $\psi_l(r) = (1/\sqrt{\pi k})(1/r)\sin(k(r-R) - l\pi/2 + \delta_l/2)$ for $r \geqslant R$.

Therefore we have $\delta_l = 2\eta_l + 2kR$. The relation between Σ and $\tilde{\Sigma}$ is also explained in detail in the one-dimensional case in appendix B.

It is convenient to introduce the Friedel phase defined as $\delta^f(E) = -\mathrm{i}\ln\det\Sigma(E)$ with the additional constraint to be a continuous function of the energy. It is the sum of the cumulative phases of the eigenvalues $\mathrm{e}^{\mathrm{i}\delta_a}$ of the scattering matrix Σ: $\delta^f(E) = \sum_a \delta_a(E)$. The Friedel phase counts the number of resonance peaks: if they are sufficiently narrow to be well separated, in the neighbourhood of a resonance, the determinant behaves like

$$\mathrm{e}^{\mathrm{i}\delta^f(E)} = \det\Sigma(E) \underset{E\sim E_n}{\propto} \left(\frac{E - E_n - \mathrm{i}\Delta_n}{E - E_n + \mathrm{i}\Delta_n}\right)^{d_n}, \tag{17}$$

up to a constant phase. E_n is the position of the resonance, Δ_n its width and d_n the degeneracy of the state. This expression shows that the phase $\delta^f(E)$ makes a jump of $2\pi d_n$ when E crosses the resonance.

The relation (15) was derived long ago by Beth and Uhlenbeck [14] in the context of the study of a gas of interacting particles, where it is involved in the second virial coefficient (related to the two-body problem). The generalization for a systematic expansion of the grand potential was provided in [15]. The demonstration of the Krein–Friedel relation [16–19], also called the FSR, is given in standard textbooks for rotational invariant potentials [20, 21]. It is also worth mentioning the existence of a vast literature in mathematical physics dealing with the scattering theory. Many references can be found in [22] which devotes its last chapter to the study of the Krein spectral shift function (the Friedel phase) and trace formula. The matrix $-\mathrm{i}\Sigma^\dagger \mathrm{d}\Sigma/\mathrm{d}E$ whose trace is computed in (16) is the matrix of Wigner time delays (note also the existence of a classical formulation of the second virial coefficient in terms of classical time delays in [23]). It is worth mentioning that (16) is exact, which is the beauty of this relation (its validity is not restricted to a high-energy regime for example). Integrated over the interval of energy below the Fermi energy, (15) and (16) give the accumulation of charge due to the presence of the potential, to use the language of [16].

Instead of considering the variation of the DoS of the whole space, it is also possible to study the LDoS integrated over the interacting region only. This quantity is also related to scattering properties through the Smith formula [24], which defines the time delay. For a rotational invariant potential the relation reads

$$2\pi\int_0^R \mathrm{d}r\, r^2|\psi_l(r)|^2 = 2\frac{\mathrm{d}\eta_l}{\mathrm{d}E} + \frac{R}{k} - \frac{1}{2E}\sin(2kR + 2\eta_l - l\pi) = \frac{\mathrm{d}\delta_l}{\mathrm{d}E} - \frac{1}{2E}\sin(\delta_l - l\pi). \tag{18}$$

Note that this relation was also derived in [16] as an intermediate result for the demonstration of (15). With a summation over the angular quantum numbers[2], we obtain the LDoS integrated over the sphere:

$$\begin{aligned}\int_{r<R} \mathrm{d}\vec{r}\,\rho(\vec{r};E) &= \sum_{l=0}^{\infty}(2l+1)\int_0^R \mathrm{d}r\, r^2|\psi_l(r)|^2 \\ &= \frac{1}{2\pi}\sum_{l=0}^{\infty}(2l+1)\left(\frac{\mathrm{d}\delta_l}{\mathrm{d}E} - \frac{1}{2E}\sin(\delta_l - l\pi)\right).\end{aligned} \tag{19}$$

If the coupling between the scattering region (sphere of radius R) and the exterior is adjustable, this quantity corresponds to the DoS of the scattering region when it is isolated. If we are interested in the Weyl contribution of the DoS of the scattering region we can forget the second term of (19) and consider only the Weyl term of the Friedel phase.

[2] The choice of normalization for the stationary scattering states $\psi_{E,l,m} = \psi_l(r)Y_l^m(\theta,\varphi)$ introduced above corresponds to associating with these states a measure $\mathrm{d}E$ (it implies for example that $\int \mathrm{d}\vec{r}\,\psi^*_{E,l,m}\psi_{E',l',m'} = \delta_{l,l'}\delta_{m,m'}\delta(E-E')$).

Due to the central position of the scattering approach in mesoscopic physics, the FSR plays an important role in the study of many physical quantities: for example the FSR allows us to relate the persistent current to scattering properties [25] and is also involved in electrochemical capacitance [26, 27]. A local formulation was also developed in [26, 28] to relate the LDoS to scattering properties (a general discussion of the role of the local FSR is provided in [29]). Since graphs are widely used to model mesoscopic networks they have been considered to apply concepts involving the FSR, as in [25] for the persistent current in a loop connected to one lead, or in the recent work [30], in which graphs provided examples to illustrate a general discussion about a subtle point related to phases.

Recently there has been some confusion about the FSR in [31]. Starting from a misinterpretation of the FSR, these authors claimed that the relation does not hold in the one-dimensional case if the potential is made of two δ peaks, which is not true. We repeat that the general demonstration of (16) in [15] covers the one-dimensional situation. The one-dimensional case is reviewed in detail in appendix B, where we consider as an example the case of one δ peak (it is not difficult to check that the FSR works perfectly well, as it should, for two δ peaks, a little exercise following the same lines).

The FSR has been proven in arbitrary dimension; however, it has not been demonstrated for graphs which are intermediate objects between one-dimensional and higher-dimensional systems. Then it is important to clarify some points in this context. The FSR (15), (16) counts the variation of the DoS due to a scattering potential. The Smith relation (19) measures the LDoS integrated in the scattering region. Both are based on the idea of counting the number of states of the scattering region by counting the resonance peaks of the phase shifts derivatives. We shall show that this procedure is not always applicable for graphs: for example, in the case of the complete graph that will be studied in detail below, some states of the isolated graph are not manifested by a resonance peak or give rise to a resonance peak that does not carry the correct spectral weight (the degeneracy of the level). To study this problem it will be sufficient to consider the Weyl part of the Friedel phase to notice some discrepancy with the Weyl part of the DoS of the graph. Before following this programme and to settle the discussion on more precise grounds, we shall generalize the Smith formula (18) to the case of graphs, although it does not always concern the DoS, as we shall see.

3. Generalization of the Smith relation

The Smith relation was derived for a one-dimensional system with one scattering channel [24] (or rotational invariant potentials in three dimensions) and involves the Wigner time delay [32]. We generalize this relation to the case of a perfectly connected graph ($w_\alpha = 1$). The starting point is to introduce

$$\Omega = (\mathrm{D}_x\psi)^* \frac{\mathrm{d}\psi}{\mathrm{d}E} - \psi^* \left(\mathrm{D}_x \frac{\mathrm{d}\psi}{\mathrm{d}E} \right) \tag{20}$$

which satisfies the following relation:

$$\frac{\mathrm{d}}{\mathrm{d}x}\Omega(x) = |\psi(x)|^2 \tag{21}$$

for any solution ψ of the Schrödinger equation $(-\mathrm{D}_x^2 + V(x))\psi(x) = E\psi(x)$; we recall that $\mathrm{D}_x = \mathrm{d}_x - \mathrm{i}A(x)$ is the covariant derivative. Applied to a graph, the relation (21) should be written for the B components of the wavefunction on the bonds (and also on the L leads).

