LECTURE 8

Trace formula I: a proof

This chapter is devoted to the trace formula connecting the spectrum of a finite compact metric graph with the set of closed paths on it. In other words this formula establishes a relation between spectral and geometric/topologic properties of metric graphs.

Such a formula was first proved for the Laplacian Δ defined on a Riemannian manifold X [?CdV72, ?Cha74, ?DuGu75, ?GuMe79] and is known now as Chazarain-Duistermaat-Guillemin-Melrose trace formula

$$\sum_{\lambda_j \in \mathrm{Spec}\,\Delta} \cos \lambda_j^{1/2} t = \sum_{\gamma} \frac{\ell(\mathrm{prim}(\gamma))}{|I - P_\gamma|^{1/2}} \delta(t - \ell(\gamma)) + R, \quad t > 0. \tag{8.1}$$

The sum on the left hand side is taken over all eigenvalues of the Laplacian Δ, the sum on the right hand side – over all closed geodesics on the manifold X. $\ell(\gamma)$ denotes the length of the geodesic γ and $\mathrm{prim}(\gamma)$ – the length of the primitive geodesic. P_γ is the Poincaré map around γ. The remainder term R is a certain (non-specified) function in $L_{1,\mathrm{loc}}$, which means that this formula holds modulo $L_{1,\mathrm{loc}}$-function. Formula (8.1) can be seen as a generalisation of the classical Poisson summation formula in Fourier analysis (see (7.12) below) as well as Selberg's trace formula.

We are going to prove a direct analog of formula (8.1) for the case of metric graphs. For simplicity we consider first the standard Laplacian, which is uniquely determined by the metric graph Γ. In contrast to (8.1) the formula we are going to prove is exact and does not contain any reminder term. This formula first appeared in a paper by J.-P. Roth [?Ro], but we follow scattering matrix approach suggested in [?KoSm0, ?KoSm, ?GuSm] and developed further in [?KuNo]. This formula will be used to prove that the spectrum of a quantum graph determines its Euler characteristic. Despite the fact that that the original formula is proven for standard Laplacians, it can be generalised to the case of standard Schrödinger operators.

8.1. The trace formula for standard Laplacians

We prove now the trace formula relating the spectrum of the standard Laplacian to the set of oriented closed paths on the graph. We consider only those paths γ which do not turn back in the interior of any edge, but which may turn back at the vertices.

DEFINITION 8.1. *Let $\{y_j\}_{j=1}^{2d}$ be a finite sequence of edge end points on a finite compact metric graph Γ*

$$y_1, y_2, y_3, \dots, y_{2d}, \quad y_j \in \mathbf{V} = \{x_i\}_{i=1}^{2N},$$

such that

- *y_{2j-1} and y_{2j} are end points of a certain edge, $j = 1, 2, \ldots, d$,*
- *y_{2j} and y_{2j+1} belong to a certain vertex, $j = 1, 2, \ldots, d$,*

where we used natural cyclic identification $y_{2d+1} = y_1$. Then the **oriented closed path** $\gamma = (y_1, y_2, y_3, \ldots, y_{2d})$ *is a union of edges*

$$\gamma = [y_1, y_2] \cup [y_3, y_4] \cup \ldots [y_{2d-1}, y_{2d}]$$

with end points y_{2j} and y_{2j+1} identified and inherited orientation. The paths obtained from each other by cyclically permuting the end points $y_j(\gamma)$ are identified.

Each pair (y_{2j-1}, y_{2j}) determines not only the edge the path traverses but also the direction of the path on it. The pairs (y_{2j}, y_{2j+1}) determine the vertices and their order on the path. Every closed path can be equivalently defined by the sequence of edges indicating path's direction on each edge.

Topologically every closed path γ is a cycle which can be continuously imbedded in Γ locally preserving the distances. Certain edges may appear in γ multiple times. Consider the graph Γ^γ obtained from Γ by substituting each edge E_n with as many parallel edges identical to E_n as it appears in γ. If γ does not pass along a certain edge, then this edge is missing in Γ^*. Therefore the path γ can be obtained by cutting Γ^γ through the vertices. In other words γ can be seen as an Eulerian path on Γ^γ, *i.e.* a closed path visiting each edge precisely once.

If the graph has no loops and parallel edges, then every oriented closed path is uniquely determined by the sequence of edges this path goes along. In this case the order of the edges determines the direction in which the path crosses every edge. Alternatively every oriented path is determined by the sequence of vertices in this case.

The **discrete length** $d = d(\gamma)$ counts how many times the path γ comes across an edge, so that contribution from every edge in Γ is equal to its multiplicity in γ (independently of the direction). The discrete length should not be mixed up with the **geometric length** $\ell = \ell(\gamma)$ obtained by summing the lengths of the edges respecting their multiplicities in γ

$$\ell(\gamma) = \sum_{j=1}^{d(\gamma)} \big(y_{2j} - y_{2j-1}\big). \tag{8.2}$$

The paths having opposite orientations are distinguished, then the path going along the same edges as γ in the opposite direction and order can be seen as its inverse.

