Laplace operator on weighted graphs

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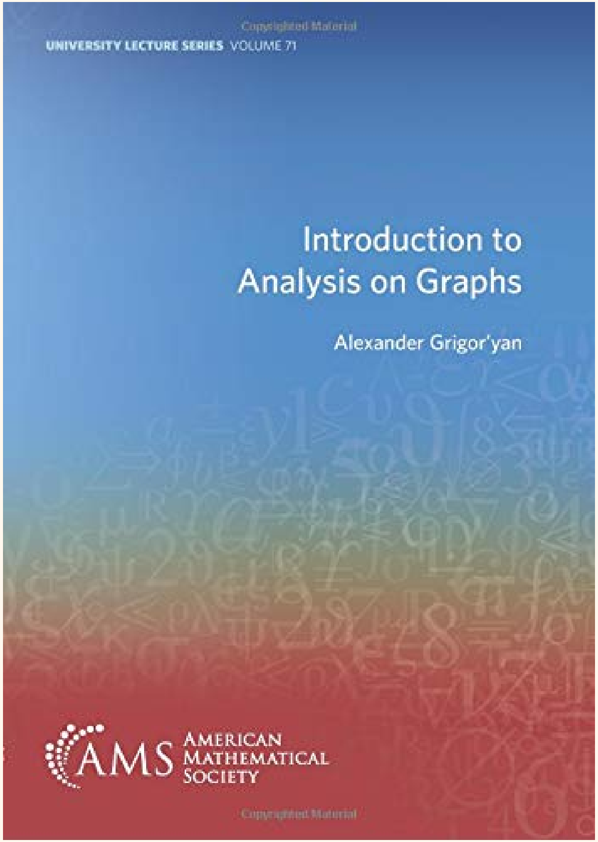
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1 Laplace operator on finite graphs

1.1 The notion of graph

A graph is a pair (V, E) where V is a set of *vertices* and E is a set of *edges*, that is, E consists of some unordered pairs (x, y) where x, y are distinct vertices. We write

$$x \sim y \quad \text{if} \quad (x, y) \in E.$$

In this case we say: x is connected to y, or x is joint to y, or x is adjacent to y, or x is a neighbor of y.

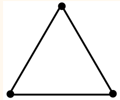
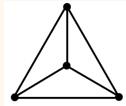
The edge (x, y) will also be denoted by $\overline{xy}$.

A graph (V, E) is called *finite* if the number $|V|$ of vertices is finite. For each vertex x, define its degree

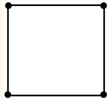
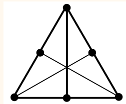
$$\deg(x) = \#\{y \in V : x \sim y\}.$$

The graph is called *regular* if $\deg(x)$ is the same for all $x \in V$. Consider some examples.

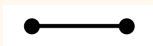
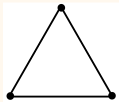
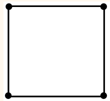
1. A complete graph K_n: $|V| = n$ and $i \sim j$ for any two distinct $i, j \in V$.

$K_2 =$  $K_3 =$  $K_4 =$ 

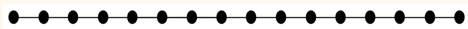
2. A complete bipartite graph $K_{n,m}$: $V = V^+ \sqcup V^-$, where $|V^+| = n$ and $|V^-| = m$, and the edges are defined as follows: $i \sim j$ if either $i \in V^+$ and $j \in V^-$ or $i \in V^-$ and $j \in V^+$.

$K_{1,1} =$  $K_{2,2} =$  $K_{3,3} =$ 

3. A cycle graph $C_m = \mathbb{Z}_m$: $V = \{0, 1, ..., m-1\}$, and $i \sim j$ if $i - j = \pm 1 \bmod m$.

$\mathbb{Z}_2 =$  $\mathbb{Z}_3 =$  $\mathbb{Z}_4 =$ 

3. A path graph P_m : $V = \{0, 1, ..., m-1\}$, and $i \sim j$ if $|i - j| = 1$.

$P_{16} =$ 

Product of graphs.

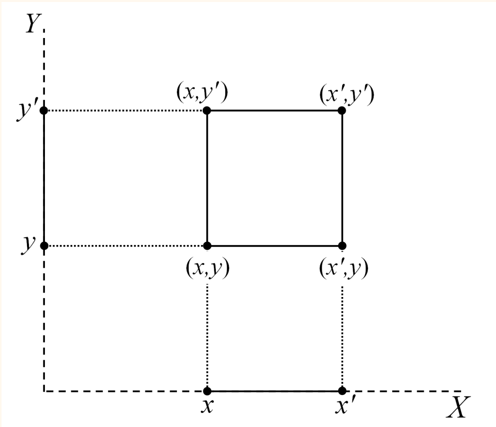
Definition. The *Cartesian product* of graphs (X, E_1) and (Y, E_2) is the graph

$$(V, E) = (X, E_1) \,\square\, (Y, E_2)\,,$$

where $V = X \times Y$ is the set of pairs (x, y) where $x \in X$ and $y \in Y$, and the set E of edges is defined by

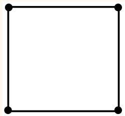
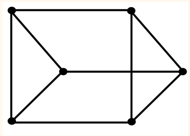
$$(x, y) \sim (x', y) \text{ if } x' \sim x \quad \text{and} \quad (x, y) \sim (x, y') \quad \text{if } y \sim y', \tag{1.1}$$

which is illustrated on the following diagram:



Clearly, we have $|V| = |X|\,|Y|$ and $\deg(x,y) = \deg(x) + \deg(y)$ for all $x \in X$ and $y \in Y$.

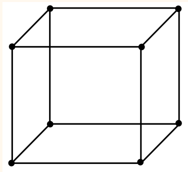
For example, we have

$\mathbb{Z}_2 \square \mathbb{Z}_2 = \mathbb{Z}_4 =$  and $\mathbb{Z}_2 \square \mathbb{Z}_3 =$ 

This definition can be iterated to define the product of a finite sequence of graphs. The graph

$$\mathbb{Z}_2^n := \underbrace{\mathbb{Z}_2 \square \mathbb{Z}_2 \square \ldots \square \mathbb{Z}_2}_{n}$$

is called the n-dimensional *binary cube*. For example,

$\mathbb{Z}_2^3 =$ 

Cayley graphs. Let $(G, *)$ be a group and S be a subset of G with the property that if $x \in S$ then $x^{-1} \in S$ and that $e \notin S$. Such a set S will be called *symmetric*.

A group G and a symmetric set $S \subset G$ determine a graph (V, E) as follows: the set V of vertices coincides with G, and the set E of edges is defined by the relation $\sim$ as follows:

$$x \sim y \ \Leftrightarrow \ x^{-1} * y \in S,$$

or, equivalently,

$$x \sim y \Leftrightarrow \ y = x * s \text{ for some } s \in S.$$

Note that the relation $x \sim y$ is symmetric in x, y, that is, $x \sim y$ implies $y \sim x$, because, by the symmetry of S,

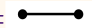
$$y^{-1} * x = \left(x^{-1} * y\right)^{-1} \in S.$$

Hence, (V, E) is indeed a graph.

Definition. The graph (V, E) defined as above is denoted by (G, S) and is called the *Cayley graph* of the group G with the *edge generating* set S.

There may be many different Cayley graphs based on the same group since they depend also on the choice of S. It follows from the construction that $\deg(x) = |S|$ for any $x \in V$. In particular, if S is finite then the graph (V, E) is locally finite.

Consider some example. Here $(\mathbb{Z}_m, +)$ is the additive group of residues $\bmod\, m$ and $\mathbb{Z}_m = \{0, 1, ..., m-1\}$, and $(\mathbb{Z}^n, +)$ is the additive group of n-tuples $(x_1, ..., x_n)$ with $x_k \in \mathbb{Z}$.

1. Let $G = (\mathbb{Z}_2, +)$. The only possibility for S is $S = \{1\}$. Then $(\mathbb{Z}_2, S) =$ .

2. Let $G = (\mathbb{Z}_m, +)$ where $m > 2$, and $S = \{\pm 1\}$. That is, each residue $k = 0, 1, ..., m-1$ has two neighbors: $k-1$ and $k+1 \bmod m$. The graph $(\mathbb{Z}_m, S)$ coincides with the m-cycle.

3. Let $G = (\mathbb{Z}_m, +)$ with the symmetric set $S = \mathbb{Z}_m \setminus \{0\}$. That is, every two distinct elements $x, y \in \mathbb{Z}_m$ are connected by an edge. Hence, $(\mathbb{Z}_m, S) = K_m$.

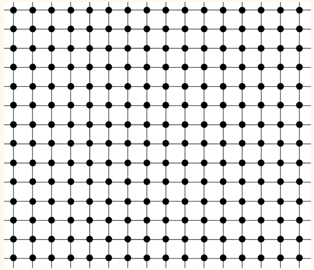
4. $G = (\mathbb{Z}, +)$ and $S = \{1, -1\}$. Then $x \sim y$ if $x - y = 1$ or $x - y = -1$. Hence, (G, S) coincides with the lattice graph $\mathbb{Z}$:

If $S = \{\pm 1, \pm 2\}$ then $x \sim y$ if $|x-y| = 1$ or $|x-y| = 2$ so that we obtain a different graph.

5. Let $G = (\mathbb{Z}^n, +)$. Let S consist of points $(x_1, ..., x_n) \in \mathbb{Z}^n$ such that exactly one of x_i is equal to ± 1 and the others are 0. The connection $x \sim y$ means that $x - y$ has exactly one component ± 1, and all others are 0.

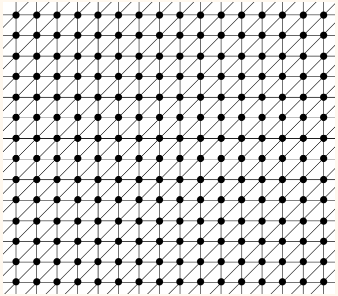
The Cayley graph of $(\mathbb{Z}^n, S)$ with this S is called the lattice graph $\mathbb{Z}^n$.

For example, in the case $n = 2$ we have $S = \{(1,0), (-1,0), (0,1), (0,-1)\}$ and $(\mathbb{Z}^2, S)$ is



6. Here is the Cayley graph $(\mathbb{Z}^2, S)$ with another edge generating set

$$S = \{(1,0), (-1,0), (0,1), (0,-1), (1,1), (-1,-1)\}.$$



1.2 The weighted Laplace operator

Definition. A *weighted graph* is a couple $((V, E), \mu)$ where (V, E) is a graph and μ_{xy} is a non-negative function on $V \times V$ such that

1. $\mu_{xy} = \mu_{yx}$;
2. $\mu_{xy} > 0$ if and only if $x \sim y$.

The weighted graph is also denoted by (V, μ) because μ determines the set of edges E.

Example. Set $\mu_{xy} = 1$ if $x \sim y$ and $\mu_{xy} = 0$ otherwise. Then μ_{xy} is a weight. This specific weight is called *simple*.

Any weight μ_{xy} gives rise to a function on vertices as follows:

$$\mu(x) = \sum_{\{y \in V, y \sim x\}} \mu_{xy} = \sum_{y \in V} \mu_{xy}. \tag{1.2}$$

Then $\mu(x)$ is called the weight of the vertex x. It can be extended to a measure of subsets: for any subset $A \subset V$, set $\mu(A) = \sum_{x \in A} \mu(x)$.

For example, if the weight μ_{xy} is simple then $\mu(x) = \deg(x)$ and $\mu(A) = \sum_{x \in A} \deg(x)$.

Definition. Let (V, μ) be a finite weighted graph without isolated points. For any function $f : V \to \mathbb{R}$, define the function $\Delta_\mu f$ by

$$\Delta_\mu f(x) = \frac{1}{\mu(x)} \sum_{y \sim x} f(y)\, \mu_{xy} - f(x)\,. \tag{1.3}$$

The operator Δ_μ is called the (*weighted*) *Laplace operator* of (V, μ).

This operator can also be written in equivalent forms as follows:

$$\Delta_\mu f(x) = \frac{1}{\mu(x)} \sum_{y \in V} f(y)\, \mu_{xy} - f(x) = \frac{1}{\mu(x)} \sum_{y \in V} (f(y) - f(x))\, \mu_{xy}. \tag{1.4}$$

Example. If μ is a simple weight then we obtain the Laplace operator of the graph (V, E):

$$\Delta f(x) = \frac{1}{\deg(x)} \sum_{y \sim x} f(y) - f(x)\,.$$

Denote by $\mathcal{F}$ the set of all real-valued functions on V. Then $\mathcal{F}$ is a linear space with respect to addition of functions and multiplication by a constant, and $\dim \mathcal{F} = |V|$. The Laplace operator Δ_μ is a linear operator in $\mathcal{F}$, and $\Delta_\mu 1 = 0$.