We first derive two properties involving $\Omega_{\alpha\beta}(x_{\alpha\beta})$, the quantity (20) related to the component of the wavefunction $\psi_{(\alpha\beta)}(x_{\alpha\beta})$ (we shall denote by $\Omega_{\mathrm{lead}\,\mu}(x)$ that associated with the component $\psi_{\mathrm{lead}\,\mu}(x)$ on the lead attached to the vertex μ). Obviously, we have

$\Omega_{\alpha\beta}(x_{\alpha\beta}) = -\Omega_{\beta\alpha}(x_{\beta\alpha})$. Due to the conservation of the current, ensured by (3), the sum of all $\Omega_{\mu\beta}$ associated with the arcs issuing from the vertex μ and computed at the position of the vertex ($x_{\mu\beta} = 0$) is zero:

$$\sum_{\beta} a_{\mu\beta}\, \Omega_{\mu\beta}(\mu) + (W^{\mathrm{T}}W)_{\mu\mu}\, \Omega_{\mathrm{lead}\,\mu}(\mu) = 0. \tag{22}$$

We have used the obvious notation $\Omega_{\mu\beta}(\mu) \equiv \Omega_{\mu\beta}(x_{\mu\beta} = 0)$. The second term is the contribution of a lead, if one is plugged in at vertex μ (due to the definition of W, we recall that $(W^{\mathrm{T}}W)_{\mu\mu} = 1$ if a lead issues from μ and 0 otherwise). The second useful property is obtained by integration of (21) on the bond $(\mu\beta)$:

$$\int_0^{l_{\mu\beta}} \mathrm{d}x\, |\psi_{(\mu\beta)}(x)|^2 = -\Omega_{\mu\beta}(\mu) - \Omega_{\beta\mu}(\beta). \tag{23}$$

We now consider the stationary scattering state $\psi^{(\alpha)}(x)$ of energy $E = k^2$, associated with the injection of a plane wave from the lead connected at vertex α. The construction of these eigenstates is briefly recalled in appendix A (see [1]). From the expression (47) of the wavefunction on the lead we see that

$$\Omega^{(\alpha)}_{\mathrm{lead}\,\mu}(\mu) = -2\mathrm{i}k\, \Sigma^*_{\mu\alpha} \frac{\mathrm{d}\Sigma_{\mu\alpha}}{\mathrm{d}E} - \frac{\mathrm{i}}{2k}(\delta_{\mu\alpha} + \Sigma^*_{\mu\alpha})(-\delta_{\mu\alpha} + \Sigma_{\mu\alpha}). \tag{24}$$

We now compute the integral of $|\psi^{(\alpha)}(x)|^2$ on the graph (the 'graph' refers to internal bonds):

$$\int_{\mathrm{Graph}} \mathrm{d}x\, |\psi^{(\alpha)}(x)|^2 = \sum_{(\mu\beta)} \int_0^{l_{\mu\beta}} \mathrm{d}x\, |\psi^{(\alpha)}_{(\mu\beta)}(x)|^2 = -\sum_{\mathrm{arc}\,\mu\nu} \Omega^{(\alpha)}_{\mu\nu}(\mu), \tag{25}$$

where we have used (23). The summation $\sum_{(\mu\beta)}$ is over the B bonds of the graph, whereas the last summation runs over the $2B$ internal arcs. We see that the contributions from the arcs issuing from an internal vertex vanish due to (22). The contributions of the internal arcs issuing from connected vertices can be replaced by the contributions of external leads due to (22). Therefore we obtain

$$\int_{\mathrm{Graph}} \mathrm{d}x\, |\psi^{(\alpha)}(x)|^2 = \sum_{\mu} \Omega^{(\alpha)}_{\mathrm{lead}\,\mu}(\mu) = -2\mathrm{i}k \left(\Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E} \right)_{\alpha\alpha} - \frac{\mathrm{i}}{2k}(\Sigma_{\alpha\alpha} - \Sigma^*_{\alpha\alpha}) \tag{26}$$

where the sum over μ is obviously over the L connected vertices.

In order to associate a measure $\mathrm{d}E$ with the stationary scattering states, we change the normalization. The scattering states (47), (50) are related to the new ones by $\tilde{\psi}^{(\alpha)}_E(x) = (1/\sqrt{4\pi k})\psi^{(\alpha)}(x)$. If we sum the contributions (26) of the L stationary scattering states of energy E, we obtain

$$\sum_{\alpha} \int_{\mathrm{Graph}} \mathrm{d}x\, |\tilde{\psi}^{(\alpha)}_E(x)|^2 = \frac{1}{2\mathrm{i}\pi} \left(\mathrm{Tr} \left\{ \Sigma^\dagger \frac{\mathrm{d}\Sigma}{\mathrm{d}E} \right\} + \frac{1}{4E}\, \mathrm{Tr}\left\{ \Sigma - \Sigma^\dagger \right\} \right) \tag{27}$$

which generalizes the Smith relation (18) to the case of graphs. The term $-\mathrm{i}\,\mathrm{Tr}\{\Sigma^\dagger \mathrm{d}\Sigma/\mathrm{d}E\}$ is the time delay.

To compute the Friedel phase of a graph appearing in the above relation, it is useful to note that[3]

$$\det \Sigma = (-1)^{V-L} \frac{\det(W^{\mathrm{T}} W - M)}{\det(W^{\mathrm{T}} W + M)}. \tag{28}$$

For one channel (one lead) we have $\Sigma = \mathrm{e}^{\mathrm{i}\delta}$, therefore we obtain

$$\int_{\mathrm{Graph}} \mathrm{d}x \, |\tilde{\psi}_E(x)|^2 = \frac{1}{2\pi}\left(\frac{\mathrm{d}\delta}{\mathrm{d}E} + \frac{1}{2E}\sin\delta\right), \tag{29}$$

which would be the relation (18) obtained by Smith if the graph reduced to a line (one-dimensional case with one channel). The different sign of the second term is only a matter of definition of the phase shift δ, in the one-dimensional case, and δ_0, in the $l = 0$ channel of the three-dimensional case, which differ by π.

Case $w_\alpha \neq 1$. When we introduce arbitrary couplings between the leads and the graph, the application of formula (27) means that we are also taking into account the integral over the bonds on which are the barriers characterized by the w_α (see [1], where the introduction of these parameters is explained in detail).

4. Violation of the Friedel sum rule for certain graphs

The idea of the FSR is to count the states in the scattering region by studying the Friedel phase. We have seen that the Smith formula (18) relates the LDoS integrated over the scattering region to the Friedel phase and we have found its generalization (27) for graphs. We call $\mathcal{N}(E) = \int_{-\infty}^{E} \mathrm{d}E' \int_{\mathrm{Graph}} \mathrm{d}x \, \rho(x; E')$ the integrated density of states (IDoS) of the graph. If we are not interested in the details of the spectrum but only in the Weyl term of the IDoS of the scattering region, and if we believe the FSR, the relation (19) shows that $\mathcal{N}_{\mathrm{Weyl}}(E) \simeq (1/2\pi)\delta^f(E)$ up to some oscillatory part. As a matter of fact this is not always true for graphs and we shall now give several examples where $\mathcal{N}_{\mathrm{Weyl}}(E)$ is not given by the dominant contribution of $\delta^f(E)$.

