2

Graph Laplacians

In this chapter we recall the definition of (generalized) graph Laplacians and present the basic properties of their eigenfunctions. Moreover, we establish the main tools that will be used throughout the book. For a thorough overview of other properties of graph Laplacians not required for our investigations of eigenfunctions we refer the interested reader to the survey by Merris [133].

2.1 Basic Properties of Graph Laplacians

Let $G(V, E)$ be a simple graph with vertex set V and edge set E. We use the convention that $|V| = n$ and $|E| = m$, i.e., G is a graph with n vertices and m edges. The *Laplacian* of G is the matrix

$$\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G) \tag{2.1}$$

where $\mathbf{D}(G)$ is the diagonal matrix whose entries are the degrees of the vertices of G, i.e. $D_{vv} = d(v)$, and $\mathbf{A}(G)$ denotes the adjacency matrix of G. For the function $\mathbf{L}f$ we find

$$(\mathbf{L}f)(x) = \sum_{y \sim x} [f(x) - f(y)] = d(x)\, f(x) - \sum_{y \sim x} f(y)\ . \tag{2.2}$$

We denote the eigenvalues of $\mathbf{L}$ by λ_i enumerated in increasing order, i.e.,

$$0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n\ . \tag{2.3}$$

The quadratic form of the graph Laplacian can be computed via Green's formula as

$$\langle f, \mathbf{L}f \rangle = \sum_{x,y \in V} L_{xy} f(x) f(y) = \sum_{xy \in E} (f(x) - f(y))^2\ . \tag{2.4}$$

This equality immediately shows that the graph Laplacian is a nonnegative operator, i.e., all eigenvalues are greater than or equal to 0.

A symmetric matrix $\mathbf{M}(G)$ is called a *generalized Laplacian* (or *discrete Schrödinger operator*) of G if it has nonpositive off-diagonal entries and for $x \neq y$, $M_{xy} < 0$ if and only if the vertices x and y are adjacent. On the other hand, for each symmetric matrix with nonpositive off-diagonal entries there exists a graph where two distinct vertices x and y are adjacent if and only if $M_{xy} < 0$. Similarly to (2.2) we have

$$(\mathbf{M}f)(x) = \sum_{y\sim x}(-M_{xy})[f(x) - f(y)] + p(x)\, f(x)\ , \tag{2.5}$$

where $p(x) = M_{xx} + \sum_{y\sim x} M_{xy}$. The last part $p(x)$ can be viewed as some potential on vertex x. Defining a matrix $\mathbf{W}$ consisting of $W_{xy} = M_{xy}$ for $x \neq y$ and $W_{xx} = -\sum_{y\neq x} M_{xy}$ and a diagonal matrix $\mathbf{P}$ with the potentials $p(x)$ as its entries we can decompose every generalized Laplacian as

$$\mathbf{M} = \mathbf{W} + \mathbf{P}\ .$$

$\mathbf{W}$ can be seen as *discrete elliptic operator*. The quadratic form of the generalized Laplacian can then be computed as

$$\langle f, \mathbf{M}f\rangle = \sum_{xy\in E}(-M_{xy})(f(x) - f(y))^2 + \sum_{x\in V} p(x)\, f(x)^2\ ; \tag{2.6}$$

an alternative presentation is

$$\langle f, \mathbf{M}f\rangle = \sum_{x\in V} M_{xx} f(x)^2 + 2\sum_{xy\in E} M_{xy} f(x) f(y)\ . \tag{2.7}$$

The following remarkable result for the eigenvalues of a generalized Laplacian can be easily derived.

Theorem 2.1 ([22]). *Let λ be an eigenvalue of a generalized Laplacian $\mathbf{M} = \mathbf{W} + \mathbf{P}$ with eigenfunction f. Then either $\sum_{v\in V} f(v) = \sum_{v\in V} p(v)\, f(v) = 0$, or*

$$\lambda = \frac{\sum_{v\in V} p(v)\, f(v)}{\sum_{v\in V} f(v)}\ .$$

Proof. Let $\mathbf{1} = (1, \ldots, 1)^\mathsf{T}$. Then a straightforward computation gives

$$\begin{aligned}
\langle \mathbf{1}, \mathbf{M}f\rangle &= \textstyle\sum_{v\in V} \left(\sum_{w\sim v}(-M_{vw})(f(v) - f(w)) + p(v)\, f(v)\right) \\
&= \textstyle\sum_{v,w\in V}(-M_{vw})(f(v) - f(w)) + \sum_{v\in V} p(v)\, f(v) \\
&= \textstyle\sum_{v,w\in V} M_{vw} f(w) - \sum_{v,w\in V} M_{vw} f(v) + \sum_{v\in V} p(v)\, f(v) \\
&= \textstyle\sum_{v\in V} p(v)\, f(v)\ .
\end{aligned}$$

Since f is an eigenfunction we find $\langle \mathbf{1}, \mathbf{M}f\rangle = \lambda \sum_{v\in V} f(v)$, and thus the proposition follows. □

Remark 2.2. The case $\sum_{v \in V} f(v) = 0$ happens, for example, for all eigenfunctions corresponding to an eigenvalue $\lambda > \lambda_1$ when the eigenfunction f_1 of λ_1 is constant. This is the case if and and only if $p(v)$ is constant for all $v \in V$.