Define the *Markov kernel* $P(x,y) = \frac{\mu_{xy}}{\mu(x)}$ so that

$$\Delta_\mu f(x) = \sum_y P(x,y) f(y) - f(x).$$

Defining the Markov operator P on $\mathcal{F}$ by

$$Pf(x) = \sum_y P(x,y) f(y),$$

we see that the Laplace operator Δ_μ and the Markov operator P are related by a simple identity $\Delta_\mu = P - \mathrm{id}$, where id is the identity operator in $\mathcal{F}$.

Since

$$\sum_{y \in V} P(x,y) \equiv 1,$$

the Markov kernel determine the Markov chain on V, that is, a random walk $\{X_n\}_{n=0}^{\infty}$ such that

$$\mathbb{P}(X_{n+1} = y \mid X_n = x) = P(x,y).$$

Moreover, this random walk is reversible because

$$P(x,y)\mu(x) = \mu_{xy} = P(y,x)\mu(y).$$

The operator Δ_μ is the generator of this random walk.

Green's formula. Define for all $x, y \in V$ the *difference operator* $\nabla_{xy} : \mathcal{F} \to \mathbb{R}$:

$$\nabla_{xy} f = f(y) - f(x),$$

so that

$$\Delta_\mu f(x) = \frac{1}{\mu(x)} \sum_{y \in V} (\nabla_{xy} f) \mu_{xy}.$$

For any set $\Omega \subset V$ denote $\Omega^c = V \setminus \Omega$.

Theorem 1.1 (Green's formula) *Let (V, μ) be a weighted graph without isolated points, and let Ω be a non-empty finite subset of V. Then, for any two functions f, g on V,*

$$\sum_{x \in \Omega} \Delta_\mu f(x) g(x) \mu(x) = -\frac{1}{2} \sum_{x,y \in \Omega} (\nabla_{xy} f)(\nabla_{xy} g) \mu_{xy} + \sum_{x \in \Omega, y \in \Omega^c} (\nabla_{xy} f) g(x) \mu_{xy} \tag{1.5}$$

If $\Omega = V$ then Ω^c is empty so that the last "boundary" term in (1.5) vanishes, and we obtain

$$\sum_{x \in V} \Delta_\mu f(x) g(x) \mu(x) = -\frac{1}{2} \sum_{x,y \in V} (\nabla_{xy} f)(\nabla_{xy} g) \mu_{xy}. \tag{1.6}$$

Proof. We have

$$
\begin{aligned}
\sum_{x\in\Omega}\Delta_\mu f(x)g(x)\mu(x) &= \sum_{x\in\Omega}\left(\frac{1}{\mu(x)}\sum_{y\in V}\left(\nabla_{xy}f\right)\mu_{xy}\right)g(x)\mu(x) \\
&= \sum_{x\in\Omega}\sum_{y\in V}\left(\nabla_{xy}f\right)g(x)\mu_{xy} \\
&= \sum_{x\in\Omega}\sum_{y\in\Omega}\left(\nabla_{xy}f\right)g(x)\mu_{xy}+\sum_{x\in\Omega}\sum_{y\in\Omega^c}\left(\nabla_{xy}f\right)g(x)\mu_{xy} \\
&= \sum_{y\in\Omega}\sum_{x\in\Omega}\left(\nabla_{yx}f\right)g(y)\mu_{xy}+\sum_{x\in\Omega}\sum_{y\in\Omega^c}\left(\nabla_{xy}f\right)g(x)\mu_{xy},
\end{aligned}
$$

where in the last line we have switched notation of the variables x and y in the first sum using $\mu_{xy}=\mu_{yx}$. Adding together the last two lines and dividing by 2, we obtain

$$
\sum_{x\in\Omega}\Delta_\mu f(x)g(x)\mu(x)=\frac{1}{2}\sum_{x,y\in\Omega}\left(\nabla_{xy}f\right)\left(g(x)-g(y)\right)\mu_{xy}+\sum_{x\in\Omega,y\in\Omega^c}\left(\nabla_{xy}f\right)g(x)\mu_{xy},
$$

which was to be proved. ∎

Eigenvalues of the Laplace operator. Let $|V| = N$ so that $\dim \mathcal{F} = N$. We investigate the spectrum of the operator $\mathcal{L} = -\Delta_\mu$ that is called *positive definite Laplace operator*. This operator acts in $\mathcal{F}$ and, hence, has N (complex) eigenvalues λ determined by $\mathcal{L}f = \lambda f$ for some $f \in \mathcal{F} \setminus \{0\}$ that is called an *eigenfunction* of $\mathcal{L}$.

In the next examples the weight μ_{xy} is simple so that

$$\mathcal{L}f(x) = f(x) - \frac{1}{\deg(x)} \sum_{y \sim x} f(y).$$

1. For $\mathbb{Z}_2 = \bullet_0 - \bullet_1$ we have

$$\mathcal{L}f(0) = f(0) - f(1), \quad \mathcal{L}f(1) = f(1) - f(0)$$

and, in the matrix form,

$$\begin{pmatrix} \mathcal{L}f(0) \\ \mathcal{L}f(1) \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} f(0) \\ f(1) \end{pmatrix}.$$

Hence, the eigenvalues of $\mathcal{L}$ coincide with those of the matrix $\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$. Its characteristic equation is $(1-\lambda)^2 - 1 = 0$, whence we obtain two eigenvalues $\lambda = 0$ and $\lambda = 2$.

2. For $\mathbb{Z}_3$ we have

$$\mathcal{L}f(x) = f(x) - \frac{1}{2}\left(f(x-1) + f(x+1)\right), \quad x = 0, 1, 2 \bmod 3.$$

The action of $\mathcal{L}$ can be written as a matrix multiplication:

$$\begin{pmatrix} \mathcal{L}f(0) \\ \mathcal{L}f(1) \\ \mathcal{L}f(2) \end{pmatrix} = \begin{pmatrix} 1 & -1/2 & -1/2 \\ -1/2 & 1 & -1/2 \\ -1/2 & -1/2 & 1 \end{pmatrix} \begin{pmatrix} f(0) \\ f(1) \\ f(2) \end{pmatrix}.$$

The characteristic equation of the above 3×3 matrix is $\lambda^3 - 3\lambda^2 + \frac{9}{4}\lambda = 0$. Hence, we obtain the following eigenvalues of $\mathcal{L}$: $\lambda = 0$ (simple) and $\lambda = 3/2$ with multiplicity 2.

3. For the path graph $P_3 = \bullet_0 - \bullet_1 - \bullet_2$ we have

$$\mathcal{L}f(0) = f(0) - f(1), \quad \mathcal{L}f(1) = f(1) - \frac{1}{2}\left(f(0) + f(2)\right), \quad \mathcal{L}f(2) = f(2) - f(1),$$

$$\text{the matrix of } \mathcal{L} = \begin{pmatrix} 1 & -1 & 0 \\ -1/2 & 1 & -1/2 \\ 0 & -1 & 1 \end{pmatrix}.$$

The characteristic equation is $\lambda^3 - 3\lambda^2 + 2\lambda = 0$ whence $\lambda = 0$, $\lambda = 1$, $\lambda = 2$.

Let (V, μ) be any finite weighted graph. Define in $\mathcal{F}$ an inner product by

$$(f, g) := \sum_{x \in V} f(x)\, g(x)\, \mu(x).$$

Lemma 1.2 *The operator $\mathcal{L}$ is symmetric: $(\mathcal{L}f, g) = (f, \mathcal{L}g)$ for all $f, g \in \mathcal{F}$.*

Proof. Indeed, by the Green formula (1.6), we have

$$(\mathcal{L}f, g) = -\sum_{x \in V} \Delta_\mu f(x)\, g(x)\, \mu(x) = \frac{1}{2} \sum_{x,y \in V} (\nabla_{xy} f)(\nabla_{xy} g)\, \mu_{xy} = (f, \mathcal{L}g).$$

Alternatively, since $\mathcal{L} = \mathrm{id} - P$, it suffices to prove that P is symmetric. Using the reversibility of P, we obtain

$$\begin{aligned} (Pf, g) &= \sum\nolimits_x Pf(x)\, g(x)\, \mu(x) = \sum\nolimits_x \sum\nolimits_y P(x, y)\, f(y)\, g(x)\, \mu(x) \\ &= \sum\nolimits_x \sum\nolimits_y P(y, x)\, f(y)\, g(x)\, \mu(y) = (Pg, f). \end{aligned}$$

∎

Corollary 1.3 *All the eigenvalues of $\mathcal{L}$ are real.*

To state the next theorem, we need the notion of a bipartite graph.

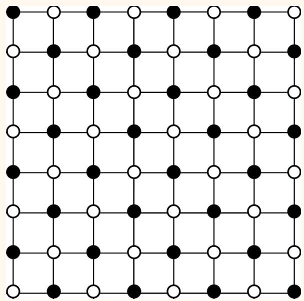
Definition. A graph (V, E) is called *bipartite* if V admits a partition into two non-empty disjoint subsets V^+, V^- such that if both x, y are contained in the same set V^+ or V^- then $x \not\sim y$.

In terms of coloring, one can say that a graph is bipartite if its vertices can be colored by two colors, so that the vertices of the same color are not connected by an edge.

Here are some examples of bipartite graphs.

1. A complete bipartite graph $K_{n,m}$ is bipartite.
2. The cycle graph $\mathbb{Z}_m$ and the path graph P_m are bipartite provided m is even.
3. Product of bipartite graphs is bipartite.

In particular, $\mathbb{Z}_m^n$ and P_m^n are bipartite provided m is even. For the example, here is P_8^2 – a chessboard:



Theorem 1.4 *For any finite, connected, weighted graph (V, μ) with $N = |V| > 1$, the following is true.*

(a) Zero is a simple eigenvalue of $\mathcal{L}$.

(b) All the eigenvalues of $\mathcal{L}$ are contained in $[0, 2]$.

(c) If (V, μ) is not bipartite then all the eigenvalues of $\mathcal{L}$ lie in $[0, 2)$.

Proof. (a) Since $\mathcal{L}1 = 0$, the constant function is an eigenfunction with the eigenvalue 0. Assume now that f is an eigenfunction of the eigenvalue 0 and prove that $f \equiv \text{const}$, which will imply that 0 is a simple eigenvalue. If $\mathcal{L}f = 0$ then it follows from (1.6) with $g = f$ that

$$\sum_{\{x,y \in V : x \sim y\}} (f(y) - f(x))^2 \mu_{xy} = 0.$$

In particular, $f(x) = f(y)$ for any two neighboring vertices x, y. The connectedness of the graph means that any two vertices $x, y \in V$ can be connected to each other by a path $\{x_k\}_{k=0}^m$ where

$$x = x_0 \sim x_1 \sim \ldots \sim x_m = y$$

whence it follows that $f(x_0) = f(x_1) = \ldots = f(x_m)$ and $f(x) = f(y)$. Since this is true for all couples $x, y \in V$, we obtain $f \equiv \text{const}$.

(b) Let λ be an eigenvalue of $\mathcal{L}$ with an eigenfunction f. Using $\mathcal{L}f = \lambda f$ and the Green formula (1.6), we obtain

$$\begin{aligned} \lambda \sum_{x \in V} f^2(x)\mu(x) &= \sum_{x \in V} \mathcal{L}f(x) f(x) \mu(x) \\ &= \frac{1}{2} \sum_{\{x,y \in V : x \sim y\}} (f(y) - f(x))^2 \mu_{xy}. \end{aligned} \tag{1.7}$$

It follows from (1.7) that $\lambda \geq 0$. Using $(a+b)^2 \leq 2(a^2+b^2)$, we obtain

$$\begin{aligned} \lambda \sum_{x \in V} f^2(x)\mu(x) &\leq \sum_{\{x,y \in V : x \sim y\}} \left(f(y)^2 + f(x)^2\right) \mu_{xy} \\ &= \sum_{x,y \in V} f(y)^2 \mu_{xy} + \sum_{x,y \in V} f(x)^2 \mu_{xy} \\ &= \sum_{y \in V} f(y)^2 \mu(y) + \sum_{x \in V} f(x)^2 \mu(x) \\ &= 2 \sum_{x \in V} f(x)^2 \mu(x). \end{aligned} \tag{1.8}$$

It follows from (1.8) that $\lambda \leq 2$.

Alternatively, one can first prove that $\|P\| \leq 1$, which follows from $\sum_y P(x,y) = 1$ and which implies spec $P \subset [-1,1]$, and then conclude that spec $\mathcal{L} = 1 - \operatorname{spec} P \subset [0,2]$.