All the examples we are going to consider are free graphs, with $V(x) = 0$, but the ideas that will come out are not specific to free graphs. We recall that in the absence of a potential we have[4] $\mathcal{N}_{\mathrm{Weyl}}(E) = \mathcal{L}k/\pi$, where $\mathcal{L} = \frac{1}{2}\sum_{\alpha,\beta} a_{\alpha\beta} l_{\alpha\beta}$ is the total length of the graph. As we shall see, one of the reasons for the violation of the FSR is the occurrence of degeneracies in the spectrum. Graphs with symmetries present many degeneracies. This is why it is interesting to start by studying the complete graph K_V, which is the most symmetric simply connected graph with V vertices.

4.1. The complete graph K_V connected to one lead.

The graph K_V is made of V vertices, each being connected to the others by bonds of same length ℓ. The matrix M takes a simple form (see equation (64) in appendix C).

[3] The proof is easily achieved by considering the graph $\mathcal{G}'$ related to the original graph $\mathcal{G}$ by attaching to each of the $V - L$ internal vertices of $\mathcal{G}$ (labelled for convenience with prime indices: $\alpha', \ldots$) a lead with tunable coupling. If these couplings are switched off ($w_{\alpha'} \to 0$), the $V \times V$ scattering matrix Σ' of $\mathcal{G}'$ is block diagonal with an $L \times L$ block being the scattering matrix Σ of $\mathcal{G}$, the other $(V - L) \times (V - L)$ block corresponding to the additional leads being -1. Let us now compute $\det \Sigma'$: for finite couplings $w_{\alpha'}$, the matrix W' describing the coupling of $\mathcal{G}'$ to the V leads is square and possesses an inverse. It follows from (13) that $\Sigma' = W'^{-1}(W'^2 - M)(W'^2 + M)^{-1}W'$. Then $\det \Sigma' = \det(W'^2 - M)/\det(W'^2 + M)$. If the couplings to the additional leads now vanish, $w_{\alpha'} \to 0$, we have $\det \Sigma' = (-1)^{V-L} \det \Sigma$ and $W'^2 = W^{\mathrm{T}} W$.

[4] The Weyl term appears in the trace formula originally derived by Roth [33] (see also [4, 7]).

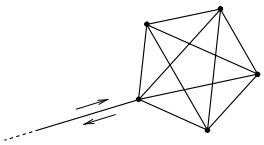

Figure 1. Complete graph K_5 connected to one lead.

The graph is connected to one lead (figure 1) and the scattering matrix is characterized by a unique phase: $\Sigma = \mathrm{e}^{\mathrm{i}\delta^f}$. Using (13) we recover after a little algebra the expression [7, formula (119)]

$$\operatorname{cotg}(\delta^f/2) = \cos\varphi \frac{\cos k\ell + \cos\varphi - 1}{\cos k\ell + \cos\varphi} \operatorname{cotg}(k\ell/2), \tag{30}$$

where $k = \sqrt{E}$ and $\cos\varphi = 1/(V-1)$. This expression shows that $\delta^f(k^2) = 3k\ell + (\text{fluct.})$, where (fluct.) represents a fluctuating term of order π, whereas the Weyl part of the IDoS is $\mathcal{N}_{\text{Weyl}}(E) = B\ell k/\pi = V(V-1)k\ell/2\pi$, which clearly shows the discrepancy between $\mathcal{N}(E)$ and $\delta^f(E)/2\pi$.

A more detailed analysis of the position of the resonance peaks of $\mathrm{d}\delta^f/\mathrm{d}E$ shows that the Friedel phase does not measure the degeneracies of the energies of the isolated graph (see appendix C, where the spectrum of K_V is recalled), and moreover even misses some energies: there is no resonance peak at k_{2+4n}.

To understand in more general terms the origin of the failure of the FSR when only one lead is plugged in on the graph, we consider the simple case of a graph with no potential ($V(x) = 0$ and $\lambda_\alpha = 0$) connected to only one external lead. The formula [7]

$$\operatorname{cotg}(\delta^f(E)/2) = -\sqrt{E}\frac{S_{\text{Dir.}}(-E - \mathrm{i}0^+)}{S_{\text{Neu.}}(-E - \mathrm{i}0^+)} \tag{31}$$

relates the phase shift $\delta^f(E)$ to the ratio of two spectral determinants. On the one hand $S_{\text{Dir.}}(\gamma)$ is the spectral determinant $\det(-\mathrm{D}_x^2+\gamma)$ calculated with a Dirichlet boundary condition ($\lambda_{\alpha_0} = \infty$) at the vertex α_0 where the lead is plugged in, and Neumann boundary conditions at all other vertices ($\lambda_\alpha = 0$). On the other hand $S_{\text{Neu.}}(\gamma)$ is calculated with Neumann boundary conditions at all vertices. The sum rule means that each state in the isolated graph is associated with a jump of 2π of the phase δ^f. Due to (31) we see that a jump of 2π occurs when the expression (31) diverges. Then we identify two reasons why the FSR fails: (i) if the spectrum of the graph is degenerate and (ii) if $S_{\text{Dir.}}(\gamma)$ vanishes for the same energy as $S_{\text{Neu.}}(\gamma)$, then (31) diverges a number of times which is not related to the number of states in the graph.

4.2. The complete graph K_V connected to V leads

To convince ourselves that the breakdown of the Krein–Friedel relation is not specific to graphs connected to one lead only, we consider now the case where K_V is attached to V leads connected to each vertex (figure 2).

If all the vertices of the graph are connected to leads ($L = V$), the matrix W is square. The determinant (28) is $\mathrm{e}^{\mathrm{i}\delta^f(E)} = \det(W^2 - M)/\det(W^2 + M)$. For simplicity we consider the case of equal couplings: $w_1 = w_2 = \cdots = w_V = w$. Using (64) we obtain

$$\mathrm{e}^{\mathrm{i}\delta^f(k^2)} = (-1)^V \frac{\sin(k\ell/2) - \mathrm{i}w^2\cos\varphi\cos(k\ell/2)}{\sin(k\ell/2) + \mathrm{i}w^2\cos\varphi\cos(k\ell/2)} \left(\frac{\cos k\ell + \cos\varphi + \mathrm{i}w^2\cos\varphi\sin k\ell}{\cos k\ell + \cos\varphi - \mathrm{i}w^2\cos\varphi\sin k\ell}\right)^{V-1}. \tag{32}$$

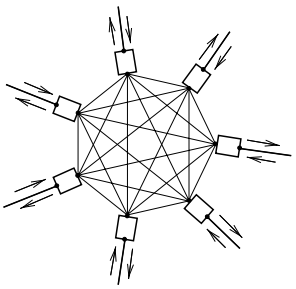

Figure 2. Complete graph K_7 connected to seven leads. The small boxes represent the couplings characterized by the parameter w [1].

This expression shows that $\delta^f(k^2) = (2V-1)k\ell + (\text{fluct.})$, which disagrees once again with $\mathcal{N}_{\text{Weyl}}(E) = V(V-1)k\ell/2\pi$.

It is interesting to provide a more detailed analysis by studying the behaviour of the Friedel phase in the neighbourhood of the energies of the graph (the spectrum is recalled in appendix C). We consider the limit $w \to 0$ for which the resonance profile of $\mathrm{d}\delta^f/\mathrm{d}E$ emerges clearly.