The spectrum of the (generalized) Laplacian provides quite detailed information on the structure of the underlying graph. We refer the interested reader to classical books and surveys, e.g. [17, 35, 41, 46, 85, 133, 137].

One of these basic results is related to the multiplicity of the first eigenvalue and the connectivity of the graph. Notice, that all eigenvalues of a discrete elliptic matrix $\mathbf{W}$ are nonnegative as an immediate consequence of (2.6). Moreover, its smallest eigenvalue is $\lambda_1 = 0$.

Theorem 2.3. *Let $\mathbf{W}(G)$ be a generalized Laplacian without potential (i.e. $\mathbf{P} = 0$). Then the multiplicity of the smallest eigenvalue λ_1 of $\mathbf{W}(G)$ is equal to the number of components of G. In particular, λ_1 is simple if and only if G is connected.*

Proof. Assume G is the disjoint sum of connected components $H_1, \dots, H_k$. Denote by f_i the characteristic function of $V(H_i)$, i.e. $f(v) = 1$ if $v \in V(H_i)$ and 0 otherwise. Obviously, $\mathbf{M}(G) f_i = 0$. Since $f_1, \dots, f_k$ are linearly independent, the multiplicity of eigenvalue 0 is at least k.

Conversely, if f is an eigenfunction of eigenvalue 0, then by (2.6) f must be constant on each edge of G and hence on each component H_i. Therefore f is a linear combination of the characteristic functions f_i. □

We assume throughout this book that all graphs are connected unless stated otherwise explicitly.

2.2 Weighted Graphs

We have introduced Laplacian and generalized Laplacian matrices on simple unweighted graphs. However, it is straightforward to generalize these concepts to *weighted graphs*. Let $w_{xy} > 0$ denote the weight for edge xy; we set $w_{xy} = 0$ if x and y are not adjacent. Then we can define the Laplacian $\mathbf{L}_w$ as

$$(\mathbf{L}_w f)(x) = \sum_{y \sim x} w_{xy}(f(x) - f(y)) \; . \tag{2.8}$$

Obviously this is a special case of (2.5) with $-M_{xy} = w_{xy}$ and $p(x) = 0$. Thus $\mathbf{L}_w$ can be seen as a generalized Laplacian on the corresponding unweighted graph (where two vertices x and y are adjacent if and only if $w_{xy} > 0$). Thus without loss of generality we will restrict our interest to generalized Laplacian on unweighted graphs.

2.3 The Rayleigh Quotient

The *Rayleigh quotient* $\mathcal{R}_\mathbf{M}(f)$ of a function $f\colon V \to \mathbb{R}$ with respect to a generalized Laplacian $\mathbf{M}$ is defined as the fraction

$$\mathcal{R}_\mathbf{M}(f) = \frac{\langle f, \mathbf{M}f\rangle}{\langle f, f\rangle} . \tag{2.9}$$

For the graph Laplacian $\mathbf{L}$ this can equivalently be written as

$$\mathcal{R}_\mathbf{L}(f) = \frac{\sum_{xy\in E}(f(x) - f(y))^2}{\sum_{x\in V} f(x)^2} .$$

The Rayleigh quotient plays a crucial rôle in our investigations. Its importance is based on the following fundamental theorem from spectral theory for symmetric matrices (which we restate here for graph Laplacians), see e.g. [100].

Proposition 2.4 (Spectral Decomposition). *For a generalized Laplacian* $\mathbf{M}$ *for a graph* G *there exists an orthonormal basis of the* $\mathbb{R}^n$ *that consists of eigenfunctions* $f_1, \dots, f_n$ *corresponding to the eigenvalues* $\lambda_1, \dots, \lambda_n$*. Moreover, for every function* $g\colon V \to \mathbb{R}$ *we find*

$$\mathbf{M}g = \sum_{i=1}^{n} \lambda_i \langle g, f_i\rangle\, f_i$$

and for the quadratic form,

$$\langle g, \mathbf{M}g\rangle = \sum_{i=1}^{n} \lambda_i \langle g, f_i\rangle^2 .$$

As an immediate consequence we have the following corollary.