(c) We need to prove that $\lambda = 2$ is not an eigenvalue. Assume from the contrary that $\lambda = 2$ is an eigenvalue with an eigenfunction f, and prove that (V,μ) is bipartite. Since $\lambda = 2$, all the inequalities in the above calculation (1.8) must become equalities. In particular, we must have for all $x \sim y$ that

$$(f(x) - f(y))^2 = 2\left(f(x)^2 + f(y)^2\right),$$

which is equivalent to

$$f(x) + f(y) = 0.$$

If $f(x_0) = 0$ for some x_0 then it follows that $f(x) = 0$ for all neighbors of x_0. Since the graph is connected, we obtain that $f(x) \equiv 0$, which is not possible for an eigenfunction. Hence, $f(x) \neq 0$ for all $x \in \Gamma$. Then V splits into a disjoint union of two sets:

$$V^+ = \{x \in V : f(x) > 0\} \text{ and } V^- = \{x \in V : f(x) < 0\}.$$

The above argument shows that if $x \in V^+$ then all neighbors of x are in V^-, and vice versa. Hence, (V,μ) is bipartite, which finishes the proof. ∎

Hence, we can enumerate all the eigenvalues of $\mathcal{L}$ in the increasing order as follows:

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_{N-1} \leq 2.$$

Example. As an example of application of Theorem 1.4, let us investigate the solvability of the equation $\mathcal{L}u = f$ for a given $f \in \mathcal{F}$. Since by the Green formula (1.6)

$$\sum_x (\mathcal{L}u)(x)\,\mu(x) = 0,$$

a necessary condition for solvability is

$$\sum_x f(x)\,\mu(x) = 0. \tag{1.9}$$

Assuming that, let us show that the equation $\mathcal{L}u = f$ has a solution. Indeed, condition (1.9) means that $f \perp 1$. Consider the subspace $\mathcal{F}_0$ of $\mathcal{F}$ that consists of all functions orthogonal to 1. Since 1 is the eigenfunction of $\mathcal{L}$ with eigenvalue $\lambda_0 = 0$, the space $\mathcal{F}_0$ is invariant for the operator $\mathcal{L}$, and the spectrum of $\mathcal{L}$ in $\mathcal{F}_0$ is $\lambda_1, ...\lambda_{N-1}$. Since all $\lambda_j > 0$, we see that $\mathcal{L}$ is invertible in $\mathcal{F}_0$, that is, the equation $\mathcal{L}u = f$ has for any $f \in \mathcal{F}_0$ a unique solution $u \in \mathcal{F}_0$ given by $u = \mathcal{L}^{-1}f$.

The next statement contains an additional information about the spectrum of $\mathcal{L}$ for bipartite graphs.

Theorem 1.5 *Let (V,μ) be finite, connected, and bipartite. If λ is an eigenvalue of $\mathcal{L}$ then $2-\lambda$ is also an eigenvalue of $\mathcal{L}$, with the same multiplicity. In particular, 2 is a simple eigenvalue of $\mathcal{L}$.*

Hence, we conclude that a graph is bipartite if and only if $\lambda_{N-1}=2$.

Proof. Since the eigenvalues α of the Markov operator $P=\mathrm{id}-\mathcal{L}$ are related to the eigenvalues λ of $\mathcal{L}$ by $\alpha=1-\lambda$, the claim is equivalent to the following: if α is an eigenvalue of P then $-\alpha$ is also an eigenvalue of P with the same multiplicity (indeed, $\alpha=1-\lambda$ implies $-\alpha=1-(2-\lambda)$). Let V^+,V^- be a partition of V such that $x\sim y$ only if x and y belong to same of the subset V^+,V^-. Given an eigenfunction f of P with the eigenvalue α, consider

$$g(x)=\begin{cases} f(x), & x\in V^+ \\ -f(x), & x\in V^- \end{cases}. \tag{1.10}$$

Let us show that g is an eigenfunction of P with the eigenvalue $-\alpha$. For all $x\in V^+$, we have

$$\begin{aligned} Pg(x) &= \sum_{y\in V} P(x,y)\,g(y)=\sum_{y\in V^-} P(x,y)\,g(y) \\ &= -\sum_{y\in V^-} P(x,y)\,f(y) = -Pf(x) = -\alpha f(x) = -\alpha g(x), \end{aligned}$$

and for $x \in V^-$ we obtain in the same way

$$\begin{aligned} Pg(x) &= \sum_{y \in V^+} P(x,y)\, g(y) \\ &= \sum_{y \in V^+} P(x,y)\, f(y) = Pf(x) = \alpha f(x) = -\alpha g(x)\,. \end{aligned}$$

Hence, $-\alpha$ is an eigenvalue of P with the eigenfunction g.

Let m be the multiplicity of α as an eigenvalue of P, and m' be the multiplicity of $-\alpha$. Let us prove that $m' = m$. There exist m linearly independent eigenfunctions $f_1, ..., f_m$ of the eigenvalue α. Using (1.10), we construct m eigenfunctions $g_1, ..., g_m$ of the eigenvalue $-\alpha$, that are obviously linearly independent, whence we conclude that $m' \geq m$. Since $-(-\alpha) = \alpha$, applying the same argument to the eigenvalue $-\alpha$ instead of α, we obtain the opposite inequality $m \geq m'$, whence $m = m'$.

Finally, since 0 is a simple eigenvalue of $\mathcal{L}$, it follows that 2 is also a simple eigenvalue of $\mathcal{L}$. It follows from the proof that the eigenfunction $g(x)$ with the eigenvalue 2 is as follows: $g(x) = c$ on V^+ and $g(x) = -c$ on V^-, for any non-zero constant c. ∎

1.3 Distance function and expansion rate

Definition. A finite sequence $\{x_k\}_{k=0}^{n}$ of vertices on a graph (V, E) is called a *path* if

$$x_0 \sim x_1 \sim \ldots \sim x_k \sim x_{k+1} \sim \ldots \sim x_n$$

The number n of edges in the path is referred to as the *length* of the path. We say that the path $\{x_k\}_{k=0}^{n}$ connects x_0 and x_n.

Definition. A graph (V, E) is called *connected* if, for any two vertices $x, y \in V$, there is a path connecting x and y. If (V, E) is connected then define the *graph distance* $d(x, y)$ between any two distinct vertices x, y as the minimal length of a path that connects x and y.

The connectedness here is needed to ensure that $d(x, y) < \infty$ for any two points. It is easy to see that on any connected graph, the graph distance is a metric, so that (V, d) is a metric space. For any two non-empty subsets $X, Y \subset V$, set

$$d(X, Y) = \min_{x \in X, y \in Y} d(x, y)$$

Note that $d(X, Y) \geq 0$ and $d(X, Y) > 0$ if and only if X and Y are disjoint.

Let now (V,μ) be a weighted connected graph. For disjoint subsets X,Y of V define one more quantity:

$$l(X,Y)=\frac{1}{2}\ln\frac{\mu(X^c)\,\mu(Y^c)}{\mu(X)\,\mu(Y)},$$

Since $X\subset Y^c$ and $Y\subset X^c$, it follows that $l(X,Y)\geq 0$. Furthermore, $l(X,Y)=0$ if and only if $X=Y^c$. To understand better $l(X,Y)$, express it in terms of the set $Z=V\setminus(X\cup Y)$ so that

$$l(X,Y)=\frac{1}{2}\ln\left(1+\frac{\mu(Z)}{\mu(X)}\right)\left(1+\frac{\mu(Z)}{\mu(Y)}\right).$$

Hence, the quantity $l(X,Y)$ measures "space" between X and Y in terms of the measure of the set Z.

Let $|V|=N$ and let the eigenvalues of the Laplace operator $\mathcal{L}$ on (V,μ) be

$$0=\lambda_0<\lambda_1\leq\ldots\leq\lambda_{N-1}\leq 2.$$

We will use the following notation:

$$\delta=\frac{\lambda_{N-1}-\lambda_1}{\lambda_{N-1}+\lambda_1}, \tag{1.11}$$

so that $\delta\in[0,1)$.

Theorem 1.6 (F.Chung, AG, S.-T.Yau '96) *For any two disjoint sets $X, Y \subset V$, we have*

$$d(X, Y) \leq 1 + \frac{l(X, Y)}{\ln \frac{1}{\delta}} \tag{1.12}$$

(if $\delta = 0$ then set by definition $\frac{l(X,Y)}{\ln \frac{1}{\delta}} = 0$).

Example. Let us show that

$$\operatorname{diam}(V) \leq 1 + \frac{1}{\ln \frac{1}{\delta}} \ln \frac{\mu(V)}{m}, \tag{1.13}$$

where $m = \min_{x \in V} \mu(x)$. Indeed, set in (1.12) $X = \{x\}$, $Y = \{y\}$ where x, y are two distinct vertices. Then

$$l(X, Y) \leq \frac{1}{2} \ln \frac{\mu(V)^2}{\mu(x)\,\mu(y)} \leq \ln \frac{\mu(V)}{m}$$

whence

$$d(x, y) \leq 1 + \frac{1}{\ln \frac{1}{\delta}} \ln \frac{\mu(V)}{m}.$$

Taking in the left hand side the supremum in all $x, y \in V$, we obtain (1.13).

For any subset $X \subset V$, denote by $U_r(X)$ the r-neighborhood of X, that is,

$$U_r(X) = \{y \in V : d(y, X) \leq r\}.$$

Corollary 1.7 *For any non-empty set $X \subset V$ and any integer $r \geq 1$, we have*

$$\mu(U_r(X)) \geq \frac{\mu(V)}{1 + \frac{\mu(X^c)}{\mu(X)}\delta^{2r}}. \tag{1.14}$$

Proof. Set $Y = V \setminus U_r(X)$ so that $U_r(X) = Y^c$ and $d(X, Y) = r + 1$. By (1.12), we have

$$r \leq \frac{1}{2}\frac{1}{\ln\frac{1}{\delta}} \ln \frac{\mu(X^c)\,\mu(Y^c)}{\mu(X)\,\mu(Y)},$$

which implies

$$\delta^{2r}\frac{\mu(X^c)}{\mu(X)} \geq \frac{\mu(Y)}{\mu(Y^c)} = \frac{\mu(V) - \mu(Y^c)}{\mu(Y^c)} = \frac{\mu(V)}{\mu(U_r(X))} - 1,$$

whence (1.14) follows. ■

Example. Given a non-empty set $X \subset V$, define the *expansion rate* of X to be the minimal positive integer R such that

$$\mu\left(U_R\left(X\right)\right) \geq \frac{1}{2}\mu\left(V\right).$$

Imagine a communication network as a graph where the vertices are the communication centers (like computer servers) and the edges are direct links between the centers. If X is a set of selected centers, then it is reasonable to ask, how many steps from X are required to reach the majority (at least 50%) of all centers? This is exactly the expansion rate of X, and the networks with short expansion rate provide better connectivity.

Let X consist of a singe vertex. Then

$$\frac{\mu\left(X^c\right)}{\mu\left(X\right)} \leq \frac{\mu\left(V\right)}{\min_{x\in V}\mu\left(x\right)} =: M, \tag{1.15}$$

and (1.14) yields

$$\mu\left(U_r\left(X\right)\right) \geq \frac{\mu\left(V\right)}{1+M\delta^{2r}}.$$

Hence, if

$$M\delta^{2r} \leq 1, \tag{1.16}$$

then $\mu(U_r(X)) \geq \frac{1}{2}\mu(V)$. The condition (1.16) is equivalent to

$$r \geq \frac{1}{2}\frac{M}{\ln\frac{1}{\delta}},$$

from where we see that the expansion rate R of any singleton satisfies

$$R \leq \frac{1}{2}\left\lceil\frac{\ln M}{\ln\frac{1}{\delta}}\right\rceil. \tag{1.17}$$

Hence, a good communication network should have the number δ as small as possible. For that, all non-zero eigenvalues of $\mathcal{L}$ must lie in a neighborhood of 1. Indeed, if

$$\lambda_1 \text{ and } \lambda_{N-1} \in [1-\varepsilon, 1+\varepsilon] \tag{1.18}$$

then

$$\delta = \frac{\lambda_{N-1}-\lambda_1}{\lambda_{N-1}+\lambda_1} \leq \frac{2\varepsilon}{2-\varepsilon} = \frac{\varepsilon}{1-\varepsilon} \simeq \varepsilon.$$

For many large practical networks, (1.18) holds with

$$\varepsilon \simeq \frac{1}{\ln N}$$

which implies

$$\delta \lesssim \frac{1}{\ln N}.$$

In this case we obtain the following estimate of the expansion rate:

$$R \leq \frac{1}{2} \frac{\ln M}{\ln \frac{1}{\delta}} \lesssim \frac{\ln M}{\ln \ln N}. \tag{1.19}$$

Typically $M \simeq N$ so that M in (1.19) can be replaced by N.