For any edge the path γ going back and forth along it coincides with its inverse. Moreover, for any even $d = 2j$, $j \in \mathbb{N}$, there exists a unique oriented path supported only by the edge and having discrete length d. It is a multiple of the primitive path going once back and forth.

For a loop the two paths going in opposite directions are distinguished. For example among the paths supported by the loop there are 3 paths of discrete length $d = 2$:

- going twice in the positive direction;
- going twice in the negative direction;
- going once in each direction.

Note that the later path coincides with its inverse and is primitive.

By the **primitive path** of γ, prim (γ), we denote the shortest closed path, such that the path γ can be obtained by repeating the path prim (γ) several times. For example every path supported by an edge E_0 is a multiple of the primitive path going back and forth E_0 just once.

The set $\mathscr{P}$ of all closed paths is infinite, but countable.

Assume that the set of edges is fixed, then the flower graph has the largest set of closed paths since any sequence of edges with arbitrary directions is allowed. Otherwise topology of the graph provides certain restrictions on the sequence.

We are ready to formulate the main result of this chapter.

THEOREM 8.2 (Trace formula). *Let Γ be a finite compact metric graph with Euler characteristic χ and the total length $\mathscr{L}$, and let $L^{\rm st}(\Gamma)$ be the corresponding standard Laplacian. Then the spectral measure*

$$\mu := 2\delta + \sum_{k_n \neq 0} \left(\delta_{k_n} + \delta_{-k_n} \right) \tag{8.3}$$

is a positive distribution.

The following two exact trace formulae establish the relation between the spectrum $\{k_n^2\}$ of $L^{\rm st}(\Gamma)$ and the set $\mathscr{P}$ of closed paths on the metric graph Γ

$$\begin{aligned} \mu(k) &= 2\delta(k) + \sum_{k_n \neq 0} \left(\delta_{k_n}(k) + \delta_{-k_n}(k) \right) \\ &= \chi \delta(k) + \frac{\mathscr{L}}{\pi} + \frac{1}{\pi} \sum_{\gamma \in \mathscr{P}} \ell(\text{prim}\,(\gamma)) \mathbf{S_v}(\gamma) \cos k \ell(\gamma), \end{aligned} \tag{8.4}$$

and

$$\begin{aligned} \hat{\mu}(l) &\equiv 2 + \sum_{k_n \neq 0} 2 \cos k_n l \\ &= \chi + 2\mathscr{L}\delta(l) + \sum_{\gamma \in \mathscr{P}} \ell(\text{prim}\,(\gamma)) \mathbf{S_v}(\gamma) \Big(\delta_{\ell(\gamma)}(l) + \delta_{-\ell(\gamma)}(l) \Big), \end{aligned} \tag{8.5}$$

where

- *$m_s(0)$ is the (spectral) multiplicity of the eigenvalue zero*[1]*;*
- *$\mathscr{P}$ is the set of closed oriented paths on Γ;*
- *$\ell(\gamma)$ is the length of the closed path γ;*
- prim (γ) *is the primitive path for γ;*
- *$\mathbf{S_v}(\gamma)$ is the product of all vertex scattering coefficients along the path γ.*

PROOF. We divide the proof of theorem into two parts. The first part concerns general properties of the spectral measure establishing that μ is a positive distribution. This will be important in Section **??**, where we show that spectral measures for metric graphs provide explicit examples of crystalline measures and Fourier quasicrystals. In the second part we prove trace formula connecting the spectral measure associated with the standard Laplacian to the set of periodic orbits on the metric graph.

Part I. General properties of the spectral measure.

Step 1. Measure μ as a positive distribution. Consider the spectral measure given by (8.3) where the sum is taken over all non-zero eigenvalues $\lambda_n > 0$, $k_n^2 =$

[1] It is equal to the number β_0 of connected components in accordance to Theorem 5.5.

$\lambda_n,\ k_n > 0$ respecting multiplicities. The formula determines a (tempered) distribution since the eigenvalues accumulate towards ∞ satisfying Weyl's asymptotics (4.14). All non-zero points (including correct multiplicities) are given by zeros of the analytic secular function p determined by (5.17). The distribution is positive as a sum of delta distributions with non-negative integer amplitudes. The Fourier transform $\hat{\mu}$ is also a (tempered) distribution, but it is not anymore positive (see Appendix).

Step 2. Spectral measure and logarithmic derivative of the secular function. The distribution μ can be obtained by integrating the jump of the logarithmic derivative of $p(k)$ on the real exis as it was done in Example **??**. The function $(p(k)$ is given now by formula (5.17) and all its zeroes are on the real axis. More precisely we have

$$\mu(k) = (2 - m_a(0))\delta(k) + \frac{1}{2\pi i}\lim_{\epsilon\searrow 0}\left(\frac{d}{dk}\log p(k - i\epsilon) - \frac{d}{dk}\log p(k + i\epsilon)\right). \tag{8.6}$$

We used here the fact that $p(k)$ has zero of order $m_a(0)$ at the origin.