Corollary 2.5. *Let* $f_1, \dots, f_n$ *denote orthogonal eigenfunctions corresponding to the eigenvalues* $\lambda_1 \le \lambda_2 \le \dots \le \lambda_n$ *of a generalized Laplacian* $\mathbf{M}$*. Let* $F_i = \{f_1, \dots, f_i\}$ *be the set of the first* i *eigenfunctions and* $F_i^\perp$ *its orthogonal complement. Then*

$$\lambda_k = \min_{g\in F_{k-1}^\perp} \mathcal{R}_\mathbf{M}(g) = \min_{g\in F_{k-1}^\perp} \frac{\langle g, \mathbf{M}g\rangle}{\langle g, g\rangle} .$$

Moreover, $\mathcal{R}_\mathbf{M}(g) = \lambda_k$ *for some* $g \in F_{k-1}^\perp$ *if and only if* g *is an eigenfunction corresponding to* λ_k*.*

Proof. Every function $g \in F_{k-1}^\perp$ can be written as $g = \sum_{i=k}^n a_i\, f_i$. Hence $\mathcal{R}_\mathbf{M}(g) = \sum_{i=k}^n \lambda_i\, a_i^2 / \sum_{i=k}^n a_i^2 \ge \sum_{i=k}^n \lambda_k\, a_i^2 / \sum_{i=k}^n a_i^2 = \lambda_k$ and equality holds if and only if all terms with eigenvalues $\lambda_i > \lambda_k$ vanish. Thus the result follows. □

Corollary 2.6 (Minimax-Theorem). *Let $\mathcal{W}_k$ and $\mathcal{W}_k^\perp$ denote the sets of subspaces of $\mathbb{R}^n$ of dimension at least k and of codimension at most k, respectively. Then*

$$\lambda_k = \min_{W\in\mathcal{W}_k} \max_{0\neq g\in W} \frac{\langle g, \mathbf{M}g\rangle}{\langle g, g\rangle} = \max_{W\in\mathcal{W}_{k-1}^\perp} \min_{0\neq g\in W} \frac{\langle g, \mathbf{M}g\rangle}{\langle g, g\rangle}$$

Proof. Every function g can be written as $g = \sum_{i=1}^n a_i f_i$ for some a_i where $\{f_1, \dots, f_n\}$ is the orthonormal basis of eigenfunctions from Prop. 2.4. Hence $\mathcal{R}_\mathbf{M}(g) = \frac{\langle g,\mathbf{M}g\rangle}{\langle g,g\rangle} = \sum_{i=1}^n a_i^2\lambda_i / \sum_{i=1}^n a_i^2$. Then for every $W \in \mathcal{W}_k$ we can find some $g \in W$ where $a_1 = \dots a_{k-1} = 0$ and thus $\sup_{g\in W} \mathcal{R}_\mathbf{M}(g) \geq \sup_{g\in W, a_1=\dots=a_{k-1}=0} \sum_{i=k}^n a_i^2\lambda_i / \sum_{i=k}^n a_i^2 \geq \lambda_k$. Consequently,

$$\inf_{W\in\mathcal{W}_k} \sup_{g\in W} \mathcal{R}_\mathbf{M}(g) \geq \lambda_k \ .$$

Equality holds if W is the subspace that is spanned by the first k eigenfunctions. Thus the first equality follows. The second equality is shown analogously. □

2.4 Calculus on Graphs

Friedman and Tillich [76, 77] developed a *Calculus on Graphs* where ideas for motivating the discrete Dirichlet matrix [75] are extended to a more general setting; see Sect. 1.5 for a more detailed description.

The *geometric realization* of a graph $G(V, E)$ is the metric space $\mathcal{G}$ consisting of V and arcs of length 1 glued between u and v for every edge $e = uv \in E$. For weighted graphs these arcs have length $1/w_{uv}$. This definition of the arc lengths needs some explanation. Setting the length of such arcs to the reciprocal of weights of the corresponding edge is motivated by the application of graphs in physical models (see e.g. Hückel theory in Sect. 1.6) or in numerical approximations of the continuous operators (see e.g. Sect. 1.2). Shorter distances between the nodes (i.e., smaller arc lengths) result in stronger coupling in these systems and hence are modeled by higher weights for these connections.

We define two measures on $\mathcal{G}$ (and G). A *vertex measure*, μ_V, is supported on the vertex set V with $\mu_V(v) > 0$ for all $v \in V$; and an *edge measure* μ_E, supported on the union of arcs of $\mathcal{G}$, with $\mu_E(v) = 0$ for all $v \in V$ and whose restriction to any open subinterval of an edge (arc) $e \in E$ is its Lebesgue measure times a constant $a_e > 0$. In our setup we have the measures $\mu_V(v) = 1$ and $a_e = 1$ (which are called *traditional* in [76]). Hence for any graph G, $\mu_V(G) = |V|$ and $\mu_E(G) = |E|$ (or $\sum_{e\in E} 1/w_e$ in case of a weighted graph).