For the internet graph, we have $N \simeq 10^9$ and, hence, $R \lesssim 7$. This very fast expansion rate is called "a small world" phenomenon, and it is actually observed in large communication networks.

The same phenomenon occurs in the *coauthor network*: two mathematicians are connected by an edge if they have a joint publication. Although the number of recorded mathematicians is quite high ($\simeq 10^5$), a few links are normally enough to get from one mathematician to a substantial portion of the entire network. Formula (1.19) gives in this case $R \lesssim 5$.

Proof of Theorem 1.6. Recall that (V, μ) is a weighted connected graph, $N = |V| > 1$. For non-empty disjoint subsets X, Y of V, we define

$$d(X, Y) = \inf_{x \in X, y \in Y} d(x, y)$$

and

$$l(X, Y) = \frac{1}{2} \ln \frac{\mu(X^c)\, \mu(Y^c)}{\mu(X)\, \mu(Y)}. \tag{1.20}$$

Let $0 = \lambda_0 < \lambda_1 \leq ... \leq \lambda_{N-1}$ be the eigenvalues of the weighted Laplacian $\mathcal{L}$. Set

$$\delta = \frac{\lambda_{N-1} - \lambda_1}{\lambda_{N-1} + \lambda_1}. \tag{1.21}$$

We need to prove that

$$\boxed{d(X, Y) \leq 1 + \frac{l(X, Y)}{\ln \frac{1}{\delta}}}. \tag{1.22}$$

As before, $\mathcal{F}$ is the space of all functions $V \to \mathbb{R}$. Let $w_0, w_1, ..., w_{N-1}$ be an orthonormal basis in $\mathcal{F}$ that consists of the eigenfunctions of $\mathcal{L}$, so that $\mathcal{L} w_k = \lambda_k w_k$.

Any function $u \in \mathcal{F}$ admits an expansion in the basis $\{w_k\}$ as follows:

$$u = \sum_{k=0}^{N-1} a_k w_k \tag{1.23}$$

with some coefficients a_k. Since $w_0 = \frac{1}{\|1\|}$ and $a_0 = (u, w_0)$, we obtain

$$a_0 w_0 = \frac{(u,1)}{\|1\|^2} = \frac{1}{\mu(V)} \sum_{x \in V} u(x) \mu(x) =: \bar{u}$$

Denote

$$u' = u - \bar{u} = \sum_{k=1}^{N-1} a_k w_k$$

so that $u = \bar{u} + u'$ and $u' \perp \bar{u}$.

Let $\Phi(\lambda)$ be a polynomial with real coefficient. We have

$$\Phi(\mathcal{L}) u = \sum_{k=0}^{N-1} a_k \Phi(\lambda_k) w_k = \Phi(0) \bar{u} + \sum_{k=1}^{N-1} a_k \Phi(\lambda_k) w_k.$$

If v is another function from $\mathcal{F}$ with expansion

$$v=\sum_{k=0}^{N-1} b_k w_k=\bar{v}+\sum_{k=1}^{N-1} b_k w_k=\bar{v}+v',$$

then

$$\begin{aligned}
(\Phi(\mathcal{L}) u, v) &= (\Phi(0)\,\bar{u}, \bar{v})+\sum_{k=1}^{N-1} a_k b_k \Phi(\lambda_k) \\
&\geq \Phi(0)\,\bar{u}\bar{v}\mu(V)-\max_{1\leq k\leq N-1}|\Phi(\lambda_k)| \sum_{k=1}^{N-1}|a_k|\,|b_k| \\
&\geq \Phi(0)\,\bar{u}\bar{v}\mu(V)-\max_{1\leq k\leq N-1}|\Phi(\lambda_k)|\,\|u'\|\,\|v'\|\,. \qquad (1.24)
\end{aligned}$$

Assume now that $\operatorname{supp} u \subset X$, $\operatorname{supp} v \subset Y$ and that

$$D:=d(X, Y) \geq 2$$

(if $D \leq 1$ then (1.12) is trivially satisfied). Let us show that if $\deg \Phi \leq D-1$ then

$$(\Phi(\mathcal{L}) u, v)=0. \qquad (1.25)$$

Indeed, the function $\mathcal{L}^k u$ is supported in $U_k(\operatorname{supp} u)$, whence it follows that $\Phi(\mathcal{L})u$ is supported in $U_{D-1}(X)$. Since $U_{D-1}(X)$ is disjoint with Y, we obtain (1.25). Comparing (1.25) and (1.24), we obtain

$$\max_{1\leq k\leq N-1}|\Phi(\lambda_k)| \geq \Phi(0)\,\frac{\bar{u}\bar{v}\mu(V)}{\|u'\|\,\|v'\|}. \tag{1.26}$$

Let us take now $u = \mathbf{1}_X$ and $v = \mathbf{1}_Y$. We have

$$\bar{u} = \frac{\mu(X)}{\mu(V)}, \qquad \|\bar{u}\|^2 = \frac{\mu(X)^2}{\mu(V)}, \qquad \|u\|^2 = \mu(X),$$

whence

$$\|u'\| = \sqrt{\|u\|^2 - \|\bar{u}\|^2} = \sqrt{\mu(X) - \frac{\mu(X)^2}{\mu(V)}} = \sqrt{\frac{\mu(X)\,\mu(X^c)}{\mu(V)}}.$$

Using similar identities for v and substituting into (1.26), we obtain

$$\max_{1\leq k\leq N-1}|\Phi(\lambda_k)| \geq \Phi(0)\sqrt{\frac{\mu(X)\,\mu(Y)}{\mu(X^c)\,\mu(Y^c)}}. \tag{1.27}$$

Finally, let us specify $\Phi(\lambda)$ as follows:

$$\Phi(\lambda) = \left(\frac{\lambda_1 + \lambda_{N-1}}{2} - \lambda\right)^{D-1}.$$

Since $\max|\Phi(\lambda)|$ on the set $\lambda \in [\lambda_1, \lambda_{N-1}]$ is attained at $\lambda = \lambda_1$ and $\lambda = \lambda_{N-1}$ and

$$\max_{[\lambda_1, \lambda_{N-1}]} |\Phi(\lambda)| = \left(\frac{\lambda_{N-1} - \lambda_1}{2}\right)^{D-1},$$

it follows from (1.27) that

$$\left(\frac{\lambda_{N-1} - \lambda_1}{2}\right)^{D-1} \geq \left(\frac{\lambda_{N-1} + \lambda_1}{2}\right)^{D-1} \sqrt{\frac{\mu(X)\,\mu(Y)}{\mu(X^c)\,\mu(Y^c)}}.$$

Using definitions (1.20) of $l(X, Y)$ and (1.21) of δ, we obtain

$$\exp(l(X, Y)) \geq \left(\frac{1}{\delta}\right)^{D-1}.$$

Taking ln, we obtain (1.12). ∎

1.4 Cheeger's inequality

Let (V, μ) be a weighted graph with the edges set E. Recall that, for any vertex subset $\Omega \subset V$, its measure $\mu(\Omega)$ is defined by

$$\mu(\Omega) = \sum_{x \in \Omega} \mu(x).$$

Similarly, for any edge subset $S \subset E$, define its measure $\mu(S)$ by

$$\mu(S) = \sum_{\xi \in S} \mu_\xi,$$

where $\mu_\xi := \mu_{xy}$ for any edge $\xi = \overline{xy}$.

For any set $\Omega \subset V$, define its *edge boundary* $\partial\Omega$ by

$$\partial\Omega = \{\overline{xy} \in E : x \in \Omega, y \notin \Omega\}.$$

Definition. Given a finite weighted graph (V, μ), define its *Cheeger constant* by

$$h = h(V, \mu) = \inf_{\substack{\Omega \subset V \\ \mu(\Omega) \leq \frac{1}{2}\mu(V)}} \frac{\mu(\partial\Omega)}{\mu(\Omega)}. \tag{1.28}$$

In other words, h is the largest constant such that the following inequality is true

$$\mu(\partial\Omega) \geq h\mu(\Omega) \tag{1.29}$$

for any subset Ω of V with measure $\mu(\Omega) \leq \frac{1}{2}\mu(V)$.

Lemma 1.8 *We have $\lambda_1 \leq 2h$.*

Proof. For any $f \in \mathcal{F} \setminus \{0\}$, consider the *Rayleigh quotient*

$$\mathcal{R}(f) := \frac{(\mathcal{L}f, f)}{(f, f)}.$$

Since

$$\lambda_1 = \inf_{f \in \mathcal{F},\ f \perp 1} \mathcal{R}(f),$$

it suffices to find a function f such that $f \perp 1$ and $\mathcal{R}(f) \leq 2h$.

Let Ω be a set at which the infimum in (1.28) is attained. Consider the following function

$$f(x) = \begin{cases} 1, & x \in \Omega \\ -a, & x \in \Omega^c \end{cases}$$

where a is chosen so that $f \perp 1$, that is, $\mu(\Omega) = a\mu(\Omega^c)$ whence

$$a = \frac{\mu(\Omega)}{\mu(\Omega^c)} \leq 1.$$

We have

$$(f, f) = \sum_{x \in V} f(x)^2 \mu(x) = \mu(\Omega) + a^2 \mu(\Omega^c) = (1+a)\mu(\Omega)$$

and by the Green formula (1.6)

$$\begin{aligned}(\mathcal{L}f, f) &= \frac{1}{2}\sum_{x,y} (\nabla f_{xy})^2 \mu_{xy} = \sum_{x \in \Omega, y \in \Omega^c} (\nabla_{xy} f)^2 \mu_{xy} \\ &= (1+a)^2 \sum_{x \in \Omega, y \in \Omega^c} \mu_{xy} = (1+a)^2 \mu(\partial\Omega).\end{aligned}$$

Hence,

$$\mathcal{R}(f) \leq \frac{(1+a)^2 \mu(\partial\Omega)}{(1+a)\mu(\Omega)} = (1+a)h \leq 2h,$$

which was to be proved. ■

Theorem 1.9 (Alon, Milman '86) *We have*

$$\lambda_1 \geq \frac{h^2}{2}. \tag{1.30}$$

The inequality (1.30) is called *Cheeger's inequality* because it is similar to an inequality proved by J.Cheeger '70 for Riemannian manifolds.

We precede the proof Theorem 1.9 by two lemmas. Given a function $f : V \to \mathbb{R}$ and an edge $\xi = \overline{xy}$, let us use the following notation:

$$|\nabla_\xi f| := |\nabla_{xy} f| = |f(y) - f(x)|.$$

Lemma 1.10 (Co-area formula). *Given any real-valued function f on V, set for any $t \in \mathbb{R}$*

$$\Omega_t = \{x \in V : f(x) > t\}.$$

Then the following identity holds:

$$\sum_{\xi \in E} |\nabla_\xi f| \, \mu_\xi = \int_{-\infty}^{\infty} \mu(\partial \Omega_t) \, dt. \tag{1.31}$$

A similar formula holds for differentiable functions on $\mathbb{R}$:

$$\int_a^b |f'(x)| = \int_{-\infty}^{\infty} \# \{x : f(x) = t\} \, dt,$$

and the common value of the both sides is called the *total variation* of f.

Proof. For any edge $\xi = \overline{xy}$, there corresponds an interval $I_\xi \subset \mathbb{R}$ that is defined as follows:

$$I_\xi = [f(x), f(y))$$

where we assume that $f(x) \le f(y)$ (otherwise, switch the notations x and y). Denoting by $|I_\xi|$ the Euclidean length of the interval I_ξ, we see that $|\nabla_\xi f| = |I_\xi|$.

Claim. $\xi \in \partial\Omega_t \Longleftrightarrow t \in I_\xi$.

Indeed, $\partial\Omega_t$ consists of edges $\xi = \overline{xy}$ such that

$$x \in \Omega_t^c \text{ and } y \in \Omega_t \iff f(x) \le t \text{ and } f(y) > t \iff t \in [f(x), f(y)) = I_\xi$$

Thus, we have

$$\mu(\partial\Omega_t) = \sum_{\xi \in \partial\Omega_t} \mu_\xi = \sum_{\xi \in E : t \in I_\xi} \mu_\xi = \sum_{\xi \in E} \mu_\xi \, \mathbf{1}_{I_\xi}(t),$$

whence

$$\begin{aligned}\int_{-\infty}^{+\infty} \mu(\partial\Omega_t)\, dt &= \int_{-\infty}^{+\infty} \sum_{\xi\in E} \mu_\xi \,\mathbf{1}_{I_\xi}(t) dt \\ &= \sum_{\xi\in E} \int_{-\infty}^{+\infty} \mu_\xi \,\mathbf{1}_{I_\xi}(t) dt \\ &= \sum_{\xi\in E} \mu_\xi \left|I_\xi\right| = \sum_{\xi\in E} \mu_\xi |\nabla_\xi f| \,.\end{aligned}$$

■

Lemma 1.11 *For any non-negative function f on V, such that*

$$\mu \left\{x \in V : f(x) > 0\right\} \leq \frac{1}{2} \mu(V), \tag{1.32}$$

the following is true:

$$\sum_{\xi\in E} |\nabla_\xi f| \, \mu_\xi \geq h \sum_{x\in V} f(x)\, \mu(x), \tag{1.33}$$

where h is the Cheeger constant of (V, μ).