- Near the first energy level (for $k \sim k_1$) we see from (32) that $\mathrm{e}^{\mathrm{i}\delta^f} \propto [(k-k_1-\mathrm{i}\Delta k_1)/(k-k_1+\mathrm{i}\Delta k_1)]^{V-1}$ with $\Delta k_1 \ell = w^2/(V-1)$. The exponent is the degeneracy of the level, which means that the resonance peak of $\mathrm{d}\delta^f/\mathrm{d}E$ has the correct spectral weight and counts correctly the $V-1$ states.
- In the neighbourhood of the second energy level (for $k \sim k_2$) $\mathrm{d}\delta^f/\mathrm{d}E$ is flat: δ^f is not sensitive to the presence of states at this energy.
- The situation at $k \sim k_3$ is the same as that at $k \sim k_1$ (with $\Delta k_3 = \Delta k_1$).
- At $k \sim k_4$ we have $\mathrm{e}^{\mathrm{i}\delta^f} \propto (k-k_4-\mathrm{i}\Delta k_4)/(k-k_4+\mathrm{i}\Delta k_4)$ with $\Delta k_4 = 2\Delta k_1$: the Friedel phase misses the degeneracy.

One may now ask why the Friedel phase sometimes misses some states and sometimes does not. To answer this question we can study the structure of the wavefunctions of the isolated graph (see appendix C). Whereas the wavefunction is finite at the nodes at energies k_{1+2m} where the Friedel phase is sensitive to the degeneracy, all the $V(V-3)/2$ degenerate wavefunctions vanish at all the nodes at energies k_{2+4m} as well as at energies k_{4+4m}, which means that the wave sent from the lead does not enter the graph at these energies.

4.3. The ring connected with two leads

To understand better the remark that closed the previous subsection we consider next a simpler case: a ring connected to two leads (figure 3). The arms of the ring are of lengths l_a and l_b with $l = l_a + l_b$.

Let us first recall the spectrum of the isolated ring of perimeter l threatened by a flux θ: the energies are $E_m(\theta) = (2\pi/l)^2(m-\theta/2\pi)^2$ associated with wavefunctions $\varphi_m(x) = (1/\sqrt{l})\mathrm{e}^{2\mathrm{i}\pi mx/l}$ for $m \in \mathbb{Z}$. If $\theta = 0$ the states φ_m and φ_{-m} are degenerate. Therefore we can introduce in this case a different basis: a symmetric function $\varphi_n^+ = (\varphi_n + \varphi_{-n})/\sqrt{2} = \sqrt{2/l}\cos(2\pi nx/l)$ with $n \in \mathbb{N}$, and an antisymmetric one $\varphi_n^- = (\varphi_n - \varphi_{-n})/\mathrm{i}\sqrt{2} = \sqrt{2/l}\sin(2\pi nx/l)$ with $n \in \mathbb{N}^*$.

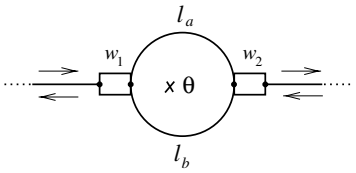

Figure 3. The ring connected to two leads and threatened by a flux θ. The two arms have lengths l_a and l_b. The parameters w_1 and w_2 allow us to tune the coupling of the ring.

We now consider the graph when it is coupled to two leads with coupling parameters w_1 and w_2 (see figure 3). The Friedel phase $e^{i\delta^f} = \det(W^2 - M)/\det(W^2 + M)$ is

$$e^{i\delta^f} = \frac{2(\cos\theta - \cos kl) + w_1^2 w_2^2 \sin kl_a \sin kl_b - i(w_1^2 + w_2^2)\sin kl}{2(\cos\theta - \cos kl) + w_1^2 w_2^2 \sin kl_a \sin kl_b + i(w_1^2 + w_2^2)\sin kl} \tag{33}$$

($\det(W^2 + M)$ was calculated in [1]). If $\theta \neq 0$ the spectrum is non-degenerate and δ^f counts the states correctly. Now we focus on the degenerate case $\theta = 0$ for which we have

$$\tan(\delta^f/2) = -\frac{(w_1^2 + w_2^2)\sin kl}{4\sin^2(kl/2) + w_1^2 w_2^2 \sin kl_a \sin kl_b}. \tag{34}$$

Each interval of width $\Delta k = 2\pi/l$ contains two states of the ring. Let us now examine under what condition (34) counts these states correctly. We can identify the position of the resonances with the value of k for which the denominator of (34) vanishes[5]. Then we distinguish two different cases:

- l_a/l is an irrational number. Then the denominator of (34) vanishes twice per interval $k \in [2m\pi/l; 2(m+1)\pi/l[$, which means that δ^f counts the correct number of states.
- l_a/l is a rational number: $l_a/l = \frac{p}{2q}$ with $(p, q) \in \mathbb{N}^2$. If $(q - p)(m + 1)$ is an integer multiple of q, the denominator vanishes only once in $[2m\pi/l; 2(m+1)\pi/l[$. The intervals for which $(q - p)(m + 1)$ is an integer multiple of q are those in which one of the two degenerate wavefunctions φ^+_{m+1} and φ^-_{m+1} vanishes on the vertices where the leads are plugged in.

4.4. The ring connected with one lead. Why cannot the lhs of (27) always be identified with the DoS?

We have given a general argument to explain how the degeneracies of the spectrum lead to a failure of the FSR; however, it is surprising that the quantity in the left-hand side of (27) cannot always be identified with the DoS of the graph since the sum runs over the complete

[5] The denominator is of the form

$$f_a(x) = \sin^2(x/2) + b\sin(ax)\sin((1-a)x) = (1+b)\sin^2(x/2) - b\sin^2((1/2-a)x), \tag{35}$$

with $a \in]0; 1/2[$ and $b \in]0; +\infty[$. We are interested in the number of zeros of $f_a(x)$ in the interval $[2m\pi; 2(m+1)\pi[$. We distinguish two cases:

- a is not a rational number ($a \notin \mathbb{Q}$). Since $f_a(2m\pi) < 0\ \forall m \in \mathbb{N}$ and the amplitude of the first positive term in the rhs of (35) is larger than the second, it follows that $f_a(x) = 0$ has exactly two solutions in $[2m\pi; 2(m+1)\pi[$.
- $a \in \mathbb{Q}$: we write $a = p/2q$ where $(p, q) \in \mathbb{N}^2$ with $p < q$. We have $f_a(2m\pi) = -b\sin^2((q-p)m\pi/q) \leqslant 0$. If $(q - p)(m + 1)$ is not an integer multiple of q the interval $[2m\pi; 2(m + 1)\pi[$ contains two solutions of $f_a(x) = 0$.
  If $(q - p)(m + 1) = rq$ with $r \in \mathbb{N}$ the interval contains only one solution of $f_a(x) = 0$.

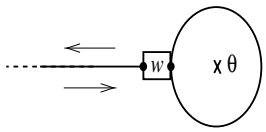

Figure 4. The ring connected to one lead.

set of L stationary scattering states of energy E. This point needs clarification, that we shall give now by studying again the case of the ring.