Let $\mathcal{S}$ denote the set of all continuous functions on $\mathcal{G}$ which are differentiable on $\mathcal{G}\setminus V$. Then we introduce a Laplacian operator $\mathcal{L}(\mathcal{G})$ by the Rayleigh quotient for functions $f \in \mathcal{S}$ given as

$$\mathcal{R}_{\mathcal{L}}(f) = \frac{\int_{\mathcal{G}} |\nabla f|^2 d\mu_E}{\int_{\mathcal{G}} |f|^2 d\mu_V} \ .$$

The operator $\mathcal{L}(\mathcal{G})$ can be seen as the continuous version of the corresponding graph Laplacian $\mathbf{L}(G)$. On $\mathcal{G}$ we can avoid the problems that arise from the discreteness of our situation. Many concepts in analysis translate almost immediately to this setting. For example, nodal domains (Sect. 3.1) of an (eigen-)function f are separated by points in $\mathcal{G}$ where f vanishes; in opposition to the traditional setting where such points need not exist as f is supported on V only (see Sect. 3.1).

These two concepts, $\mathbf{L}(G)$ and $\mathcal{L}(\mathcal{G})$, coincide [75, 76]. The Rayleigh quotient $\mathcal{R}_{\mathcal{L}}(f)$ is minimized if and only if $f \in \mathcal{S}$ is an edgewise linear function, i.e. a function whose restriction to an edge is linear. The eigenvalues and eigenfunctions of $\mathcal{L}(\mathcal{G})$ exist and are those of $\mathbf{L}(G)$, i.e. the restrictions of the $\mathcal{L}(\mathcal{G})$-eigenfunctions to V are the graph Laplacian eigenfunctions.

In this setting the motivation for the Dirichlet operator, introduced in Sect. 1.5, is obvious: Restrict $\mathcal{S}$ to $\{f \in \mathcal{S} \colon f(v) = 0 \text{ for all } v \in \partial V\}$. We then have the following analog to eigenfunctions of the classical Laplace-Beltrami operator. If G_1 and G_2 are graphs with boundary, then we say that G_2 is an extension of G_1, written $G_1 \subseteq G_2$, if there exists an isometric embedding of the realization of G_1 into G_2 which preserves the degree of each interior vertex. If G_1 and G_2 are connected graphs and the above embedding is not onto, we say that G_2 is a strict extension, $G_1 \subset G_2$.

Proposition 2.7 ([75]). *Let $\lambda^\circ(G)$ denote the first Dirichlet eigenvalue. Then the following holds:*

(1) $\lambda^\circ(G)$ is continuous as a function of G in the metric $\rho(G, G') = \mu_E(G - G') + \mu_E(G' - G)$.
(2) $\lambda^\circ(G)$ is monotone in G, i.e., if $G \subset G'$ then $\lambda^\circ(G) > \lambda^\circ(G')$.

2.5 Basic Properties of Eigenfunctions

As we have already seen the graph Laplacian is a nonnegative operator. If G is a connected graph with n vertices then the constant function $\mathbf{1} \colon x \mapsto 1$ is the unique eigenfunction with eigenvalue 0, $\mathbf{L1} = 0$ (for a proof see Cor. 2.23). Each eigenfunction of an eigenvalue greater than 0 is orthogonal to $\mathbf{1}$ by Prop. 2.4. Thus there are at least two vertices with values of opposite sign, and of course $\sum_{x \in V} f(x) = 0$. For vertices where an eigenfunction vanishes we have the following important property which holds for every generalized Laplacian.

Lemma 2.8. *Let f be an eigenfunction of $\mathbf{M}(G)$ with a zero vertex z, i.e., a vertex where f vanishes, $f(z) = 0$. Then $\sum_{y \sim z} M_{yz} f(y) = 0$. Moreover, either all neighbors of the zero vertex z are zero vertices themselves, or z is adjacent to vertices of both strict signs.*

Proof. $0 = f(z) = \sum_{y \in V} M_{yz} f(y) = \sum_{y \sim z} M_{yz} f(y) + M_{zz} f(z) = \sum_{y \sim z} M_{yz} f(y).$ □

The next property can be interpreted as a discrete analog of the *maximum principle* for the Laplace operator. We say that x is a *local maximum* of a function f if $f(x) \geq f(y)$ for all $y \sim x$ and $f(x) > f(z)$ for at least one $z \sim x$. A *local minimum* is defined analogously.

Theorem 2.9 ([81, 90]). *An eigenfunction f of a graph Laplacian $\mathbf{L}(G)$ cannot have a nonnegative local minimum or a nonpositive local maximum.*

Proof. Suppose x is a local minimum of f with $f(x) \geq 0$. Then $\sum_{y \sim x}[f(x) - f(y)] < 0$ and thus by (2.2), $0 \leq \lambda f(x) = (\mathbf{L}f)(x) = \sum_{y \sim x}[f(x) - f(y)] < 0$, a contradiction. □

Remark 2.10. This theorem analogously holds for generalized Laplacians without a potential $p(x)$ in (2.5). However, if $p(x) \neq 0$ for some vertices then it might fail. For example, consider a simple path P_3, with generalized Laplacian

$$\mathbf{M} = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} .$$

Then $\lambda_1 = 2 - \sqrt{3}$ has an eigenfunction with a positive minimum on the second vertex.