Part II. Trace formula.
Step 3. Spectral measure via the trace of the scattering matrices.

Our next goal will be to use secular equation to calculate the spectral measure. In this way we shall express the spectral measure using periodic orbits on Γ. Let us remind that $\mathbb{S}(k)$ is a product of the edge and vertex scattering matrices $\mathbb{S}(k) = \mathbf{S}\mathbf{S}_{\mathbf{e}}(k)$ and $\mathbf{S}$ is energy independent. Moreover we use the fact that

$$\| \mathbb{S}^{\pm 1}(k \pm i\epsilon) \| < 1, \quad \epsilon > 0, \tag{8.7}$$

since $\mathbf{S}$ is unitary and $\mathbf{S}_{\mathbf{e}}$ satisfies the same inequality. We can repeat calculations carried deriving Poisson's summation formula now taking into account that we are dealing with matrix valued functions. The spectral measure is given by

$$\begin{aligned}
\mu(k) &= (2 - m_a(0))\delta(k) \\
&\quad + \frac{1}{2\pi i}\lim_{\epsilon\searrow 0}\Big(\frac{d}{dk}\log\det\big(\mathbb{S}(k - i\epsilon) - I\big) - \frac{d}{dk}\log\det\big((\mathbb{S}(k + i\epsilon) - I\big)\Big) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\lim_{\epsilon\searrow 0}\Big(\mathrm{Tr}\,\frac{d}{dk}\log\big(\mathbb{S}(k - i\epsilon) - I\big) - \mathrm{Tr}\,\frac{d}{dk}\log\big(\mathbb{S}(k + i\epsilon) - I\big)\Big) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\lim_{\epsilon\searrow 0}\Big(\mathrm{Tr}\,\frac{d}{dk}\Big(- \sum_{m=1}^{\infty}\frac{1}{m}\mathbb{S}^{-m}(k - i\epsilon) \\
&\qquad\qquad + \log\mathbb{S}(k - i\epsilon) + \sum_{m=1}^{\infty}\frac{1}{m}\mathbb{S}^{m}(k + i\epsilon)\Big)\Big) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\left(\mathrm{Tr}\sum_{m=-\infty}^{+\infty}\mathbb{S}^{m}(k)\mathbb{S}'(k)\right),
\end{aligned}$$

where we used

- formula $\log\det A = \mathrm{Tr}\,\log A$ is valid modulo $2\pi i$ for any diagonalisable matrix A;
- the fact that $\mathbb{S}(k \pm i\epsilon)$ are diagonalisable being close to a unitary matrix;
- the series expansion (7.10) for $\log(1 - x)$;

- the fact that under Tr the matrices may be permuted cyclically.

Taking into account that $\mathbb{S}'(k) = \mathbf{S}\mathbf{S}_\mathbf{e}'(k) = \mathbf{S}\mathbf{S}_\mathbf{e}(k)i\mathbf{D} = \mathbb{S}(k)i\mathbf{D}$, where $\mathbf{D}$ is the diagonal matrix given by (5.21) we see that the distribution μ is given by the sum of the series

$$\mu(k) = \chi\delta(k) + \frac{1}{2\pi}\left(\operatorname{Tr}\sum_{m=-\infty}^{+\infty}\mathbb{S}^m(k)\mathbf{D}\right).$$

Our next goal is to calculate the trace having a geometric picture in mind. We are going to calculate the traces corresponding to each power m separately in direct correspondence with formula (9.13), where the Taylor series was summed putting together terms having the same degree m. It is reasonable to start with small powers.

Step 4. Oriented closed paths of discrete lengths 1, 2, 3. The trace of a matrix B can be calculated by choosing an arbitrary orthonormal basis $\vec{e}_j$ and calculating the sum $\sum_j\langle\vec{e}_j, B\vec{e}_j\rangle$. In our case it is natural to choose the standard basis of edge incoming waves, so that all except one coordinates of $\vec{e}_j$ are equal to zero and the j-th coordinate is just 1. Then every vector $\vec{e}_j$ is naturally associated with one of the edge end points. We start by calculating contribution from the first few terms corresponding to $m = 0, 1, 2$.

$m = 0$ It is trivial to calculate the contribution from the zero term in the series

$$\operatorname{Tr}\mathbb{S}^0(k)\mathbf{D} = \operatorname{Tr}\mathbf{D} = 2\mathscr{L}.$$

$m = 1$ We calculate the contribution $\langle\vec{e}_1, \mathbb{S}(k)\mathbf{D}\vec{e}_1\rangle$. Let us assume *w.l.o.g.* that the edge $[x_1, x_2]$ connects together vertices V^1 and V^2. We get $\mathbb{S}(k)\mathbf{D}\vec{e}_1 = \mathbf{S}\mathbf{S}_\mathbf{e}(k)\mathbf{D}\vec{e}_1$ by applying the three matrices one after the other:

$$\vec{e}_1 \xrightarrow{\mathbf{D}} \ell_1\vec{e}_1 \xrightarrow{\mathbf{S}_\mathbf{e}} \ell_1 e^{ik\ell_1}\vec{e}_2 \xrightarrow{\mathbf{S}} \ell_1 e^{ik\ell_1}\underbrace{\sum_{x_j\in V^2}\mathbf{S}_{j2}\vec{e}_j}_{\equiv\sum_{x_j}\mathbf{S}_{j2}\vec{e}_j}, \tag{8.8}$$