Note that for the function $f = \mathbf{1}_\Omega$ the condition (1.32) means that $\mu(\Omega) \le \frac{1}{2}\mu(V)$, and the inequality (1.33) is equivalent to

$$\mu(\partial\Omega) \ge h\mu(\Omega),$$

because

$$\sum_{x\in V} f(x)\,\mu(x) = \sum_{x\in\Omega}\mu(x) = \mu(\Omega)$$

and

$$\sum_{\xi\in E} |\nabla_\xi f|\,\mu_\xi = \sum_{x\in\Omega, y\in\Omega^c} |f(y) - f(x)|\,\mu_{xy} = \sum_{x\in\Omega, y\in\Omega^c} \mu_{xy} = \mu(\partial\Omega).$$

Proof. By the co-area formula, we have

$$\sum_{\xi\in E} |\nabla_\xi f|\,\mu_\xi = \int_{-\infty}^{\infty} \mu(\partial\Omega_t)\,dt \ge \int_0^\infty \mu(\partial\Omega_t)\,dt.$$

By (1.32), the set $\Omega_t = \{x \in V : f(x) > t\}$ has measure $\le \frac{1}{2}\mu(V)$ for any $t \ge 0$. Therefore, by (1.29)

$$\mu(\partial\Omega_t) \ge h\mu(\Omega_t).$$

It follows that

$$\sum_{\xi \in E} |\nabla_\xi f| \, \mu_\xi \geq h \int_0^\infty \mu(\Omega_t) \, dt$$

Observe that, for $t \geq 0$,

$$x \in \Omega_t \Longleftrightarrow t \in [0, f(x)),$$

we obtain

$$\begin{aligned}
\int_0^\infty \mu(\Omega_t) \, dt &= \int_0^\infty \sum_{x \in \Omega_t} \mu(x) \, dt \\
&= \int_0^\infty \sum_{x \in V} \mu(x) \, \mathbf{1}_{[0, f(x))}(t) \, dt \\
&= \sum_{x \in V} \mu(x) \int_0^\infty \mathbf{1}_{[0, f(x))}(t) \, dt \\
&= \sum_{x \in V} \mu(x) \, f(x) \, .
\end{aligned}$$

■

Proof of Theorem 1.9. Let f be the eigenfunction of λ_1. Consider two sets

$$V^+ = \{x \in V : f(x) \geq 0\} \quad \text{and } V^- = \{x \in V : f(x) < 0\}.$$

Without loss of generality, we can assume that $\mu(V^+) \leq \mu(V^-)$ (if not then replace f by $-f$). It follows that $\mu(V^+) \leq \frac{1}{2}\mu(V)$. Consider the function

$$g = f_+ := \begin{cases} f, & f \geq 0, \\ 0, & f < 0. \end{cases}$$

Applying the Green formula (1.6)

$$(\mathcal{L}f, g) = \frac{1}{2} \sum_{x,y \in V} (\nabla_{xy} f)(\nabla_{xy} g)\, \mu_{xy}$$

and using so that $\mathcal{L}f = \lambda_1 f$, we obtain

$$\lambda_1 \sum_{x \in V} f(x) g(x) \mu(x) = \frac{1}{2} \sum_{x,y \in V} (\nabla_{xy} f)(\nabla_{xy} g)\, \mu_{xy}.$$

Observing that $fg = g^2$ and

$$(\nabla_{xy} f)(\nabla_{xy} g) = (f(y) - f(x))(g(y) - g(x)) \geq (g(y) - g(x))^2 = |\nabla_{xy} g|^2.$$

we obtain

$$\lambda_1 \geq \frac{\sum\limits_{\xi \in E} \left|\nabla_\xi g\right|^2 \mu_\xi}{\sum\limits_{x \in V} g^2 (x) \mu (x)}.$$

Note that $g \not\equiv 0$ because otherwise $f_+ \equiv 0$ and $(f, 1) = 0$ imply that $f_- \equiv 0$ whereas $f \not\equiv 0$.

Hence, to prove (1.30) it suffices to verify that

$$\sum_{\xi \in E} \left|\nabla_\xi g\right|^2 \mu_\xi \geq \frac{h^2}{2} \sum_{x \in V} g^2 (x) \mu (x) . \tag{1.34}$$

Since

$$\mu (x \in V : g (x) > 0) \leq \mu \left(V^+\right) \leq \frac{1}{2} \mu (V) ,$$

we can apply Lemma 1.11 to function g^2 and obtain

$$\sum_{\xi \in E} \left|\nabla_\xi \left(g^2\right)\right| \mu_\xi \geq h \sum_{x \in V} g^2 (x) \mu (x) . \tag{1.35}$$

Let us estimate from above the left hand side as follows:

$$
\begin{aligned}
\sum_{\xi\in E}\left|\nabla_\xi\left(g^2\right)\right|\mu_\xi &= \frac{1}{2}\sum_{x,y\in V}\left|g^2(x)-g^2(y)\right|\mu_{xy}\\
&= \frac{1}{2}\sum_{x,y}|g(x)-g(y)|\mu_{xy}^{1/2}|g(x)+g(y)|\mu_{xy}^{1/2}\\
&\le \left(\frac{1}{2}(\sum_{x,y}(g(x)-g(y))^2\mu_{xy})\frac{1}{2}(\sum_{x,y}(g(x)+g(y))^2\mu_{xy})\right)^{1/2},
\end{aligned}
$$

where we have used the Cauchy-Schwarz inequality

$$
\sum_k a_k b_k \le \left(\sum_k a_k^2\right)^{1/2}\left(\sum_k b_k^2\right)^{1/2}
$$

that is true for arbitrary sequences of non-negative reals a_k, b_k. Next, using the inequality

$$
\frac{1}{2}\left(a+b\right)^2 \le a^2+b^2,
$$

we obtain

$$
\begin{aligned}
\sum_{\xi\in E}\left|\nabla_\xi\left(g^2\right)\right|\mu_\xi &\le \left(\sum_{\xi\in E}\left|\nabla_\xi g\right|^2\mu_\xi\sum_{x,y}\left(g^2(x)+g^2(y)\right)\mu_{xy}\right)^{1/2}\\
&= \left(2\sum_{\xi\in E}\left|\nabla_\xi g\right|^2\mu_\xi\sum_{x,y}g^2(x)\mu_{xy}\right)^{1/2}\\
&= \left(2\sum_{\xi\in E}\left|\nabla_\xi g\right|^2\mu_\xi\sum_{x\in V}g^2(x)\mu\left(x\right)\right)^{1/2},
\end{aligned}
$$

which together with (1.35) yields

$$
h\sum_{x\in V}g^2\left(x\right)\mu\left(x\right)\le\left(2\sum_{\xi\in E}\left|\nabla_\xi g\right|^2\mu_\xi\right)^{1/2}\left(\sum_{x\in V}g^2(x)\mu\left(x\right)\right)^{1/2}.
$$

Dividing by $\left(\sum_{x\in V}g^2\left(x\right)\mu\left(x\right)\right)^{1/2}$ and taking square, we obtain (1.34). ■

Go to Chapter 2

1.5 Eigenvalues in a weighted path graph

Consider a path graph P_N with the set of vertices $V = \{0, 1, ...N - 1\}$ and the edges

$$0 \sim 1 \sim 2 \sim ... \sim N - 1.$$

Define the weights $\mu_{k-1,k} := m_k$, where $\{m_k\}_{k=1}^{N-1}$ is a given sequence of positive numbers. Then, for $1 \le k \le N - 2$, we have

$$\mu(k) = \mu_{k-1,k} + \mu_{k,k+1} = m_k + m_{k+1},$$

and the same is true also for $k = 0, N - 1$ if we define $m_{-1} = m_N = 0$. The Markov kernel is then

$$P(k, k+1) = \frac{\mu_{k,k+1}}{\mu(k)} = \frac{m_{k+1}}{m_k + m_{k+1}}.$$

Claim. *Assume that the sequence $\{m_k\}_{k=1}^{N-1}$ is increasing, that is, $m_k \le m_{k+1}$. Then $h \ge \frac{1}{2N}$.*

Proof. Let Ω be a subset of V with $\mu(\Omega) \le \frac{1}{2}\mu(V)$, and let $\overline{k-1,k}$ be an edge of the boundary $\partial\Omega$ with the largest possible k. We claim that either Ω or Ω^c is contained in $[0, k - 1]$. Indeed, if there were vertices from both sets Ω and Ω^c outside $[0, k-1]$, that is, in $[k, N-1]$, then there would have been an edge $\overline{j-1,j} \in \partial\Omega$ with $j > k$, which contradicts the choice of k. It follows that either $\mu(\Omega) \leq \mu([0, k-1])$ or $\mu(\Omega^c) \leq \mu([0, k-1])$. However, since $\mu(\Omega) \leq \mu(\Omega^c)$, we obtain that in the both cases $\mu(\Omega) \leq \mu([0, k-1])$. We have

$$\begin{aligned}
\mu([0, k-1]) &= \sum_{j=0}^{k-1} \mu(j) = \sum_{j=0}^{k-1} \left(\mu_{j-1,j} + \mu_{j,j+1}\right) \\
&= \sum_{j=0}^{k-1} (m_j + m_{j+1}) \\
&\leq 2km_k
\end{aligned} \tag{1.36}$$

where we have used that $m_j \leq m_{j+1} \leq m_k$. Therefore

$$\mu(\Omega) \leq 2km_k.$$

On the other hand, we have

$$\mu(\partial\Omega) \geq \mu_{k-1,k} = m_k,$$

whence it follows that

$$\frac{\mu(\partial\Omega)}{\mu(\Omega)} \geq \frac{m_k}{2km_k} = \frac{1}{2k} \geq \frac{1}{2N},$$

which proves that $h \geq \frac{1}{2N}$. ■

Consequently, Theorem 1.9 yields

$$\lambda_1 \geq \frac{1}{8N^2}. \tag{1.37}$$

If the weight μ is simple then $\lambda_1 = 1 - \cos\frac{\pi}{N-1}$ so that, for large N,

$$\lambda_1 \approx \frac{\pi^2}{2\,(N-1)^2} \approx \frac{5}{N^2},$$

which is of the same order in N as the estimate (1.37).

Let us estimate the expansion rate of (V, μ). Since this graph is bipartite, we have

$$\delta := \frac{\lambda_{N-1} - \lambda_1}{\lambda_{N-1} + \lambda_1} = \frac{2 - \lambda_1}{2 + \lambda_1} \leq 1 - \frac{\lambda_1}{2}$$

and by (1.17)

$$R \leq \frac{1}{2}\lceil \frac{\ln M}{\ln\frac{1}{\delta}} \rceil \leq \frac{1}{2}\lceil \frac{\ln M}{\ln\frac{1}{1-\lambda_1/2}} \rceil \leq \frac{1}{2}\lceil \frac{\ln M}{\lambda_1/2} \rceil \leq \frac{\ln M}{\lambda_1} + 1$$

where

$$M = \max_k \frac{\mu\,(V)}{\mu\,(k)}.$$

Observe that

$$\mu(V) = \sum_{j=0}^{N-1} (m_j + m_{j+1}) \le 2 \sum_{j=1}^{N-1} m_j$$

where we put $m_0 = m_N = 0$, whence

$$M = \max_k \frac{\mu(V)}{\mu(k)} \le \frac{2\sum_{j=1}^{N-1} m_j}{m_1} =: M_0,$$

It follows

$$R \le \frac{\ln M_0}{\lambda_1} + 1. \tag{1.38}$$

For an arbitrary increasing sequence $\{m_k\}$, we obtain using (1.37) that

$$R \le 8N^2 \ln M_0 + 1.$$

If the sequence $\{m_k\}$ increases at most polynomially, say $m_k \le k^p m_0$, then

$$M_0 \lesssim N^{p+1},$$

and we obtain

$$R \lesssim CN^2 \ln N.$$

Now assume that the weights m_k satisfy a stronger condition

$$m_{k+1} \geq c m_k,$$

for some constant $c > 1$ and all $k = 0, ..., N - 2$. Then $m_k \geq c^{k-j} m_j$ for all $k \geq j$, which allows to improve the estimate (1.36) as follows

$$\begin{aligned}
\mu([0, k-1]) &= \sum_{j=0}^{k-1} (m_j + m_{j+1}) \leq \sum_{j=0}^{k-1} \left(c^{j-k} m_k + c^{j+1-k} m_k\right) \\
&= m_k \left(c^{-k} + c^{1-k}\right) \left(1 + c + ... c^{k-1}\right) = m_k \left(c^{-k} + c^{1-k}\right) \frac{c^k - 1}{c - 1} \\
&\leq m_k \frac{c+1}{c-1}.
\end{aligned}$$

Therefore, we obtain

$$\frac{\mu(\partial\Omega)}{\mu(\Omega)} \geq \frac{c-1}{c+1}$$

whence $h \geq \frac{c-1}{c+1}$ and, by Theorem 1.9,

$$\lambda_1 \geq \frac{1}{2} \left(\frac{c-1}{c+1}\right)^2. \tag{1.39}$$

Consider the specific weights $m_k = c^k$ where $c > 1$. Then we have

$$M_0 = 2 \sum_{j=1}^{N-1} c^{j-1} = 2 \frac{c^{N-1} - 1}{c - 1}$$

whence

$$\ln M_0 \approx N \ln c.$$

By (1.38) and (1.39), we obtain

$$R \lesssim 2 \left(\frac{c+1}{c-1} \right)^2 N \ln c.$$

Note that in this case R is linear in N!