Merris [134] considers several “eigenfunction principles” for the graph Laplacian. In the following we review some of them.

Theorem 2.11 ([134]). *Let G be a graph with n vertices. If $0 \neq \lambda < n$ is an eigenvalue of $\mathbf{L}(G)$, then any eigenfunction affording λ takes the value 0 on every vertex of degree $n - 1$.*

Proof. Let v be a vertex of degree $n-1$. $(\mathbf{L}f)(v) = (n-1)\,f(v) - \sum_{x \neq v} f(x) = \lambda\, f(v)$, hence $n\, f(v) = \lambda\, f(v)$ and $f(v) = 0$. □

Theorem 2.12 ([134]). *Let λ be an eigenvalue of $\mathbf{L}(G)$ afforded by eigenfunction f. If $f(u) = f(v)$, then λ is an eigenvalue of $\mathbf{L}(G')$ afforded by f, where G' is the graph obtained from G by deleting or adding the edge $e = uv$ depending on whether or not $e = uv$ is an edge of G.*

The *reduced graph* $G\{W\}$ is obtained from G by deleting all vertices in $V \setminus W$ that are not adjacent to a vertex of W and subsequent deletion of any remaining edges that are not incident with a vertex of W.

Theorem 2.13 ([134]). *For a graph $G(V, E)$ fix a nonempty subset W of V. Suppose f is an eigenfunction of the reduced graph $G\{W\}$ that affords λ and is supported by W in the sense that if $f(u) \neq 0$, then $u \in W$. Then the extension f' with $f'(v) = f(v)$ for $v \in W$ and $f'(v) = 0$ otherwise is an eigenfunction of G affording λ.*

Theorem 2.14 ([134]). *Let f be an eigenfunction affording λ of a graph G with n vertices. Let N_v be the set of neighbors of v. Suppose $f(u) = f(v) = 0$, where $N_u \cap N_v = \emptyset$. Let G' be the graph on $n-1$ vertices obtained by coalescing u and v into a single vertex, which is adjacent in G' precisely to those vertices that are adjacent in G to u or to v. The function f' obtained by restricting f to $V(G) \setminus \{u\}$ is an eigenfunction of G' affording λ.*

If G is a regular graph, then the eigenvalues of the Laplacian are determined by the eigenvalues of the adjacency matrix.

Proposition 2.15. *Let G be a k-regular graph. If the adjacency matrix $\mathbf{A}(G)$ has eigenvalues $\lambda_1, \ldots, \lambda_n$, then the Laplacian $\mathbf{L}(G)$ has eigenvalues $k - \lambda_1, \ldots, k - \lambda_n$.*

Proof. If G is k-regular, then $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G) = k\mathbf{I} - \mathbf{A}$. Thus every eigenfunction of $\mathbf{A}$ with eigenvalue λ is an eigenfunction of $\mathbf{L}(G)$ with eigenvalue $k - \lambda$. □

The next well-known result describes the relation between the Laplacian spectrum of G and the Laplacian spectrum of its complement G^c. The matrix $\mathbf{J}$ is the $n \times n$ matrix each of whose entries are 1.

Theorem 2.16. *If G is a graph with n vertices and f is an eigenfunction of $\mathbf{L}(G)$ with eigenvalue $\lambda \neq 0$, then f is an eigenfunction of $\mathbf{L}(G^c)$ with eigenvalue $n - \lambda$.*

Proof. We start observing that $\mathbf{L}(G) + \mathbf{L}(G^c) = n\mathbf{I} - \mathbf{J}$ and $\mathbf{J}f = 0$ as f is orthogonal to the constant function $\mathbf{1}$. Then,

$$nf = (n\mathbf{I} - \mathbf{J})f = \mathbf{L}(G)f + \mathbf{L}(G^c)f = \lambda f + \mathbf{L}(G^c)f \ .$$

Therefore, $\mathbf{L}(G^c)f = (n - \lambda)f$. □

2.6 Graph Automorphisms and Eigenfunctions

It is sometimes possible to infer directly from the graph structure at which vertices some or all eigenfunctions of $\mathbf{L}(G)$ vanish. Theorem 2.11 is an example. Symmetry properties of G are particularly useful for this purpose.

An automorphism of a graph G is a permutation of its vertex set $V(G)$ that maps edges onto edges and nonedges onto nonedges. The set of all automorphisms of G forms a group. We denote this *automorphism group* of G by $\mathrm{Aut}(G)$. For an $X \in \mathrm{Aut}(G)$ and a given eigenfunction f we define the function Xf by

$$Xf(v) = f(X(v)) \ .$$

Moreover

$$V_X = \{v \in V : X(v) = v\} \qquad \text{and} \qquad O_X(v) = \{X^k(v) : k \in \mathbb{Z}\}$$

denote the set of vertices that are fixed under the action of X and the orbit of the vertex v under the action of X, respectively.