(see the first three pictures in Fig. 8.1). We denote here by $\mathbf{S}_{ij}$ the entry of the matrix $\mathbf{S}$ corresponding to the transition from the end point x_j to the end point x_i. The result $\langle\vec{e}_1, \mathbb{S}(k)\mathbf{D}\vec{e}_1\rangle$ is non-zero only if both end points x_1 and x_2 belong to the same vertex, in other words if the edge $[x_1, x_2]$ forms a loop (see Fig. 8.2). The contribution is then equal to

$$\langle\vec{e}_1, \mathbb{S}(k)\mathbf{D}\vec{e}_1\rangle = \ell_1 e^{ik\ell_1}\mathbf{S}_{12}.$$

The remaining first order contributions $\langle\vec{e}_j, \mathbb{S}(k)\mathbf{D}\vec{e}_j\rangle$, $j = 1, 2, \ldots, 2N$, are calculated in the same way. Using the discrete length $d(\gamma)$ we have

$$\operatorname{Tr}\mathbb{S}(k)\mathbf{D} = \sum_{\substack{\gamma\in\mathscr{P}\\ d(\gamma)=1}}\ell(\operatorname{prim}(\gamma))\mathbf{S}_\mathbf{v}(\gamma)e^{ik\ell(\gamma)}, \tag{8.9}$$

where the product of scattering coefficients $\mathbf{S}_\mathbf{v}(\gamma)$ coincides with the single scattering coefficient on the path and every path coincides with its primitive $\ell(\gamma) = \ell(\operatorname{prim}(\gamma))$. The summation is over all loops in Γ. If the graph has no loops, then the total contribution from the first term is zero.

Note that each loop contributes twice since we distinguish paths going in the opposite direction. For example contributions from the loop presented in Fig. 8.2 are

$$\ell_1 e^{ik\ell_1}\mathbf{S}_{12} \quad \text{and} \quad \ell_1 e^{ik\ell_1}\mathbf{S}_{21}.$$