We consider the ring of figure 4 coupled to a lead and construct the stationary scattering states (47), (50). The wavefunction on the lead is

$$\tilde{\psi}_E^{\rm lead}(x) = \frac{1}{\sqrt{4\pi k}}(\mathrm{e}^{-\mathrm{i}kx} + \mathrm{e}^{\mathrm{i}kx+\mathrm{i}\delta}), \tag{36}$$

where the phase shift δ is [1]

$$\mathrm{cotg}\,(\delta/2) = \frac{w^2 \sin kl}{2(\cos\theta - \cos kl)}. \tag{37}$$

On the ring (arc a) the wavefunction reads

$$\psi_{(a)}(x) = \psi_1 \frac{\mathrm{e}^{\mathrm{i}\theta x/l}}{\sin kl}(\sin k(l-x) + \mathrm{e}^{-\mathrm{i}\theta}\sin kx) \tag{38}$$

where

$$\psi_1 = \frac{1}{\sqrt{\pi k}}\,\frac{w\sin kl}{w^2\sin kl + 2\mathrm{i}(\cos kl - \cos\theta)} = \frac{1}{w}\tilde{\psi}_E^{\rm lead}(0) \tag{39}$$

is the wavefunction at the node.

- $\theta \neq 0$. We study the limit $w \to 0$ of small coupling for which we expect to recover some features of the isolated ring. In this case $|\psi_1|$ presents sharp peaks at the positions of the energies of the isolated ring (given by $k_n^{\pm} l = \pm\theta + 2n\pi$). These resonance contributions will eventually give the main contributions to (27). Let us express the wavefunction in the ring for k in the neighbourhood of a resonance. Expressions (38) and (39) give

$$\psi_{(a)}(x) \underset{k\sim k_n^{\pm}}{\simeq} \frac{1}{\sqrt{\pi k}}\,\frac{\mathrm{i}w/2l}{k - k_n^{\pm} + \mathrm{i}w^2/2l}\,\mathrm{e}^{\mp 2\mathrm{i}\pi n x/l}. \tag{40}$$

  Up to a normalization, we recover the wavefunctions of the isolated ring recalled in the previous subsection. By integration in the ring we obtain

$$\int_0^l \mathrm{d}x\,|\psi_{(a)}(x)|^2 \underset{k\sim k_n^{\pm}}{\simeq} \frac{1}{2k}\,\frac{1}{\pi}\,\frac{w^2/2l}{(k-k_n^{\pm})^2 + (w^2/2l)^2} \underset{w\to 0}{\longrightarrow} \frac{1}{2k}\delta(k-k_n^{\pm}) = \delta(E - [k_n^{\pm}]^2), \tag{41}$$

  which is the correct DoS of the isolated ring.
- $\theta = 0$. If we now consider the degenerate case of zero flux, the resonance peaks are in $k_n = 2n\pi/l$. The wavefunction in the ring near the resonance is

$$\psi_{(a)}(x) \underset{k\sim k_n}{\simeq} \frac{1}{\sqrt{\pi k}}\,\frac{\mathrm{i}w/l}{k - k_n + \mathrm{i}w^2/l}\cos(2n\pi x/l). \tag{42}$$

  In this case the scattering state only reproduces the symmetric wavefunction $\varphi_n^+(x)$ of the isolated ring. It is now clear that the integration cannot give the DoS of the isolated ring: indeed,

$$\int_0^l \mathrm{d}x\,|\psi_{(a)}(x)|^2 \underset{k\sim k_n}{\simeq} \frac{1}{2k}\,\frac{1}{\pi}\,\frac{w^2/l}{(k-k_n)^2 + (w^2/l)^2} \underset{w\to 0}{\longrightarrow} \frac{1}{2k}\delta(k-k_n) \tag{43}$$

  misses the degeneracy 2 of the eigenstates.

In the cases studied above the stationary scattering states, computed in the limit of a graph weakly coupled to the leads ($w_\alpha \to 0$), do not reproduce all the wavefunctions of the isolated graph and the *lhs of the formula (27) cannot be identified with the DoS of the graph*. In this sense the scattering states do not form a complete basis to describe the Hilbert space of the graph.

5. Remark on free graphs connected to one lead

Note that for a free graph, i.e. with no potential and no magnetic flux, perfectly connected ($w = 1$) to only one lead, we can prove with (31) that

$$\delta^f(k^2) \underset{k\to 0}{\simeq} 2k\mathcal{L} \tag{44}$$

where $\mathcal{L} = \frac{1}{2}\sum_{\alpha,\beta} a_{\alpha\beta} l_{\alpha\beta}$ is the total length of the graph. The proof is obtained by analysing the behaviours of the two spectral determinants at small energy [7]. If the FSR fails, the total length $\mathcal{L}$ of the free graph is not encoded in the Weyl part of $\delta^f(k^2)$; however, $\mathcal{L}$ appears in the low-energy behaviour of the phase shift. For example if we consider the complete graph (figure 1), we have shown that $\delta^f_{\text{Weyl}} = 3k\ell$ and we can check on (30) that the low-energy behaviour ($k \to 0$) is $\delta^f \simeq V(V-1)k\ell = 2k\mathcal{L}$.

6. Discussion

We have shown that the well known FSR, a state counting method from the scattering properties, may be violated for certain graphs having degenerate spectra. This has been demonstrated already at the level of the Weyl term of the DoS: we have studied several examples where a discrepancy occurs between the Weyl term of the Dos of the isolated graph and the Weyl part of the derivative of the Friedel phase $(1/2\pi)\mathrm{d}\delta^f/\mathrm{d}E = (1/2\mathrm{i}\pi)\,\mathrm{tr}(\Sigma^\dagger \mathrm{d}\Sigma/\mathrm{d}E)$.

A way to understand the origin of the failure of the FSR is to compare the quantities involved in the DoS and in the Friedel phase. The DoS of an isolated graph can be obtained from the spectral determinant $S(\gamma) = \prod_n (\gamma + E_n)$ by making the substitution $\gamma \to -E - \mathrm{i}0^+$. The spectral determinant is proportional to the determinant of the matrix M introduced above: $S(\gamma) \propto \det M(\gamma)$ [6,7,10,12,34,35]. Adding a small imaginary part to the spectral parameter γ produces a resonance structure in $\partial_\gamma \ln S(\gamma)$, each peak having a weight equal to the degeneracy of the state. If we now consider the Friedel phase we note that the widths of the resonances are obtained by adding to the anti-Hermitian matrix $M(-E)$ a Hermitian matrix $W^{\mathrm{T}}W$: the Friedel phase involves $\det(M(-E) + W^{\mathrm{T}}W)$. Comparing this latter determinant with the determinant $\det M(-E - \mathrm{i}0^+)$ involved in the DoS, it is not surprising that the Friedel phase does not produce the correct spectral weights since the ways the energies (zero of determinant) acquire an imaginary part is different in the two cases.

Another way to understand the failure of the FSR for graphs is the following. For a problem invariant under rotations in a d-dimensional space, the essence of the FSR is to count the number of nodes of the wavefunction in the angular channel crossing a $(d-1)$-dimensional sphere at infinity when the energy is varied. The number of states coincides with the number of nodes, that is with the number of jumps of π of the phase shift $\eta_l(E)$ of the partial wave of orbital momentum l. On the other hand, a graph is connected to the exterior only through leads plugged in at vertices. In a sense the Friedel phase counts the number of nodes of the wavefunction $\psi_k(x)$ that reach those vertices by varying k. The failure of the FSR is caused when several nodes of $\psi_k(x)$ reach at the same energy the same vertex from different bonds

issuing from this vertex (we can easily convince ourselves of this remark by considering the ring connected to one lead studied above).