Lemma 2.17. *Let $X \in \mathrm{Aut}(G)$ for some graph G. If f is an eigenfunction of $\mathbf{L}(G)$ corresponding to eigenvalue λ, then Xf is also an eigenfunction of λ.*

Proof. $\mathbf{L}(Xf)(v) = \sum_{w\sim v}(Xf(v) - Xf(w)) = \sum_{w\sim v}(f(X(v)) - f(X(w))) = \sum_{w\sim X(v)}(f(X(v)) - f(w)) = \mathbf{L}f(X(v)) = \lambda f(X(v)) = \lambda Xf(v)$. □

Theorem 2.18. *For an eigenfunction f and an automorphism $X \in \mathrm{Aut}(G)$ one of the following three cases holds:*

(1) $Xf = f$. In particular, f is constant on every orbit $O_X(v)$.
(2) $Xf = -f$, and f vanishes on all orbits of odd size. In particular, f vanishes on the fixed points V_X. Moreover, there must be an orbit of even size.
(3) Xf and f are linearly independent, and consequently λ is an eigenvalue of multiplicity greater than one.

Proof. Let s denote the size of the orbit $O_X(v)$ of vertex v ($s = 1$ if $v \in V_X$), i.e., $X^s v = v$. Assume $Xf = \alpha f$ for some $\alpha \in \mathbb{R}$. Then we find $f(v) = f(X^s v) = Xf(X^{s-1}v) = \alpha f(X^{s-1}v) = \cdots = \alpha^s f(v)$. Thus $f(v) = 0$ and f vanishes on the orbit of v, or $\alpha^s = 1$ and hence $\alpha = 1$ (case (1)), or $\alpha = -1$ (case (2)). Obviously if $f(v) = X^s f(v) = (-1)^s f(v)$ then f vanishes on all orbits of odd size s and there must be an orbit of even size since otherwise f would be identical to zero. Another immediate consequence of these considerations is that when neither (1) nor (2) holds, then Xf and f are linearly independent (case (3)). □

Theorem 2.19. *Let $X \in \mathrm{Aut}(G)$ and let f_1 and f_2 be Laplacian eigenfunctions of G with properties (1) and (2) of Thm. 2.18, respectively. Then f_1 and f_2 are orthogonal, i.e., $\langle f_1, f_2\rangle = 0$.*

Proof. Since X is a permutation operator on V, we have $X^t X = I$. Thus we find $\langle f_1, f_2\rangle = \langle X^t X f_1, f_2\rangle = \langle Xf_1, Xf_2\rangle = \langle f_1, -f_2\rangle = -\langle f_1, f_2\rangle$ and the proposition follows. □

2.7 Quasi-Abelian Cayley Graphs

In highly symmetric graphs one can expect a close connection between eigenfunctions of the graph Laplacian and group-theoretic properties. We exploit this connection here to derive explicit expressions for the eigenfunctions of the graph Laplacian of a class of highly symmetric graphs.

Let G be a finite group and let S be a symmetric set of generators of G, i.e., $\langle S\rangle = \mathsf{G}$, $S = S^{-1}$, and $\imath \notin S$, where $\imath$ is the identity of G. A graph

$\Gamma(\mathsf{G}, S)$ with vertex set G and edges $\{s, t\}$ if and only if $t^{-1}s \in S$ is called a *Cayley graph*. A Cayley graph $\Gamma(\mathsf{G}, S)$ is called *quasi-Abelian* if S is the union of some conjugacy classes of G.

Cayley graphs are vertex transitive and hence regular. The characteristic function of S will be denoted by $\Theta : \mathsf{G} \to \{0, 1\}$. Clearly, a Cayley graph on a commutative group is quasi-Abelian, because in this case each group element forms its own conjugacy class. Some interesting properties of quasi-Abelian Cayley graphs are discussed in [172, 179].

In the case of Cayley graphs we have to distinguish between the "Fourier series expansion" (1.5) with respect to the Laplacian matrix of the graph $\Gamma(\mathsf{G}, S)$, and the representation theoretical Fourier transformation on the group G itself. It should not come as a surprise that there is an intimate connection between these two. In fact, the connection between the algebraic properties of $\Gamma(\mathsf{G}, S)$ and the representation theory of the underlying group G derives from the following simple facts: The *regular representation* $\boldsymbol{\rho}_{\text{reg}}$ of G is defined by

$$\boldsymbol{\rho}_{\text{reg}}(s) f(t) = f(s^{-1}t)$$

for any $f \colon \mathsf{G} \longrightarrow \mathbb{C}$. Substituting Θ for f we find $\boldsymbol{\rho}_{\text{reg}}(s)\Theta(t) = \Theta(s^{-1}t) = 1$ if $\{t, s\}$ is an edge of $\Gamma(\mathsf{G}, S)$ and 0 otherwise. Thus we may write the adjacency matrix $\mathbf{A}(\mathsf{G}, S)$ of $\Gamma(\mathsf{G}, S)$ in the form

$$\mathbf{A}(\mathsf{G}, S) = \sum_{s \in S} \boldsymbol{\rho}_{\text{reg}}(s) \ .$$