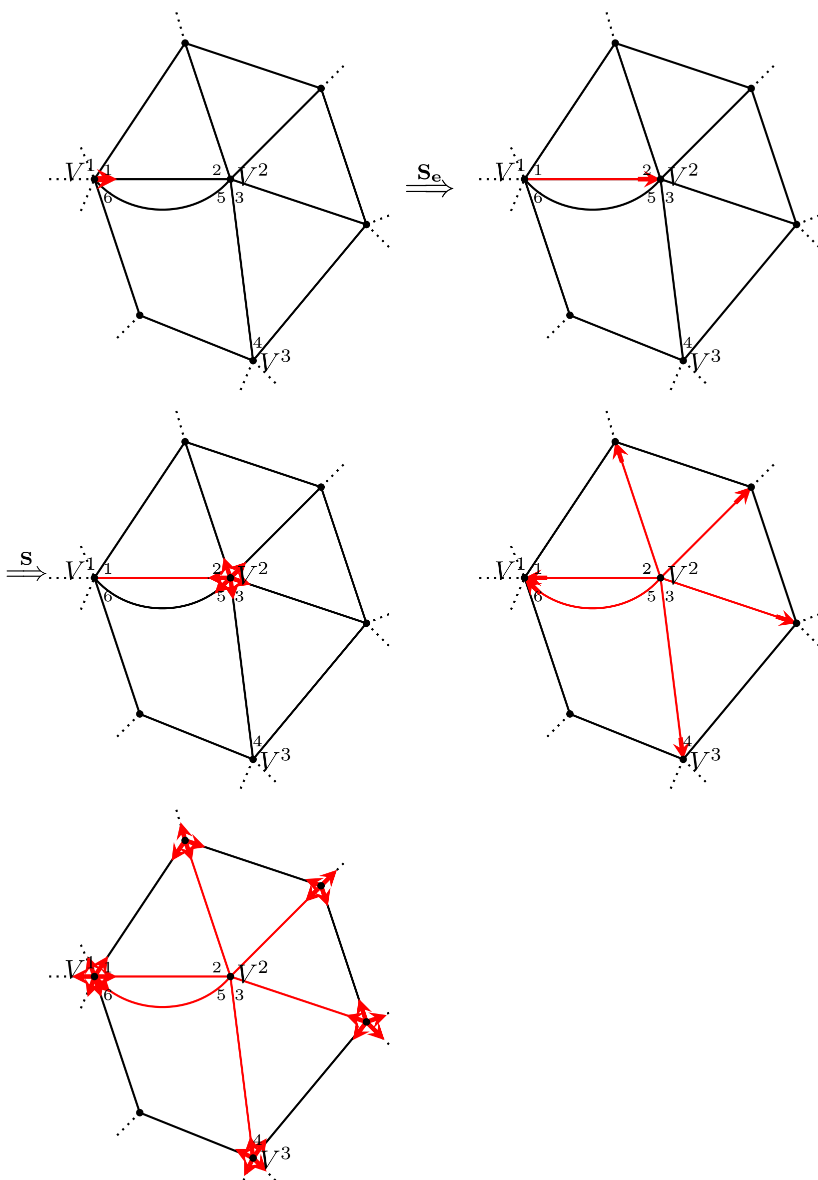

FIGURE 8.1. Edge $[x_1, x_2]$ does not form a loop. The numbers indicate positions of the end points x_j

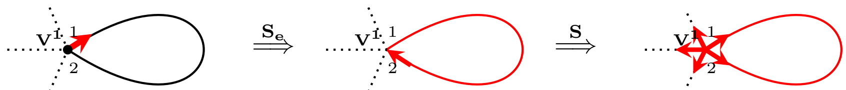

FIGURE 8.2. Edge $[x_1, x_2]$ forms a loop.
Emergence of non-zero contributions

$m = 2$ As before we start by calculating the contribution $\langle \vec{e}_1, \mathbb{S}^2(k)\mathbf{D}\vec{e}_1\rangle$. Assume first that the edge E_1 does not form a loop, then to calculate the contribution we may continue procedure presented in Fig. 8.1. We need to determine

$$\mathbf{S_e}\Big(\ell_1 e^{ik\ell_1} \sum_{x_j \in V^2} S_{j2}\vec{e}_j\Big) = \ell_1 e^{ik\ell_1} \sum_{x_j \in V^2} S_{j2}\mathbf{S_e}\vec{e}_j. \tag{8.10}$$

Each vector $\mathbf{S_e}\vec{e}_j$ is just the vector associated with the opposite end point of the edge x_j belongs to, multiplied by the exponential. For example if $x_3 \in V^2$ (as in Fig. 8.1), then

$$\mathbf{S_e}\vec{e}_3 = e^{ik\ell_2}\vec{e}_4.$$

Denoting by V^3 the vertex x_4 belongs to we obtain

$$\mathbf{S}\mathbf{S_e}\vec{e}_3 = \sum_{x_i \in V^3} \mathbf{S}_{i4} e^{ik\ell_2}\vec{e}_i.$$

The scalar product with $\vec{e}_1$ is non-zero just in two cases:

- If $\vec{e}_j$ in (8.10) coincides with $\vec{e}_2$ corresponding to the reflection at V^2. Then we have

$$\mathbb{S}(k)\vec{e}_2 = \sum_{x_i \in V^1} \mathbf{S}_{i1} e^{ik\ell_1}\vec{e}_i \Rightarrow \langle \vec{e}_1, \ell_1 e^{ik\ell_1}\mathbb{S}(k)\vec{e}_2\rangle = \ell_1 e^{2ik\ell_1}\mathbf{S}_{11}\mathbf{S}_{22}.$$

  This term is always present.
- If $\vec{e}_j$ in (8.10) is different from $\vec{e}_2$ but the corresponding edge is parallel to $[x_1, x_2]$ like the edge $[x_5, x_6]$ in Fig. 8.1. Using notations from the figure we get

$$\mathbb{S}(k)\vec{e}_5 = \sum_{x_i \in V^1} \mathbf{S}_{i6} e^{ik\ell_3}\vec{e}_i \Rightarrow \langle \vec{e}_1, \ell_1 e^{ik\ell_1}\mathbb{S}(k)\vec{e}_5\rangle = \ell_1 e^{ik(\ell_1+\ell_2)}\mathbf{S}_{16}\mathbf{S}_{52}.$$

  This term is present only if there are two parallel edges, *i.e.* there is a closed path of discrete length 2 supported by two edges.

Assume now that E_1 forms a loop, then modifying formula (8.8) we get

$$\mathbf{S}\mathbf{S_e}\mathbf{D}\vec{e}_1 = \ell_1 e^{ik\ell_1} \sum_{x_j \in V^1} \mathbf{S}_{j2}\vec{e}_j.$$

The contribution

$$\langle \vec{e}_1, \mathbf{S}\mathbf{S_e}\mathbf{S}\mathbf{S_e}\mathbf{D}\vec{e}_1\rangle$$

is non-zero in just three cases:

- the end point x_j coincides with x_2 with the contribution

$$\ell_1 e^{2ik\ell_1}\mathbf{S}_{11}\mathbf{S}_{22};$$

- the end point x_j coincides with x_1 with the contribution

$$\ell_1 e^{2ik\ell_1}\mathbf{S}_{12}\mathbf{S}_{12};$$

- the end point x_j belongs to a different from E_1 edge, say E_2, forming a loop with the contribution

$$\ell_1 e^{ik(\ell_1+\ell_2)}\mathbf{S}_{13}\mathbf{S}_{32}.$$

Summing over all $j = 1, 2, \dots, 2N$ we see that every oriented path of discrete length 2 contributes to the trace of $\mathbb{S}(k)^2\mathbf{D}$. The paths going through two vertices or two different edges contribute twice.