We can also provide a clear picture of the problem within the arc formulation introduced in [1] and recalled in section 1. In the arc formulation, the wavefunction is described by a set of amplitudes. Each arc i is associated with a couple A_i, B_i. We gather the internal amplitudes in a vector $A^{\rm int}$, the external amplitudes in a vector $A^{\rm ext}$ and all amplitudes in a vector A. The internal amplitudes of the graph are related through the bond scattering matrix: $A^{\rm int} = R\,B^{\rm int}$. All amplitudes are also related to each other by the vertex scattering matrix: $B = Q\,A$. If we eliminate $B^{\rm int}$ we obtain

$$\tilde{Q}^{\rm T}\,A^{\rm ext} = (R^\dagger - Q^{\rm int})\,A^{\rm int} \tag{45}$$

$$B^{\rm ext} = \tilde{Q}\,A^{\rm int} + Q^{\rm ext}\,A^{\rm ext}. \tag{46}$$

In general $\det(R^\dagger - Q^{\rm int}) \neq 0$ whatever k is and at all energies of the continuous spectrum, the stationary scattering states are the only solutions of the Schrödinger equation on the graph. However, for certain graphs (in particular for those examined above), there exists a discrete set of energies in the continuous spectrum for which $\det(R^\dagger - Q^{\rm int}) = 0$. This means that in addition to the scattering states we can construct at these particular energies solutions such that $A^{\rm ext} = B^{\rm ext} = 0$ while the internal amplitudes satisfy $(R^\dagger - Q^{\rm int})A^{\rm int} = 0$ and $\tilde{Q}A^{\rm int} = 0$. These two last equations describe a solution localized in the graph and that does not communicate with the leads. The stationary scattering states give the solutions of the Schrödinger equation for the continuous spectrum apart for a discrete set of energies where some additional states are localized in the graph and thus are not probed by scattering, leading to the failure of the state counting method from the scattering.

The study of the various examples of section 4 leads us to make the following conjecture for the ability of δ^f to count the states (at least at the level of the Weyl term): if there are degenerate energies of degeneracies d_n, the Friedel phase δ^f counts correctly the states of the system if $L \geqslant d_n$ leads are plugged in at vertices in such a way that the wavefunction cannot vanish at the positions of all these vertices at the same time.

Acknowledgments

I am grateful to Alain Comtet, Jean Desbois and Gilles Montambaux for many stimulating discussions. I also acknowledge Markus Büttiker for interesting remarks.

Appendix A. The stationary scattering states

In this appendix we recall briefly how the stationary scattering states are constructed [1]. We consider the stationary scattering state $\psi^{(\alpha)}(x)$ of energy $E = k^2$ which describes a plane wave entering the graph from the lead connected at vertex α and being scattered by the graph into all leads. On the lead connected to vertex μ, the wavefunction is

$$\psi^{(\alpha)}_{\text{lead }\mu}(x) = \delta_{\mu\alpha}\mathrm{e}^{-\mathrm{i}kx} + \Sigma_{\mu\alpha}\mathrm{e}^{\mathrm{i}kx}, \tag{47}$$

where $x \in [0;+\infty[$. The wavefunction on the internal bond $(\mu\beta)$ of the graph is related to the two linearly independent solutions $f_{\mu\beta}(x_{\mu\beta})$ and $f_{\beta\mu}(x_{\mu\beta})$ of the differential equation

$$(-\mathrm{d}^2_{x_{\mu\beta}} + V_{(\mu\beta)}(x_{\mu\beta}) - k^2)\,f(x_{\mu\beta}) = 0 \tag{48}$$

for $x \in [0; l_{\mu\beta}]$. The two solutions $f_{\mu\beta}$ and $f_{\beta\mu}$ satisfy the following boundary conditions at the edges of the interval:

$$\begin{matrix} f_{\mu\beta}(\mu) = 1 \\ f_{\mu\beta}(\beta) = 0 \end{matrix} \quad \text{and} \quad \begin{matrix} f_{\beta\mu}(\mu) = 0 \\ f_{\beta\mu}(\beta) = 1 \end{matrix} \tag{49}$$

where $f(\mu) \equiv f(x_{\mu\beta} = 0)$ and $f(\beta) \equiv f(x_{\mu\beta} = l_{\mu\beta})$. The stationary scattering state on the bond $(\mu\beta)$ is

$$\psi^{(\alpha)}_{(\mu\beta)}(x_{\mu\beta}) = \psi^{(\alpha)}_{\mu}\, f_{\mu\beta}(x_{\mu\beta}) + \psi^{(\alpha)}_{\beta}\, f_{\beta\mu}(x_{\mu\beta}) \tag{50}$$

which already satisfies the continuity condition (2). The relation between the functions $f_{\mu\beta}$ and $f_{\beta\mu}$ and the reflection and transmission coefficients characterizing the potential on the bond is established by computing the derivatives of $f_{\mu\beta}$ and $f_{\beta\mu}$ at the boundaries of the interval. Imposing the 'current conservation' (3) then leads to the expressions (11)–(13), that permit a systematic construction of the scattering matrix [1].

Appendix B. Friedel sum rule and Smith relation in one dimension

The one-dimensional case can be considered as a graph with one bond and two vertices and can therefore be described with the formalism presented in [1] and this paper. The FSR (16) has been demonstrated in general terms in [15]; however, it is interesting to give a rapid demonstration that follows the lines of the original one in three dimensions [14,16,20,21]. Note also that it has been demonstrated in [36] that the Friedel phase in a one-dimensional situation is related to the phase of the transmission amplitude (see also [30]). We consider the one-dimensional Hamiltonian $-\mathrm{d}_x^2 + V(x)$ with $x \in \mathbb{R}$ with a potential $V(x)$ being concentrated in some region of the space. We start by describing several possible bases of eigenstates characterizing the scattering problem.

- The stationary scattering states of energy $E = k^2$ related to the scattering matrix

$$\tilde{\Sigma} = \begin{pmatrix} \tilde{r} & \tilde{t}' \\ \tilde{t} & \tilde{r}' \end{pmatrix} \tag{51}$$

  are the state $\varphi^{(L)}(x)$ associated with a plane wave coming from the left and $\varphi^{(R)}(x)$ for an incoming wave from the right. The asymptotic behaviours of the left stationary scattering state are $\varphi^{(L)}(x) = \mathrm{e}^{\mathrm{i}kx} + \tilde{r}\,\mathrm{e}^{-\mathrm{i}kx}$ for $x \to -\infty$ and $\varphi^{(L)}(x) = \tilde{t}\,\mathrm{e}^{\mathrm{i}kx}$ for $x \to +\infty$. The state $\varphi^{(R)}(x)$ involves similarly the coefficients $\tilde{r}'$ and $\tilde{t}'$. Note that these states can be introduced even if the potential is not concentrated in a finite interval provided that it decreases sufficiently rapidly at infinity.
- If the potential has a support $[x_1; x_2]$ we introduce the stationary scattering states $\psi^{(L)}(x)$ and $\psi^{(R)}(x)$ related to the scattering matrix Σ: the left stationary scattering state behaves like $\psi^{(L)}(x) = \mathrm{e}^{\mathrm{i}k(x-x_1)} + r\,\mathrm{e}^{-\mathrm{i}k(x-x_1)}$ for $x \leqslant x_1$ and $\psi^{(L)}(x) = t\,\mathrm{e}^{\mathrm{i}k(x-x_2)}$ for $x \geqslant x_2$. A similar expression for $\psi^{(R)}(x)$ involves the coefficient r' and t': $\psi^{(R)}(x) = t'\mathrm{e}^{-\mathrm{i}k(x-x_1)}$ for $x \leqslant x_1$ and $\psi^{(R)}(x) = \mathrm{e}^{-\mathrm{i}k(x-x_2)} + r'\,\mathrm{e}^{\mathrm{i}k(x-x_2)}$ for $x \geqslant x_2$. The reflections and transmissions defined in this way are naturally involved in transfer matrices, which makes for part of the interest of this definition.
  Comparing the two sets of eigenstates it is clear that $\varphi^{(L)}(x) = \mathrm{e}^{\mathrm{i}kx_1}\psi^{(L)}(x)$ and $\varphi^{(R)}(x) = \mathrm{e}^{-\mathrm{i}kx_2}\psi^{(R)}(x)$. The relations between the coefficients of the two scattering matrices $\tilde{\Sigma}$ and Σ are then $r = \tilde{r}\,\mathrm{e}^{-2\mathrm{i}kx_1}$, $r' = \tilde{r}'\,\mathrm{e}^{2\mathrm{i}kx_2}$, $t = \tilde{t}\,\mathrm{e}^{\mathrm{i}k(x_2-x_1)}$ and $t' = \tilde{t}'\,\mathrm{e}^{\mathrm{i}k(x_2-x_1)}$. The relation between matrices reads $\Sigma = \mathcal{U}\tilde{\Sigma}\mathcal{U}$ with $\mathcal{U} = \mathrm{diag}(\mathrm{e}^{-\mathrm{i}kx_1}, \mathrm{e}^{\mathrm{i}kx_2})$.
- To derive the FSR we introduce the two eigenstates of energy $E = k^2$ labelled by the index $\sigma = 1, 2$:

$$\Psi_\sigma(x) = [a_{\sigma,+}\,\theta(x) + a_{\sigma,-}\,\theta(-x)]\,\sin(k|x| + \eta_\sigma(k^2) + \pi/2) \qquad \text{for } |x| \to \infty, \tag{52}$$

  where $\theta(x)$ is the Heaviside function. If the potential is symmetric the two amplitudes $a_{\sigma,+}$ and $a_{\sigma,-}$ are equal in modulus and $\sigma = 1, 2$ labels the symmetric and antisymmetric states. Let us establish the relation with the 2×2 scattering matrix $\tilde{\Sigma}$. We look for

the relation between this basis of eigenstates and the first basis introduced above: let us write $\Psi_\sigma(x) = \varphi^{(R)}(x) + C\,\varphi^{(L)}(x)$. Comparing their behaviours at $x \to +\infty$ we obtain $\tilde{r}' + C\,\tilde{t} = \mathrm{e}^{2\mathrm{i}\eta_\sigma}$ and at $x \to -\infty$: $\tilde{t}' + C\,\tilde{r} = C\,\mathrm{e}^{2\mathrm{i}\eta_\sigma}$. These two equations show that $\mathrm{e}^{4\mathrm{i}\eta_\sigma} - (\tilde{r} + \tilde{r}')\mathrm{e}^{2\mathrm{i}\eta_\sigma} - \tilde{t}\tilde{t}' + \tilde{r}\tilde{r}' = 0$. In other terms,

$$\det(\tilde{\Sigma} - \mathrm{e}^{2\mathrm{i}\eta_\sigma}) = 0. \tag{53}$$

Therefore $\mathrm{e}^{2\mathrm{i}\eta_1}$ and $\mathrm{e}^{2\mathrm{i}\eta_2}$ are the two eigenvalues of the scattering matrix $\tilde{\Sigma}$. To finish the proof of the FSR we consider that the system is in a large interval $[-R; +R]$ and impose Dirichlet boundary conditions. The quantification condition for $\Psi_\sigma(x)$ reads $k_n R + \eta_\sigma(k_n^2) + \pi/2 = n\pi$. We introduce $\delta k_n = k_{n+1} - k_n$, therefore in the limit $R \to \infty$

$$\frac{1}{\delta k_n} \simeq \frac{R}{\pi} + \frac{1}{\pi}\frac{\mathrm{d}\eta_\sigma(k_n^2)}{\mathrm{d}k_n} \tag{54}$$

which is the density of modes in the channel σ. The term R/π is the density of modes in the absence of the potential: $1/\delta k_n^{(0)}$. In the limit $R \to \infty$ the difference of densities of modes $1/\delta k_n - 1/\delta k_n^{(0)}$ remains finite. It follows that

$$\int_{-\infty}^{+\infty} \mathrm{d}x\,[\rho(x; E) - \rho_0(x; E)] = \frac{1}{\pi}\sum_{\sigma=1,2}\frac{\mathrm{d}\eta_\sigma(E)}{\mathrm{d}E} \tag{55}$$

where $\rho(x; E) = \langle x\,|\delta(E - H)|\,x\,\rangle$ is the LDoS and $\rho_0(x; E)$ the LDoS in the absence of the potential. Due to (53) this equation can be rewritten $\int_{-\infty}^{+\infty}\mathrm{d}x\,[\rho(x; E) - \rho_0(x; E)] = (1/2\mathrm{i}\pi)\,\mathrm{Tr}\{\tilde{\Sigma}^\dagger \mathrm{d}\tilde{\Sigma}/\mathrm{d}E\}$.

Next we would like to apply both the FSR and the Smith formula to a simple example. We now consider a potential with support $[0; \mathcal{L}]$ that vanishes elsewhere, a situation where it is meaningful to introduce Σ (instead of $\tilde{\Sigma}$).

(i) The Smith formula (27) gives the DoS of the interval $[0; \mathcal{L}]$

$$\begin{aligned}\int_0^{\mathcal{L}} \mathrm{d}x\,\rho(x; E) &= \int_0^{\mathcal{L}} \mathrm{d}x\,(|\tilde{\psi}_E^{(L)}(x)|^2 + |\tilde{\psi}_E^{(R)}(x)|^2) \\ &= \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\,\mathrm{Tr}\{\Sigma - \Sigma^\dagger\}\right).\end{aligned} \tag{56}$$

The two terms correspond to left (L) and right (R) stationary scattering states, which form a complete basis of eigenstates in one dimension. Note that this relation has also been given in [28] for the one-dimensional case.

(ii) On the other hand the FSR

$$\int_{-\infty}^{+\infty} \mathrm{d}x\,[\rho(x; E) - \rho_0(x; E)] = \frac{1}{2\mathrm{i}\pi}\left(\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} - \frac{\mathrm{i}\,\mathcal{L}}{\sqrt{E}}\right) = \frac{1}{2\mathrm{i}\pi}\,\mathrm{Tr}\left\{\tilde{\Sigma}^\dagger\frac{\mathrm{d}\tilde{\Sigma}}{\mathrm{d}E}\right\} \tag{57}$$

measures the variation of the DoS of the infinite line due to the presence of the potential in the interval $[0; \mathcal{L}]$. In particular (57) is sensitive to the effect of the potential on the wavefunction at infinity whereas (56) is a local quantity.