For any function $f \colon \mathsf{G} \to \mathbb{C}$ and any matrix representation $\varrho = \{\boldsymbol{\rho}(s)\}_{s \in \mathsf{G}}$ of G we call the matrix sum

$$\widehat{f}(\varrho) = \sum_{x \in \mathsf{G}} f(x) \boldsymbol{\rho}(x)$$

the (group theoretic) *Fourier Transform* of f at ϱ. Consider a complete set $\{\varrho^1, \dots, \varrho^h\}$ of inequivalent irreducible matrix representations of G. Let d_k denote the dimension of ϱ^k. Then

$$f(s) = \frac{1}{|\mathsf{G}|} \sum_{k=1}^{h} d_k \operatorname{tr}(\boldsymbol{\rho}^k(s^{-1}))\, \widehat{f}(\varrho^k)$$

inverts the Fourier transform.

Following e.g. [55, Sect. 8A] we assume that the irreducible representations ϱ^k are unitary, i.e., that $\boldsymbol{\rho}^k(t)^* = \boldsymbol{\rho}^k(t^{-1})$ and introduce

$$\tilde{\rho}^k_{ij}(s) := \sqrt{d_k} \boldsymbol{\rho}^k_{ji}(s^{-1}) \ .$$

These functions are orthonormal w.r.t. the scalar product

$$\langle \varphi, \psi \rangle = \frac{1}{|\mathsf{G}|} \sum_{s \in |\mathsf{G}|} \varphi(s) \psi^*(s)$$

and form a new basis for the vector space of functions of G. Now we are in the position to state the main result of this section.

Theorem 2.20 ([151]). *Let $\Gamma(\mathsf{G}, S)$ be a quasi-Abelian Cayley graph with a finite group G.*

(i) The function $\varepsilon_{ij}^k : \mathsf{G} \to \mathbb{C}$ defined as

$$\varepsilon_{ij}^k(u) = \frac{1}{\sqrt{|\mathsf{G}|}} \tilde{\rho}_{ij}^k(u) = \sqrt{\frac{d_k}{|\mathsf{G}|}} \boldsymbol{\rho}_{ij}^k(u^{-1})$$

is a normalized eigenfunction of $\mathbf{L}(\Gamma)$ with eigenvalue

$$\lambda_k = |S| - \frac{1}{d_k} \sum_{s \in S} \chi_k(s)$$

where $\chi_k(s) = \mathrm{tr}(\boldsymbol{\rho}^k(s))$ is the character of ϱ^k at s.

(ii) All quasi-Abelian Cayley graphs on G have a common basis of eigenfunctions and hence their Laplacian matrices commute.

Proof. (i) We verify by explicit computation that $\tilde{\rho}_{ij}^k$ is an eigenfunction of the adjacency matrix:

$$\begin{aligned}
\sum_{u \in \mathsf{G}} \mathbf{A}_{vu} \tilde{\rho}_{ij}^k(u) &= \sum_{u \in \mathsf{G}} \Theta(vu^{-1}) \tilde{\rho}_{ij}^k(u) \\
&= \sum_{u \in \mathsf{G}} \left\{ \frac{1}{|\mathsf{G}|} \sum_{r,s,t} \sqrt{d_r} \widehat{\Theta}_{ts}(\rho^r) \tilde{\rho}_{st}^r(uv^{-1}) \right\} \tilde{\rho}_{ij}^k(u) \\
&= \sum_{u \in \mathsf{G}} \frac{1}{|\mathsf{G}|} \sum_{r,s,t} \widehat{\Theta}_{ts}(\varrho^r) \sum_y \tilde{\rho}_{ys}^{r*}(u) \tilde{\rho}_{yt}^r(v) \tilde{\rho}_{ij}^k(u) \\
&= \sum_{r,s,t} \widehat{\Theta}_{ts}(\varrho^r) \sum_y \tilde{\rho}_{yt}^r(v) \frac{1}{|\mathsf{G}|} \sum_{u \in \mathsf{G}} \tilde{\rho}_{ij}^k(u) \tilde{\rho}_{ys}^{r*}(u) \\
&= \sum_{r,s,t} \widehat{\Theta}_{ts}(\varrho^r) \sum_y \tilde{\rho}_{yt}^r(v) \delta_{kr} \delta_{iy} \delta_{js} = \sum_t \widehat{\Theta}_{tj}(\varrho^k) \tilde{\rho}_{it}^k(v) \; .
\end{aligned}$$