Every edge E_n not forming a loop determines the unique path γ_1 going back and force along it (see Fig. 8.3 (**a**)). The contribution from this path comes from the following two scalar products $\langle e_{2n-1}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n-1}\rangle$ and $\langle e_{2n}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n}\rangle$ and is equal to

$$\ell_n e^{ik2\ell_n}\mathbf{S}_{2n-1\;2n-1}\mathbf{S}_{2n\;2n} + \ell_n e^{ik2\ell_n}\mathbf{S}_{2n\;2n}\mathbf{S}_{2n-1\;2n-1} = \ell(\mathrm{prim}\,(\gamma_1))e^{ik\ell(\gamma_1)}\mathbf{S}_{\mathbf{v}}(\gamma_1).$$

The corresponding primitiv path coincides with γ_1, hence $\ell(\mathrm{prim}\,(\gamma_1)) = \ell(\gamma_1) = 2\ell_n$. The product of scattering coefficients is $\mathbf{S}_{\mathbf{v}}(\gamma_1) = \mathbf{S}_{2n-1\;2n-1}\mathbf{S}_{2n\;2n}$.

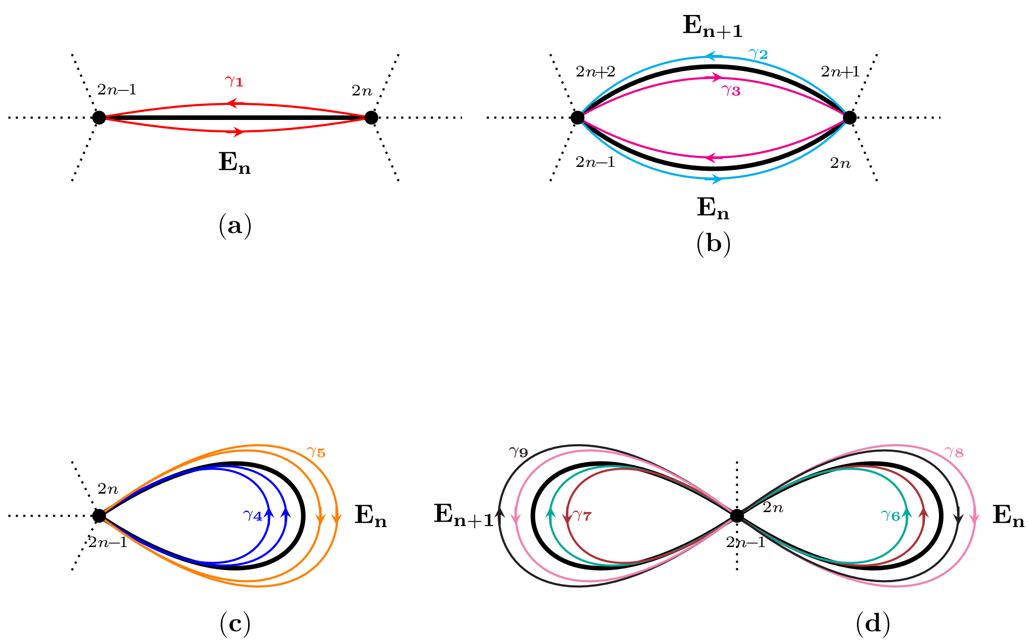

FIGURE 8.3. Different paths of discrete length 2

Consider now the case, where there is an edge parallel to E_n. We denote the parallel edge by E_{n+1} and assume E_n and E_{n+1} are oriented in the opposite directions (see Fig. 8.3 (**b**)). Then there are two more discrete length 2 paths

$$\gamma_2 = (x_{2n-1}, x_{2n}, x_{2n+1}, x_{2n+2}) \quad \text{and} \quad \gamma_3 = (x_{2n+2}, x_{2n+1}, x_{2n}, x_{2n-1})$$

(marked by cyan and magenta colours respectively) contributing via the scalar products

$$\langle e_{2n-1}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n-1}\rangle, \quad \langle e_{2n+1}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n+1}\rangle$$

and

$$\langle e_{2n}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n}\rangle, \quad \langle e_{2n+2}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n+2}\rangle,$$

respectively. The corresponding contributions are

$$\begin{aligned}\ell_n e^{ik(\ell_n+\ell_{n+1})}\mathbf{S}_{2n-1\ 2n+2}\mathbf{S}_{2n+1\ 2n} + \ell_{n+1}e^{ik(\ell_n+\ell_{n+1})}\mathbf{S}_{2n+1\ 2n}\mathbf{S}_{2n-1\ 2n+2} \\ = \ell(\text{prim}\,(\gamma_2))e^{ik\ell(\gamma_2)}\mathbf{S}_{\mathbf{v}}(\gamma_4),\end{aligned}$$