1.6 Products of weighted graphs

Definition. Let (X,a) and (Y,b) be two finite weighted graphs. Fix two numbers $p,q>0$ and define the product graph

$$(V,\mu)=(X,a)\,\Box_{p,q}\,(Y,b)$$

as follows: $V=X\times Y$ and the weight μ on V is defined by

$$\begin{aligned}\mu_{(x,y),(x',y)} &= pb\left(y\right)a_{xx'}\\ \mu_{(x,y),(x,y')} &= qa\left(x\right)b_{yy'}\end{aligned}$$

and $\mu_{(x,y),(x',y')}=0$ otherwise. The numbers p,q are called the *parameters* of the product.

Clearly, the product weight $\mu_{(x,y),(x',y')}$ is symmetric. The weight on the vertices of V is given by

$$\begin{aligned}\mu\left(x,y\right) &= \sum_{x',y'}\mu_{(x,y),(x',y')}=p\sum_{x'}a_{xx'}b\left(y\right)+q\sum_{y'}a\left(x\right)b_{yy'}\\ &= \left(p+q\right)a\left(x\right)b\left(y\right).\end{aligned}$$

Claim. *If A and B are the Markov kernels on X and Y, then the Markov kernel P on the product (V, μ) is given by*

$$P\left((x,y),(x',y')\right) = \begin{cases} \frac{p}{p+q} A(x,x'), & \text{if } y = y', \\ \frac{q}{p+q} B(y,y'), & \text{if } x = x', \\ 0, & \text{otherwise.} \end{cases} \tag{1.40}$$

Proof. Indeed, we have in the case $y = y'$ (and the case $x = x'$ is similar):

$$P\left((x,y),(x',y')\right) = \frac{\mu_{(x,y),(x',y')}}{\mu(x,y)} = \frac{p a_{xx'} b(y)}{(p+q)\, a(x)\, b(y)} = \frac{p}{p+q} \frac{a_{xx'}}{a(x)} = \frac{p}{p+q} A(x,x').$$

∎

For the random walk on (V, μ), the identity (1.40) means the following: the random walk at (x,y) chooses first between the directions X and Y with probabilities $\frac{p}{p+q}$ and $\frac{q}{p+q}$, respectively, and then chooses a vertex in the chosen direction accordingly to the Markov kernel there.

In particular, if a and b are simple weights, then we obtain

$$\begin{aligned} \mu_{(x,y),(x',y)} &= p \deg(y) \quad \text{if } x \sim x' \\ \mu_{(x,y),(x,y')} &= q \deg(x) \quad \text{if } y \sim y' \end{aligned}$$

and $\mu_{(x,y),(x',y')} = 0$ otherwise.

If in addition the graphs A and B are regular, that is, $\deg(x) = \text{const} =: \deg(A)$ and $\deg(y) = \text{const} =: \deg(B)$ then the most natural choice of the parameter p and q is as follows

$$p = \frac{1}{\deg(B)} \text{ and } \quad q = \frac{1}{\deg(A)},$$

so that the weight μ is also simple. We obtain the following statement.

Lemma 1.12 *If (X, a) and (Y, b) are regular graphs with simple weights, then the product*

$$(X, a) \,\square_{\frac{1}{\deg(B)}, \frac{1}{\deg(A)}} (Y, b) \tag{1.41}$$

is again a regular graph with a simple weight. The degree of the product graph (1.41) is $\deg(A) + \deg(B)$.

Example. Consider the graphs $\mathbb{Z}_m^n$ and $\mathbb{Z}_m^k$ with simple weights. Since their degrees are equal to $2n$ and $2k$, respectively, we obtain

$$\mathbb{Z}_m^n \square_{\frac{1}{2k}, \frac{1}{2n}} \mathbb{Z}_m^k = \mathbb{Z}_m^{n+k}.$$

Theorem 1.13 *Let (X,a) and (Y,b) be finite weighted graphs without isolated vertices, and let $\{\alpha_k\}_{k=0}^{n-1}$ and $\{\beta_l\}_{l=0}^{m-1}$ be the sequences of the eigenvalues of the Markov operators A and B respectively, counted with multiplicities. Then all the eigenvalues of the Markov operator P on the product $(V,\mu) = (X,a)\,\Box_{p,q}\,(Y,b)$ are given by the sequence $\left\{\frac{p\alpha_k+q\beta_l}{p+q}\right\}$ where $k = 0,...,n-1$ and $l = 0,...,m-1$.*

In other words, the eigenvalues of P are the convex combinations of eigenvalues of A and B, with the coefficients $\frac{p}{p+q}$ and $\frac{q}{p+q}$. The same relation holds for the eigenvalues of the Laplace operators because

$$1 - \frac{p\alpha_k + q\beta_l}{p+q} = \frac{p\left(1-\alpha_k\right) + q\left(1-\beta_l\right)}{p+q}.$$

Proof. Let f be an eigenfunction of A with the eigenvalue α and g be the eigenfunction of B with the eigenvalue β. Let us show that the function $h\left(x,y\right) = f\left(x\right)g\left(y\right)$ is the eigenvalue of P with the eigenvalue $\frac{p\alpha+q\beta}{p+q}$.

We have

$$Ph\left(x,y\right) = \sum_{x',y'} P\left(\left(x,y\right),\left(x',y'\right)\right)h\left(x',y'\right)$$

$$\begin{aligned}
&= \sum_{x'} P\left(\left(x,y\right),\left(x',y\right)\right) h\left(x',y\right) + \sum_{y'} P\left(\left(x,y\right),\left(x,y'\right)\right) h\left(x,y'\right) \\
&= \frac{p}{p+q} \sum_{x'} A\left(x,x'\right) f\left(x'\right) g\left(y\right) + \frac{q}{p+q} \sum_{y'} B\left(y,y'\right) f\left(x\right) g\left(y'\right) \\
&= \frac{p}{p+q} Af\left(x\right) g\left(y\right) + \frac{q}{p+q} f\left(x\right) Bg\left(y\right) \\
&= \frac{p}{p+q} \alpha f\left(x\right) g\left(y\right) + \frac{q}{p+q} \beta f\left(x\right) g\left(y\right) \\
&= \frac{p\alpha + q\beta}{p+q} h\left(x,y\right),
\end{aligned}$$

which was to be proved.

Let $\{f_k\}$ be a basis in the space of functions on X such that $Af_k = \alpha_k f_k$, and $\{g_l\}$ be a basis in the space of functions on Y, such that $Bg_l = \beta_l g_l$. Then $h_{kl}\left(x,y\right) = f_k\left(x\right) g_l\left(y\right)$ is a linearly independent sequence of functions on $V = X \times Y$. Since the number of such functions is $nm = |V|$, we see that $\{h_{kl}\}$ is a basis in the space of functions on V. Since h_{kl} is the eigenfunction with the eigenvalue $\frac{p\alpha_k + q\beta_l}{p+q}$, we conclude that the sequence $\left\{\frac{p\alpha_k + q\beta_l}{p+q}\right\}$ exhausts all the eigenvalues of P. ■

Corollary 1.14 *Let (V, E) be a finite connected regular graph with $N > 1$ vertices, and set $(V^n, E_n) = (V, E)^{\Box n}$. Let μ be a simple weight on V, and $\{\alpha_k\}_{k=0}^{N-1}$ be the sequence of the eigenvalues of the Markov operator on (V, μ), counted with multiplicity. Let μ_n be a simple weight on V^n. Then the eigenvalues of the Markov operator on (V^n, μ_n) are given by the sequence*

$$\left\{ \frac{\alpha_{k_1} + \alpha_{k_2} + ... + \alpha_{k_n}}{n} \right\} \tag{1.42}$$

for all $k_i \in \{0, 1, ..., N-1\}$, where each eigenvalue is counted with multiplicity.

It follows that if $\{\lambda_k\}_{k=0}^{N-1}$ is the sequence of the eigenvalues of the Laplace operator on (V, μ) then the eigenvalues of Laplace operator on (V^n, μ_n) are given by the sequence

$$\left\{ \frac{\lambda_{k_1} + \lambda_{k_2} + ... + \lambda_{k_n}}{n} \right\}. \tag{1.43}$$

Proof. Induction in n. If $n = 1$ then there is nothing to prove. Let us make the inductive step from n to $n+1$. Let degree of (V, E) be D, then $\deg(V^n) = nD$. Note that.

$$\left(V^{n+1}, E_{n+1}\right) = (V^n, E_n) \Box (V, E)$$

It follows from Lemma 1.12 that

$$\left(V^{n+1}, \mu_{n+1}\right) = (V^n, \mu_n) \, \square_{\frac{1}{D}, \frac{1}{nD}} \, (V, \mu) \, .$$

By the inductive hypothesis, the eigenvalues of the Laplacian on (V^n, μ_n) are given by the sequence (1.42). Hence, by Theorem 1.13, the eigenvalues on $\left(V^{n+1}, \mu_{n+1}\right)$ are given by

$$\begin{aligned} & \frac{1/D}{1/D + 1/(nD)} \frac{\alpha_{k_1} + \alpha_{k_2} + \ldots + \alpha_{k_n}}{n} + \frac{1/(nD)}{1/D + 1/(nD)} \alpha_k \\ = & \frac{n}{n+1} \frac{\alpha_{k_1} + \alpha_{k_2} + \ldots + \alpha_{k_n}}{n} + \frac{1}{n+1} \alpha_k \\ = & \frac{\alpha_{k_1} + \alpha_{k_2} + \ldots + \alpha_{k_n} + \alpha_k}{n+1}, \end{aligned}$$

which was to be proved. ■

1.7 Eigenvalues in $\mathbb{Z}_m$

Let us compute the eigenvalues of the Markov operator P on the cycle graph $\mathbb{Z}_m$ with simple weight:

$$0 \sim 1 \sim 2 \sim ... \sim m-1 \sim 0.$$

The Markov operator is given by

$$Pf(k) = \frac{1}{2}\left(f(k+1) + f(k-1)\right) \quad \text{for any } k = 0, ..., m-1 \bmod m.$$

The eigenvalue equation $Pf = \alpha f$ becomes

$$f(k+1) - 2\alpha f(k) + f(k-1) = 0. \tag{1.44}$$

We know already that $\alpha = 1$ is always a simple eigenvalue of P, and $\alpha = -1$ is a (simple) eigenvalue if and only if $\mathbb{Z}_m$ is bipartite, that is, if m is even. Assume in what follows that $\alpha \in (-1, 1)$.

Consider first the *difference equation* (1.44) on $\mathbb{Z}$, that is, for all $k \in \mathbb{Z}$, and find all solutions f as functions on $\mathbb{Z}$. The set of all solutions of (1.44) is a linear space, and the dimension of this space is 2, because function f is uniquely determined by (1.44) and by two initial conditions $f(0) = a$ and $f(1) = b$. Therefore, to find all solutions of (1.44), it suffices to find two linearly independent solutions and take their linear combination.