As an illustration, let us consider the extremely simple case of a potential $\lambda\delta(x)$ on a line. The corresponding graph is a vertex ($V = 1$, $B = 0$ and $L = 2$). Formulae (6)–(8) give the scattering matrix

$$\Sigma = \frac{2}{2 + \mathrm{i}\lambda/k}\begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} - 1. \tag{58}$$

It is easy to check that (56) therefore vanishes

$$\mathrm{Tr}\left\{\Sigma^\dagger\frac{\mathrm{d}\Sigma}{\mathrm{d}E}\right\} + \frac{1}{4E}\,\mathrm{Tr}\{\Sigma - \Sigma^\dagger\} = 0, \tag{59}$$

which is not surprising since the 'graph' is only a point (the support of the potential is an interval of measure 0). On the other hand the variation of the DoS of the infinite line can be computed either with the exact Green function, known for this potential, or with (57). The Green function gives

$$\int_{-\infty}^{+\infty} \mathrm{d}x\,[\rho(x;E)-\rho_0(x;E)] = \theta(-\lambda)\delta(E+\lambda^2/4) - \frac{1}{2}\delta(E) + \theta(E)\frac{\lambda}{4\pi\sqrt{E}}\frac{1}{E+\lambda^2/4}, \tag{60}$$

where $\theta(E)$ is the Heaviside function. The first term is the contribution of the bound state (that exists if $\lambda < 0$). We can check that the total number of states is conserved: $\int_{-\infty}^{+\infty}\mathrm{d}E\int_{-\infty}^{+\infty}\mathrm{d}x\,[\rho(x;E)-\rho_0(x;E)] = 0$. The Friedel phase, obtained from the above scattering matrix, is $\delta^f(E) = -\mathrm{i}\ln\det\Sigma = 2\arctan(2k/\lambda)$ and we can therefore recover the expression (60) using the FSR (57).

Appendix C. The spectrum of the complete graph K_V

We give here the spectrum of the complete graph, which is made of V vertices all connected to each other with bonds of the same length ℓ. The spectrum is easily extracted from the spectral determinant $S(-k^2) = \prod_{m=0}^{\infty}(E_m - k^2)$, which has been computed in [7]:

$$S(-k^2) \propto \left(\frac{\sin k\ell}{k}\right)^{\frac{V(V-3)}{2}} \sin^2(k\ell/2)\,(\cos k\ell + \cos\varphi)^{V-1} \tag{61}$$

up to some inessential numerical factor. The parameters λ_α that characterize the boundary condition (3) are put to zero here. We have introduced $\cos\varphi = 1/(V-1)$. The energies E_m and the corresponding degeneracies d_m are given in the following table:

$k_m = \sqrt{E_m}$	d_m
$k_0 = 0$	1
$k_1 = \dfrac{\pi-\varphi}{\ell}$	$V-1$
$k_2 = \dfrac{\pi}{\ell}$	$\dfrac{V(V-3)}{2}$
$k_3 = \dfrac{\pi+\varphi}{\ell}$	$V-1$
$k_4 = \dfrac{2\pi}{\ell}$	$2+\dfrac{V(V-3)}{2}$
$\vdots$	$\vdots$

It is obvious from the expression of the spectral determinant that the spectrum is periodic in k of period $2\pi/\ell$, that is $k_{m+4} = k_m + 2\pi/\ell$ and $d_{m+4} = d_m$ (for $m > 0$).

We next consider the corresponding eigenfunctions. The eigenfunction on the bond $(\alpha\beta)$ is given by (50)

$$\psi_{(\alpha\beta)}(x) = \frac{1}{\sin k l_{\alpha\beta}}(\psi_\alpha \sin k(l_{\alpha\beta}-x) + \psi_\beta \sin kx). \tag{62}$$

Imposing the conditions (3) leads to the V equations

$$\sum_\beta M_{\alpha\beta}\psi_\beta = 0. \tag{63}$$

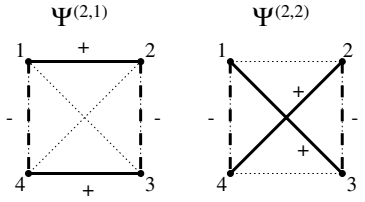

Figure C1. The two eigenstates of K_4 of energy $k = k_2$. The dotted lines are the bonds and the large dots the vertices (labelled 1, 2, 3 and 4). The thick continuous lines are put where the wavefunction is positive and the thick dashed lines where it is negative. On the other bonds the wavefunction vanishes.

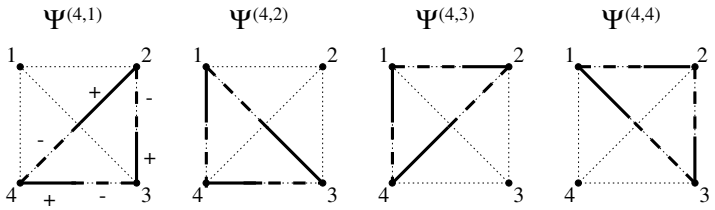

Figure C2. The four eigenstates of energy $k = k_4$.

For a free graph M is given by (14) [2]. For the complete graph we have

$$M_{\alpha\beta}(-k^2) = \frac{\mathrm{i}}{\sin k\ell}(\delta_{\alpha\beta}(V-1)\cos k\ell - a_{\alpha\beta}) \tag{64}$$

where the adjacency matrix is $a_{\alpha\beta} = 1 - \delta_{\alpha\beta}$.

- *Zero mode*. The wavefunction is constant on the graph $\psi^{(0)}(x) = 1/\sqrt{\mathcal{L}}$ where $\mathcal{L} = [V(V-1)/2]\ell$ is the total length of the graph.
- $k = k_1$. All the matrix elements of M are equal: $M_{\alpha\beta} = -I/\sin\varphi$. The equation (63) has $V-1$ solutions labelled by $j = 1, 2, \ldots, V-1$. A possible basis is $\psi_\alpha^{(1,j)} = \delta_{\alpha,1} - \delta_{\alpha,j+1}$, up to a normalization (this basis is not orthogonal).
- $k = k_2$. At this energy the matrix M is divergent and equation (63) cannot give the eigenstates. They are obtained by considering the equation $(1 - RQ)A = 0$, where R and Q are the matrices given by (5)–(8). A is the vector gathering the $2B$ amplitudes of the wavefunction (one for each arc) [1,7]. The system $(1 - RQ)A = 0$ has $V(V-3)/2$ solutions at $k = k_2$. To obtain an idea of the structure of the solution let us consider K_4. We label the nodes by 1, 2, 3 and 4, and we bring together the six components on the six bonds in a vector $\Psi(x) = (\psi_{(12)}(x), \psi_{(13)}(x), \psi_{(14)}(x), \psi_{(23)}(x), \psi_{(24)}(x), \psi_{(34)}(x))$. We have for the first state, labelled (2, 1), $\Psi^{(2,1)} = (1, 0, -1, -1, 0, 1) \times \sin(\pi x/\ell)$, and for the second eigenstate $\Psi^{(2,2)} = (0, 1, -1, -1, 1, 0) \times \sin(\pi x/\ell)$ (see figure C1).
- $k = k_3$. The matrix M is the opposite to that computed at $k = k_1$ and the wavefunctions on the nodes have the same value as for this latter energy.
- $k = k_4$. The same problem occurs as for $k = k_2$. The system $(1 - RQ)A = 0$ has $V(V-3)/2 + 2$ solutions corresponding to wavefunctions vanishing at all the nodes. Again we consider the graph K_4 and give the four degenerate states: $\Psi^{(4,1)} = (0, 0, 0, -1, 1, -1) \times \sin(2\pi x/\ell)$, $\Psi^{(4,2)} = (0, -1, 1, 0, 0, -1) \times \sin(2\pi x/\ell)$, $\Psi^{(4,3)} = (-1, 0, 1, 0, -1, 0) \times \sin(2\pi x/\ell)$ and $\Psi^{(4,4)} = (-1, 1, 0, -1, 0, 0) \times \sin(2\pi x/\ell)$ (see figure C2).

- $k = k_{m>4}$. The spectrum is periodic in k with period $2\pi/\ell$. Then the value of the wavefunctions at the nodes is the same at k_m and k_{m+4}; only the number of oscillations on the bonds changes.

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