and

$$\begin{aligned}\ell_n e^{ik(\ell_n+\ell_{n+1})}\mathbf{S}_{2n\ 2n+1}\mathbf{S}_{2n+2\ 2n-1} + \ell_{n+1}e^{ik(\ell_n+\ell_{n+1})}\mathbf{S}_{2n+2\ 2n-1}\mathbf{S}_{2n\ 2n+1} \\ = \ell(\text{prim}\,(\gamma_3))e^{ik\ell(\gamma_3)}\mathbf{S}_{\mathbf{v}}(\gamma_5),\end{aligned}$$

where $\ell(\text{prim}\,(\gamma_2))2\ell(\text{prim}\,(\gamma_3)) = \ell(\gamma_2) = \ell(\gamma_3) = \ell_n + \ell_{n+1}$ and

$$\mathbf{S}_{\mathbf{v}}(\gamma_2) = \mathbf{S}_{2n+1\ 2n}\mathbf{S}_{2n-1\ 2n+2}, \quad \text{and} \quad \mathbf{S}_{\mathbf{v}}(\gamma_3) = \mathbf{S}_{2n+2\ 2n-1}\mathbf{S}_{2n\ 2n+1}.$$

Assume now that the edge E_n forms a loop (see Fig. 8.3 (**b**)), then we have the path γ_1 going once back and force with the same contribution as above

$$\ell(\text{prim}\,(\gamma_1))e^{ik\ell(\gamma_1)}\mathbf{S}_{\mathbf{v}}(\gamma_1).$$

In addition we have two more oriented periodic paths

$$\gamma_4 = (x_{2n-1}, x_{2n}, x_{2n-1}, x_{2n}) \quad \text{and} \quad \gamma_5 = (x_{2n}, x_{2n-1}, x_{2n}, x_{2n-1})$$

going around the first loop twice in different directions marked by blue and orange colors respectively (see Fig. 8.3 (**c**)). Each of the paths contributes to just one of the two scalar products with

$$\gamma_4: \quad \langle \vec{e}_{2n-1}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n-1}\rangle = \ell_n e^{2ik\ell_n}\mathbf{S}_{2n-1\ 2n}\mathbf{S}_{2n-1\ 2n} = \ell(\text{prim}\,(\gamma_4))e^{ik\ell(\gamma_4)}\mathbf{S}_{\mathbf{v}}(\gamma_4),$$

$$\gamma_5: \quad \langle \vec{e}_{2n}, \mathbb{S}^2(k)\mathbf{D}\vec{e}_{2n}\rangle = \ell_n e^{2ik\ell_n}\mathbf{S}_{2n\ 2n-1}\mathbf{S}_{2n\ 2n-1} = \ell(\text{prim}\,(\gamma_5))e^{ik\ell(\gamma_5)}\mathbf{S}_{\mathbf{v}}(\gamma_5),$$

with $\ell(\text{prim}\,(\gamma_4)) = \ell(\text{prim}\,(\gamma_5)) = \ell_n; \ell(\gamma_2) = \ell(\gamma_3) = 2\ell_n$ and

$$\mathbf{S}_{\mathbf{v}}(\gamma_4) = \mathbf{S}_{2n-1\ 2n}\mathbf{S}_{2n-1\ 2n}, \quad \mathbf{S}_{\mathbf{v}}(\gamma_5) = \mathbf{S}_{2n\ 2n-1}\mathbf{S}_{2n\ 2n-1}.$$

If there is another edge, say E_{n+1}, forming a loop attached to the same vertex, then we have analogs of the paths γ_2 and γ_3 going first along one of the loops and returning back along the other one. There are four such paths since the loops can be passed in different directions (see Fig. 8.3 (**d**)). we denote these paths by $\gamma_6, \gamma_7, \gamma_8$, and γ_9.

The result can be written as a sum over all periodic paths with discrete length 2

$$\sum_{\substack{\gamma\in\mathscr{P}\\ d(\gamma)=2}} \ell(\text{prim}\,(\gamma))\mathbf{S}_{\mathbf{v}}(\gamma)e^{ik\ell(\gamma)}. \tag{8.11}$$

Step 5. Arbitrary oriented closed paths. We are ready now to look at the contributions from higher powers of $\mathbb{S}(k)$. Our analysis shows that a term $\langle \vec{e}_i, \mathbb{S}^m(k)\mathbf{D}\vec{e}_i\rangle$ gives a nonzero contribution only if there is a closed path γ on Γ with the discrete length $d(\gamma) = m$ passing through the end point x_i.