Let us search specific solution of (1.44) in the form $f(k) = r^k$ where the number r is to be found. Substituting into (1.44) and cancelling by r^k, we obtain the equation for r:

$$r^2 - 2\alpha r + 1 = 0.$$

It has two complex roots

$$r = \alpha \pm i\sqrt{1-\alpha^2} = e^{\pm i\theta},$$

where $\theta \in (0, \pi)$ is determined by the condition

$$\cos\theta = \alpha \ \ (\text{and } \sin\theta = \sqrt{1-\alpha^2}).$$

Hence, we obtain two independent complex-valued solutions of (1.44)

$$f_1(k) = e^{ik\theta} \ \text{ and } \ f_2(k) = e^{-ik\theta}.$$

Taking their linear combinations and using the Euler formula, we arrive at the following real-valued independent solutions:

$$f_1(k) = \cos k\theta \ \text{ and } \ f_2(k) = \sin k\theta. \tag{1.45}$$

In order to be able to consider a function $f(k)$ on $\mathbb{Z}$ as a function on $\mathbb{Z}_m$, it must be m-periodic, that is,

$$f(k+m) = f(k) \text{ for all } k \in \mathbb{Z}.$$

The functions (1.45) are m-periodic provided $m\theta$ is a multiple of 2π, that is,

$$\theta = \frac{2\pi l}{m},$$

for some integer l. The restriction $\theta \in (0, \pi)$ is equivalent to

$$l \in (0, m/2).$$

Hence, for each l from this range we obtain an eigenvalue $\alpha = \cos\theta$ of multiplicity 2 (with eigenfunctions $\cos k\theta$ and $\sin k\theta$).

Let us summarize this result in the following statement.

Proposition 1.15 *The eigenvalues of the Markov operator P on the graph $\mathbb{Z}_m$ are as follows:*

1. If m is odd then the eigenvalues are $\alpha = 1$ (simple) and $\alpha = \cos\frac{2\pi l}{m}$ for all $l = 1, ..., \frac{m-1}{2}$ (double);

2. if m is even then the eigenvalues are $\alpha = \pm 1$ (simple) and $\alpha = \cos\frac{2\pi l}{m}$ for all $l = 1, ..., \frac{m}{2} - 1$ (double).

In the both case, all the eigenvalues of P with multiplicities are listed in the following sequence:

$$\left\{\cos\frac{2\pi j}{m}\right\}_{j=0}^{m-1}.$$

For example, in the case $m = 3$ we obtain the Markov eigenvalues $\alpha = 1$ and $\alpha = \cos\frac{2\pi}{3} = -\frac{1}{2}$ (double). The eigenvalues of $\mathcal{L}$ are as follows: $\lambda = 0$ and $\lambda = 3/2$ (double). If $m = 4$ then the Markov eigenvalues are $\alpha = \pm 1$ and $\alpha = \cos\frac{2\pi}{4} = 0$ (double). The eigenvalues of $\mathcal{L}$ are as follows: $\lambda = 0$, $\lambda = 1$ (double), $\lambda = 2$.

1.8 Eigenvalues in $\mathbb{Z}_m^n$

Consider the graph $\mathbb{Z}_m^n$ with odd m. In the case $n = 1$, all the eigenvalues of P in $\mathbb{Z}_m$ are listed in the following sequence (without multiplicity):

$$\left\{\cos\frac{2\pi l}{m}\right\},\ l = 0, 1, ..., \frac{m-1}{2}. \tag{1.46}$$

This sequence is obviously decreasing in l, and its maximal and minimal values are

$$1 \quad \text{and} \quad \cos\left(\frac{2\pi}{m}\frac{m-1}{2}\right) = -\cos\frac{\pi}{m},$$

respectively. For a general n, by Corollary 1.14, the eigenvalue of P have the form

$$\frac{\alpha_{k_1} + \alpha_{k_2} + ... + \alpha_{k_n}}{n} \tag{1.47}$$

where α_{k_i} are the eigenvalues of P for $n = 1$, that is, elements of the sequence (1.46). In particular, the minimal value of (1.47) is equal to the minimal value of α_k, that is, to $-\cos\frac{\pi}{m}$.

1.9 Additional properties of eigenvalues

Theorem 1.16 *Let (V, μ) be a finite, connected, weighted graph with $N := |V| > 1$.*

(a) *Then we have*

$$\lambda_1 + ... + \lambda_{N-1} = N \tag{1.48}$$

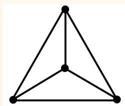
and, hence,

$$\lambda_1 \leq \frac{N}{N-1} \leq \lambda_{N-1} \tag{1.49}$$

(b) *If $(V, \mu) = K_N$, that is, (V, μ) is a complete graph with a simple weight then*

$$\lambda_1 = ... = \lambda_{N-1} = \frac{N}{N-1}.$$

(c) *If (V, μ) is non-complete then $\lambda_1 \leq 1$. Consequently, a graph with a simple weight is complete if and only if $\lambda_1 > 1$.*

For example, for $K_4 =$  , we obtain that the eigenvalues of $\mathcal{L}$ are 0 (simple) and $\frac{4}{3}$ (with multiplicity 3).

Proof. (a) Let $\{v_k\}_{k=0}^{N-1}$ be an orthonormal basis in $\mathcal{F}$ that consists of the eigenfunctions of $\mathcal{L}$, so that $\mathcal{L}v_k = \lambda_k v_k$. In the basis $\{v_k\}$, the matrix of $\mathcal{L}$ is

$$\operatorname{diag}\left(\lambda_0, \lambda_1, ...\lambda_{N-1}\right).$$

Since $\lambda_0 = 0$, we obtain

$$\operatorname{trace}\mathcal{L} = \lambda_0 + \lambda_1 + ... + \lambda_{N-1} = \lambda_1 + ... + \lambda_{N-1}. \tag{1.50}$$

Note that the trace $\operatorname{trace}\mathcal{L}$ does not depend on the choice of a basis. Let us choose another basis as follows: enumerate all the vertices of V by $0, 1, ..., N-1$ and consider the indicator functions $\mathbf{1}_{\{k\}}$ (where $k = 0, 1, ..., N-1$) that obviously form a basis in $\mathcal{F}$. The components of any function $f \in \mathcal{F}$ in this basis are the values $f(k)$. Rewrite the definition of $\mathcal{L}$ in the form

$$\mathcal{L}f(i) = f(i) - \sum_j P(i,j) f(x_j) = f(i) - \sum_{j \neq i} P(i,j) f(x_j).$$

We see that the matrix of $\mathcal{L}$ in this basis has the values 1 on the diagonal and $-P(i,j)$ in the intersection of the column i and the row j off the diagonal. It follows that $\operatorname{trace}\mathcal{L} = N$ whence (1.48) follows. Since λ_1 is the minimum of the sequence $\{\lambda_1, ..., \lambda_{N-1}\}$ of $N-1$ numbers and λ_{N-1} is its maximum, we obtain (1.49).

(b) We need to construct $N-1$ linearly independent eigenfunctions with the eigenvalue $\frac{N}{N-1}$. As above, set $V=\{0,1,...,N-1\}$ and consider the following $N-1$ functions f_k for $k=1,2,...N-1:$

$$f_k(i)=\begin{cases}1, & i=0,\\ -1, & i=k,\\ 0, & \text{otherwise.}\end{cases}$$

We have

$$\mathcal{L}f_k(i)=f_k(i)-\frac{1}{N-1}\sum_{j\neq i}f_k(j).$$

If $i=0$ then $f_k(0)=1$ and in the sum $\sum_{j\neq 0}f_k(j)$ there is exactly one term $=-1$, for $j=k$, and all others vanish, whence

$$\mathcal{L}f_k(0)=f_k(0)-\frac{1}{N-1}\sum_{j\neq 0}f_k(j)=1+\frac{1}{N-1}=\frac{N}{N-1}f_k(0).$$

If $i=k$ then $f_k(k)=-1$ and in the sum $\sum_{j\neq k}f_k(j)$ there is exactly one term $=1$, for $j=0$, whence

$$\mathcal{L}f_k(k)=f_k(k)-\frac{1}{N-1}\sum_{j\neq k}f_k(j)=-1-\frac{1}{N-1}=\frac{N}{N-1}f_k(k).$$

If $i \neq 0, k$ then $f_k(i) = 0$, while in the sum $\sum_{j \neq k} f_k(j)$ there are terms $1, -1$ and all others are 0, whence

$$\mathcal{L} f_k(i) = 0 = \frac{N}{N-1} f_k(i).$$

Hence, $\mathcal{L} f_k = \frac{N}{N-1} f_k$. Since the sequence $\{f_k\}_{k=1}^{N-1}$ is linearly independent, we see that $\frac{N}{N-1}$ is the eigenvalue of multiplicity $N-1$, which finishes the proof.

(c) By the variational principle, we have

$$\lambda_1 = \inf_{f \perp 1} \mathcal{R}(f),$$

where $\mathcal{R}(f)$ is the Rayleigh quotient and the condition $f \perp 1$ comes from the fact that the eigenfunction of λ_0 is constant. Hence, to prove that $\lambda_1 \leq 1$ it suffices to construct a function $f \perp 1$ such that $\mathcal{R}(f) \leq 1$.

Claim 1. *Fix $z \in V$ and consider the indicator function $f = \mathbf{1}_{\{z\}}$. Then $\mathcal{R}(f) \leq 1$.*

We have

$$(f, f) = \sum_{x \in V} f(x)^2 \mu(x) = \mu(z)$$

and, by the Green formula,

$$
\begin{aligned}
(\mathcal{L}f, f) &= \frac{1}{2}\sum_{x,y\in V}(f(x)-f(y))^2\mu_{xy} \\
&= \frac{1}{2}\left(\sum_{x=z,y\neq z}+\sum_{x\neq z,y=z}\right)(f(x)-f(y))^2\mu_{xy} \\
&= \sum_{y\neq z}(f(z)-f(y))^2\mu_{zy}=\sum_{y\neq z}\mu_{zy}\leq \mu(z),
\end{aligned}
$$

whence $\mathcal{R}(f)\leq 1$ (note that if the graph has no loops then we obtain the identity $\mathcal{R}(f)=1$).

Clearly, we have also $\mathcal{R}(cf)\leq 1$ for any constant c.

Claim 2. *Let f, g be two functions on V such that*

$$\mathcal{R}(f)\leq 1, \qquad \mathcal{R}(g)\leq 1,$$

and their supports

$$A=\{x\in V: f(x)\neq 0\} \quad \textit{and} \quad B=\{x\in V: g(x)\neq 0\}$$

are disjoint and not connected, that is, $x\in A$ and $y\in B$ implies that $x\neq y$ and $x\not\sim y$. Then $\mathcal{R}(f+g)\leq 1$.

It is obvious that $fg \equiv 0$. Let us show that also $(\mathcal{L}f)\,g \equiv 0$. Indeed, if $g(x) = 0$ then $(\mathcal{L}f)\,g(x) = 0$. If $g(x) \neq 0$ then $x \in B$. It follows that $f(x) = 0$ and $f(y) = 0$ for any $y \sim x$ whence

$$\mathcal{L}f(x) = f(x) - \sum_{y \sim x} P(x,y)\, f(y) = 0,$$

whence $(\mathcal{L}f)\,g(x) = 0$. Using the identities $fg = (\mathcal{L}f)\,g = (\mathcal{L}g)\,f = 0$, we obtain

$$(f+g, f+g) = (f,f) + 2(f,g) + (g,g) = (f,f) + (g,g)$$

and

$$\begin{aligned}
(\mathcal{L}(f+g), f+g) &= (\mathcal{L}f, f) + (\mathcal{L}g, f) + (\mathcal{L}f, g) + (\mathcal{L}g, g) \\
&= (\mathcal{L}f, f) + (\mathcal{L}g, g).
\end{aligned}$$

Since by hypothesis

$$(\mathcal{L}f, f) \leq (f,f) \ \text{ and } \ (\mathcal{L}g, g) \leq (g,g)$$

it follows that

$$\mathcal{R}(f+g) = \frac{(\mathcal{L}f, f) + (\mathcal{L}g, g)}{(f,f) + (g,g)} \leq 1.$$

Now we construct a function $f \perp 1$ such that $\mathcal{R}(f) \leq 1$. Since the graph is non-complete, there are two distinct vertices, say z_1 and z_2, such that $z_1 \not\sim z_2$. Consider function f in the form

$$f(x) = c_1 \mathbf{1}_{\{z_1\}} + c_2 \mathbf{1}_{\{z_2\}},$$

where the coefficients c_1 and c_2 are chosen so that $f \perp 1$ (for example, $c_1 = 1/\mu(z_1)$ and $c_2 = -1/\mu(z_2)$). Since $\mathcal{R}\left(c_i \mathbf{1}_{\{z_i\}}\right) \leq 1$ and the supports of $\mathbf{1}_{\{z_1\}}$ and $\mathbf{1}_{\{z_2\}}$ are disjoint and not connected, we obtain that also $\mathcal{R}(f) \leq 1$, which finishes the proof. $\blacksquare$

2 Infinite graphs

Here (V, μ) is always a connected locally finite weighted graph, finite or infinite, and $|V| > 1$.