Here we have used that $\boldsymbol{\rho}^k(st^{-1}) = \boldsymbol{\rho}^k(s)\boldsymbol{\rho}^k(t^{-1}) = \boldsymbol{\rho}^k(s)\boldsymbol{\rho}^{k*}(t)$ translates to

$$\sqrt{d_r} \tilde{\rho}_{st}^r(vu^{-1}) = \sum_{y=1}^{h} \tilde{\rho}_{ys}^{r*}(u) \tilde{\rho}_{yt}^r(v) \; .$$

Next we use the fact that Θ is a class function. Hence its Fourier transform is diagonal

$$\widehat{\Theta}(\rho^k) = \frac{1}{d_k} \sum_{s \in S} \chi_k(s) \, \mathbf{I}_{d_k}$$

where $\chi_k(s) = \mathrm{tr}(\boldsymbol{\rho}^k(s))$ is the character of the representation ϱ^k at s. We have therefore

$$\sum_{u \in \mathsf{G}} \mathbf{A}_{vu} \tilde{\rho}^k_{ij}(u) = \sum_t \frac{1}{d_k} \sum_{s \in S} \chi_k(s) \delta_{tj} \tilde{\rho}^k_{it}(v) = \frac{1}{d_k} \sum_{s \in S} \chi_k(s) \times \tilde{\rho}^k_{ij}(v) \ .$$

Changing the normalizations back to the standard scalar product of $\mathbb{C}$ and using $\mathbf{L} = |S|\mathbf{I} - \mathbf{A}$ leads to claim (i) of the theorem.

(ii) We have just shown that $\{\tilde{\rho}^{ij}\}$ is an orthonormal basis of eigenfunctions of $\mathbf{L}$ whenever S is the union of conjugacy classes of G. Thus the Laplacian matrices of all quasi-Abelian Cayley graphs of the group G share a common orthonormal basis of eigenfunctions. Since the graph Laplacians are symmetric matrices, they commute under these circumstances. □

Theorem 2.20 generalizes the following well known result for Abelian Cayley graphs which is discussed e.g. by Lovász [128]:

Corollary 2.21. *Let* G *be a commutative group, and let* S *be a symmetric set of generators of* G*. Then the irreducible characters* χ_k *of* G *are eigenfunctions of* $\mathbf{A}(\mathsf{G}, S)$ *with corresponding eigenvalue* $\Lambda_k = \sum_{s \in S} \chi_k(s)$*.*

2.8 The Perron-Frobenius Theorem

Let $\mathbf{A}$ be an $n \times n$ real symmetric matrix. Analogously to the generalized Laplacians we can associate a graph G such that two vertices u and v are connected by an edge if and only if $A_{uv} \neq 0$. Then $\mathbf{A}$ is called *irreducible* if its underlying graph is connected[1].

Theorem 2.22 (Perron-Frobenius Theorem). *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *be real symmetric irreducible nonnegative* $n \times n$ *matrices. Then*

(i) the spectral radius $\rho(\mathbf{A})$ *is a simple eigenvalue of* $\mathbf{A}$*. If* $\mathbf{x}$ *is an eigenfunction for* $\rho(\mathbf{A})$*, then no entries of* x *are zero, and all have the same sign.*
(ii) If moreover $\mathbf{A} - \mathbf{B}$ *is nonnegative, then* $\rho(\mathbf{B}) \leq \rho(\mathbf{A})$*, with equality if and only if* $\mathbf{B} = \mathbf{A}$*.*

For a proof see, e.g., [100].

We can apply this theorem to get a statement about the smallest eigenvalue λ_1 and its eigenfunctions of a generalized Laplacian of G.

Corollary 2.23. *Let* G *be a connected graph with a generalized Laplacian* $\mathbf{M}$*. Then the smallest eigenvalue* λ_1 *of* $\mathbf{M}$ *is simple and the corresponding eigenfunction can be taken to have all entries positive.*

[1] A nonsymmetric matrix is called irreducible if the corresponding graph is strongly connected, i.e., if, for all $u, v \in V$, there is a *directed* path from u to v. The Perron-Frobenius Theorem then holds as well.

Proof. We use an argument of Godsil and Royle [85]. If $\mathbf{M}$ is a generalized Laplacian of G, then for any c, the matrix $\mathbf{M} - c\mathbf{I}$ is a generalized Laplacian of G with the same eigenfunctions as $\mathbf{M}$. We choose a constant c such that all diagonal entries of $\mathbf{M} - c\mathbf{I}$ are nonpositive. As a consequence of the Perron-Frobenius Theorem, the largest eigenvalue of $-\mathbf{M} + c\mathbf{I}$ is simple and the associated eigenfunction may be taken to have only positive entries. □

A positive eigenfunction to the smallest eigenvalue λ_1 of $\mathbf{M}$ of a connected graph is called a *Perron vector* of G.