Let us calculate the total contribution from any path γ of discrete length $d(\gamma) = m$. Assume that the path is a multiple of the primitive path

$$\text{prim}\,(\gamma) = (x_{i_1}, x_{i_2}, x_{i_3}, \dots, x_{i_{2Q}}), \quad \gamma = R\ \text{prim}\,(\gamma),$$

where the primitive path is formed by Q edges and this path should be repeated R times to get γ so that $m = QR$. This path contributes to the scalar products

$$\langle \vec{e}_{i_{2q-1}}, \mathbf{S}^m\mathbf{D}\vec{e}_{i_{2q-1}}\rangle, \quad q = 1, 2, \dots, Q.$$

If every end point $x_{i_{2q-1}}$ appears just once in prim (γ), then the contribution from each point is equal to the length of the edge that $x_{i_{2q-1}}$ belongs multiplied by $e^{ik\ell(\gamma)}$ and the product $\mathbf{S}_{\mathbf{v}}(\gamma)$ of all vertex scattering coefficients along γ. If a certain end point appears several times, then the above contribution is multiplied by the number of times $x_{i_{2q-1}}$ appears in prim (γ). Summing up contributions from different vertices on the primitive path results in multiplication of $S_{\mathbf{v}}(\gamma)e^{ik\ell(\gamma)}$ by the length of the primitive path

$$\ell(\text{prim}(\gamma))\mathbf{S}_{\mathbf{v}}(\gamma)e^{ik\ell(\gamma)}.$$

Summation over all paths of discrete length m leads to

$$\text{Tr}\ \mathbf{S}^m(k)\mathbf{D} = \sum_{\substack{\gamma\in\mathscr{P}\\ d(\gamma)=m}} \ell(\text{prim}\,(\gamma))\mathbf{S}_{\mathbf{v}}(\gamma)e^{ik\ell(\gamma)}. \tag{8.12}$$

Formula (8.4) is obtained by summing over all m and taking into account the fact that the contribution from m and $-m$ are complex conjugates of each other.

The second trace formula (8.5) is obtained via Fourier transform. □

Formula (8.4) can be modified using summation over primitive orbits, provided the graph has more than one edge (is different from $\Gamma_{(1.1)}$ and $\Gamma_{(1.2)}$).

$$\begin{aligned} \mu(k) &= 2\delta(k) + \sum_{k_n\neq 0}(\delta_{k_n}(k) + \delta_{-k_n}(k)) \\ &= \chi\delta(k) + \frac{\mathscr{L}}{\pi} + \frac{1}{2\pi}\sum_{\gamma\in\mathscr{P}_{\text{prim}}}\ell(\gamma)\frac{2\,\mathbf{S}_{\mathbf{v}}(\gamma)(\cos k\ell(\gamma) - \mathbf{S}_{\mathbf{v}}(\gamma))}{1 - 2\cos k\ell(\gamma)\mathbf{S}_{\mathbf{v}}(\gamma) + \mathbf{S}_{\mathbf{v}}^2(\gamma)}, \end{aligned} \tag{8.13}$$

where $\mathscr{P}_{\text{prim}}$ denotes the set of primitive oriented paths, *i.e.* those oriented paths that coincide with their primitives. To prove the formula we note that every primitive path γ determines a sequence of non-primitive paths: $2\gamma, 3\gamma, \dots, n\gamma, \dots$ Taking into account that

$$e^{ik\ell(n\gamma)} = e^{ink\ell(\gamma)} = \left(e^{ik\ell(\gamma)}\right)^n, \quad \mathbf{S}_\mathbf{v}(n\gamma) = \left(\mathbf{S}_\mathbf{v}(\gamma)\right)^n, \tag{8.14}$$

we see that contributions from the multiples of γ form a converging geometric progression since $|\mathbf{S}_\mathbf{v}(\gamma)| < 1$[2]

$$\sum_{n=1}^{\infty} \ell(\text{prim }(n\gamma)) e^{ik\ell(n\gamma)} \mathbf{S}_\mathbf{v}(n\gamma) = \sum_{n=1}^{\infty} \ell(\gamma) \left(e^{ik\ell(\gamma)} \mathbf{S}_\mathbf{v}(\gamma)\right)^n = \ell(\gamma) \frac{e^{ik\ell(\gamma)} \mathbf{S}_\mathbf{v}(\gamma)}{1 - e^{ik\ell(\gamma)} \mathbf{S}_\mathbf{v}(\gamma)}.$$

Adding the conjugated contribution we get

$$\begin{aligned} \sum_{n=1}^{\infty} \ell(\text{prim }(n\gamma)) e^{ik\ell(n\gamma)} \mathbf{S}_\mathbf{v}(n\gamma) + \sum_{n=1}^{\infty} \ell(\text{prim }(n\gamma)) e^{-ik\ell(n\gamma)} \mathbf{S}_\mathbf{v}(n\gamma) \\ = \ell(\gamma) \frac{2\, \mathbf{S}_\mathbf{v}(\gamma)(\cos k\ell(\gamma) - \mathbf{S}_\mathbf{v}(\gamma))}{1 - 2\cos k\ell(\gamma) \mathbf{S}_\mathbf{v}(\gamma) + \mathbf{S}_\mathbf{v}^2(\gamma)}. \end{aligned}$$

[2]Here we use that the graph is different from $\Gamma_{(1.1)}$ and $\Gamma_{(1.2)}$ and therefore every path crosses at least one vertex of degree different from 1 and 2 – the scattering coefficients may have unit modulus only for such vertices.