2.1 The Dirichlet Laplacian and its eigenvalues

Given a finite subset $\Omega \subset V$, denote by $\mathcal{F}_\Omega$ the set of functions $V \to \mathbb{R}$ such that $f|_{\Omega^c} \equiv 0$. Then $\mathcal{F}_\Omega$ is a linear space of dimension $N = |\Omega|$. Define the operator $\mathcal{L}_\Omega$ on $\mathcal{F}_\Omega$ as follows:

$$\mathcal{L}_\Omega f = \begin{cases} \mathcal{L}f & \text{in } \Omega \\ 0 & \text{in } \Omega^c \end{cases}$$

so that $\mathcal{L}_\Omega f \in \mathcal{F}_\Omega$ and $\mathcal{L}_\Omega : \mathcal{F}_\Omega \to \mathcal{F}_\Omega$.

Definition. The operator $\mathcal{L}_\Omega$ is called the *Dirichlet Laplace operator* in Ω.

Example. Recall that the Laplace operator in $\mathbb{Z}^2$ with a simple weight is defined by

$$\mathcal{L}f(x) = f(x) - \frac{1}{4}\sum_{y \sim x} f(y).$$

Let Ω be the subset of $\mathbb{Z}^2$ that consists of three vertices $a = (0,0)$, $b = (1,0)$, $c = (2,0)$, so that $a \sim b \sim c$. Then we obtain for $\mathcal{L}_\Omega$ the following formulas:

$$\begin{aligned}
\mathcal{L}_\Omega f(a) &= f(a) - \frac{1}{4} f(b) \\
\mathcal{L}_\Omega f(b) &= f(b) - \frac{1}{4} \left(f(a) + f(c) \right) \\
\mathcal{L}_\Omega f(c) &= f(c) - \frac{1}{4} f(b) .
\end{aligned}$$

Consequently, the matrix of $\mathcal{L}_\Omega$ is

$$\begin{pmatrix} 1 & -1/4 & 0 \\ -1/4 & 1 & -1/4 \\ 0 & -1/4 & 1 \end{pmatrix}$$

and the eigenvalues are 1, $1 \pm \frac{1}{4}\sqrt{2}$.

For comparison, consider Ω as a finite graph itself. Then $\Omega = P_3$ and we know that the eigenvalues are $0, 1, 2$. As we see, the Dirichlet Laplace operator of Ω as a subset of $\mathbb{Z}^2$ and the Laplace operator of Ω as a graph are different operators with different spectra.

Returning to the general setting, introduce in $\mathcal{F}_\Omega$ the inner product

$$(f,g)=\sum_{x\in\Omega}f(x)\,g(x)\,\mu(x)\,.$$

Lemma 2.1 (Green's formula) *For any two functions $f,g\in\mathcal{F}_\Omega$, we have*

$$(\mathcal{L}_\Omega f,g)=\frac{1}{2}\sum_{x,y\in\Omega_1}(\nabla_{xy}f)\,(\nabla_{xy}g)\,\mu_{xy},\tag{2.1}$$

where $\Omega_1=U_1(\Omega)\,.$

Proof. Applying the Green formula of Theorem 1.1 in Ω_1 and using that $g=0$ outside Ω, we obtain

$$\begin{aligned}(\mathcal{L}_\Omega f,g) &= \sum_{x\in\Omega_1}\mathcal{L}f(x)\,g(x)\,\mu(x)\\ &= \frac{1}{2}\sum_{x,y\in\Omega_1}(\nabla_{xy}f)\,(\nabla_{xy}g)\,\mu_{xy}-\sum_{x\in\Omega_1,y\in\Omega_1^c}(\nabla_{xy}f)\,g(x)\mu_{xy} \qquad (2.2)\\ &= \frac{1}{2}\sum_{x,y\in\Omega_1}(\nabla_{xy}f)\,(\nabla_{xy}g)\,\mu_{xy}.\end{aligned}$$

We have used the fact that the last sum in (2.2) vanishes. Indeed, the summation can be restricted to neighboring x, y. Therefore, if $y \in \Omega_1^c$ then necessarily $x \in \Omega^c$ and $g(x) = 0$. ■

Since the right hand side of (2.1) is symmetric in f, g, we obtain the following consequence.

Corollary 2.2 *$\mathcal{L}_\Omega$ is a symmetric operator in $\mathcal{F}_\Omega$.*

Hence, the spectrum of $\mathcal{L}_\Omega$ is real. Denote the eigenvalues of $\mathcal{L}_\Omega$ in increasing order by

$$\lambda_1(\Omega) \le \lambda_2(\Omega) \le ... \le \lambda_N(\Omega),$$

Since $\mathcal{L}_\Omega$ is symmetric, the smallest eigenvalue $\lambda_1(\Omega)$ admits the variational characterization:

$$\lambda_1(\Omega) = \inf_{f \in \mathcal{F}_\Omega \setminus \{0\}} \mathcal{R}(f), \tag{2.3}$$

where the *Rayleigh quotient* $\mathcal{R}(f)$ is defined by

$$\mathcal{R}(f) := \frac{(\mathcal{L}_\Omega f, f)}{(f, f)} = \frac{\frac{1}{2}\sum_{x,y\in\Omega_1} (\nabla_{xy} f)^2 \mu_{xy}}{\sum_{x\in\Omega} f^2(x)\mu(x)}, \tag{2.4}$$

where the second equality is true by Lemma 2.1. Note that the ranges $x \in \Omega$ and $x, y \in \Omega_1$ of summations in (2.4) can be extended to $x \in V$ and $x, y \in V$ respectively, because f is supported in Ω.

Theorem 2.3 *Let Ω be a finite non-empty subset of V with non-empty Ω^c. Then the following is true.*

(a) $0 < \lambda_1(\Omega) \leq 1$.

(b) $\lambda_1(\Omega) + \lambda_N(\Omega) \leq 2$. *Consequently,*

$$\operatorname{spec} \mathcal{L}_\Omega \subset [\lambda_1(\Omega), 2 - \lambda_1(\Omega)] \subset (0, 2). \tag{2.5}$$

(c) $\lambda_1(\Omega)$ *decreases when* Ω *increases.*

Proof. (a) Let f be the eigenfunction of $\lambda_1(\Omega)$. Then we have

$$\lambda_1(\Omega) = \frac{(\mathcal{L}_\Omega f, f)}{(f, f)} = \frac{\frac{1}{2}\sum_{x,y\in\Omega_1} |\nabla_{xy} f|^2 \mu_{xy}}{\sum_{x\in\Omega} f^2(x)\mu(x)}, \tag{2.6}$$

which implies $\lambda_1(\Omega) \geq 0$. Let us show that $\lambda_1(\Omega) > 0$. Assume from the contrary that $\lambda_1(\Omega) = 0$. It follows from (2.6) that $\nabla_{xy} f = 0$ for all neighboring vertices $x, y \in \Omega_1$.

That is, $\forall x, y \in \Omega_1$, if $x \sim y$ then $f(x) = f(y)$. Since the complement Ω^c is non-empty, $\exists z \in \Omega^c$. Since (V, μ) is connected, for any $x \in \Omega$ there is a path $\{x_i\}_{i=1}^n$ connecting x and z, let $x_0 = x$ and $x_n = z$. Let k be the minimal index such that $x_k \in \Omega^c$. Since $x_{k-1} \in \Omega$ and $x_{k-1} \sim x_k$, it follows that $x_k \in \Omega_1$.

Hence, all the vertices in the path $x_0 \sim x_1 \sim ... \sim x_{k-1} \sim x_k$ belong to Ω_1 whence we conclude that

$$f(x_0) = f(x_1) = ... = f(x_k).$$

Since $f(x_k) = 0$ it follows that $f(x) = f(x_0) = 0$. Hence, $f \equiv 0$ in Ω. This contradiction proves that $\lambda_1(\Omega) > 0$.

To prove that $\lambda_1(\Omega) \leq 1$, we use the trace of the operator $\mathcal{L}_\Omega$. On the one hand,

$$\operatorname{trace}(\mathcal{L}_\Omega) = \lambda_1(\Omega) + ... + \lambda_N(\Omega) \geq N\lambda_1(\Omega). \tag{2.7}$$

On the other hand, since

$$\mathcal{L}_\Omega f(x) = f(x) - \sum_{y \neq x} P(x,y) f(y),$$

the matrix of the operator $\mathcal{L}_\Omega$ in the basis $\left\{\mathbf{1}_{\{x\}}\right\}_{x\in\Omega}$ has all diagonal values 1 so that $\operatorname{trace}(\mathcal{L}_\Omega) = N$. Comparing with (2.7), we obtain $\lambda_1(\Omega) \leq 1$.

(b) Let f be an eigenfunction with the eigenvalue $\lambda_N(\Omega)$. Then we have similarly to (2.6)

$$\lambda_N(\Omega) = \mathcal{R}(f) = \frac{\frac{1}{2}\sum_{x,y\in V}(\nabla_{xy} f)^2 \mu_{xy}}{\sum_{x\in V} f^2(x)\mu(x)}.$$

Applying (2.3) to the function $|f|$, we obtain

$$\lambda_1(\Omega) \leq \mathcal{R}(|f|) = \frac{\frac{1}{2}\sum_{x,y\in V}(\nabla_{xy}|f|)^2\mu_{xy}}{\sum_{x\in V} f^2(x)\mu(x)} .$$

Since

$$(\nabla_{xy}f)^2 + (\nabla_{xy}|f|)^2 = (f(x)-f(y))^2 + (|f(x)|-|f(y)|)^2 \leq 2\left(f^2(x)+f^2(y)\right),$$

it follows that

$$\begin{aligned}
\lambda_1(\Omega) + \lambda_N(\Omega) &\leq \frac{\sum_{x,y\in V}(f^2(x)+f^2(y))\mu_{xy}}{\sum_{x\in V} f^2(x)\mu(x)} \\
&= \frac{2\sum_{x\in V}\sum_{y\in V} f^2(x)\mu_{xy}}{\sum_{x\in V} f^2(x)\mu(x)} = \frac{2\sum_{x\in V} f^2(x)\mu(x)}{\sum_{x\in V} f^2(x)\mu(x)} = 2.
\end{aligned}$$

(c) If $\Omega \subset \Omega'$ then $\mathcal{F}_\Omega \subset \mathcal{F}_{\Omega'}$ and

$$\lambda_1(\Omega) = \inf_{f\in\mathcal{F}(\Omega)} \mathcal{R}(f) \geq \inf_{f\in\mathcal{F}(\Omega')} \mathcal{R}(f) = \lambda_1(\Omega').$$

which was to be proved. ■

2.2 The Dirichlet problem

In this section we assume that Ω is a finite non-empty subset of V such that Ω^c is non-empty.

Theorem 2.4 *Let Ω be a finite non-empty subset of V with non-empty Ω^c. Consider the following Dirichlet problem:*

$$\begin{cases} \Delta_\mu u = f & \text{in } \Omega, \\ u = g & \text{in } \Omega^c, \end{cases} \tag{2.8}$$

where $u : V \to \mathbb{R}$ is an unknown function while the functions $f : \Omega \to \mathbb{R}$ and $g : \Omega^c \to \mathbb{R}$ are given. Then (2.8) has a unique solution u.

Proof. Let us extend g arbitrarily to Ω, set $v = u - g$ and rewrite (2.8) as follows:

$$\begin{cases} \Delta_\mu v = h & \text{in } \Omega, \\ v = 0 & \text{in } \Omega^c, \end{cases} \tag{2.9}$$

where $h = f - \Delta_\mu g$. Equivalently, (2.9) means that

$$v \in \mathcal{F}_\Omega \quad \text{and} \quad \mathcal{L}_\Omega v = -h \ \text{ in } \Omega. \tag{2.10}$$

By Theorem (2.3), $\operatorname{spec} \mathcal{L}_\Omega$ does not contain 0 so that $\mathcal{L}_\Omega$ is invertible in $\mathcal{F}_\Omega$, which yields a unique solvability of (2.10) and, hence, that of (2.9) and (2.8). $\blacksquare$

For any function $u : V \to \mathbb{R}$ define its Dirichlet energy in Ω by

$$D(u) := \frac{1}{2} \sum_{x,y \in \Omega_1} (\nabla_{xy} u)^2 \mu_{xy} \qquad \text{where } \Omega_1 = U_1(\Omega).$$

Theorem 2.5 (The Dirichlet principle) *If $u \in \mathcal{F}$ is the solution of the Dirichlet problem*

$$\begin{cases} \mathcal{L}u = 0 & \text{in } \Omega \\ u = g & \text{in } \Omega^c \end{cases} \tag{2.11}$$

then $D(u) \le D(v)$ for any function $v \in \mathcal{F}$ such that $v = g$ in Ω^c.

Proof. Set $w = u - v$ so that $w = 0$ in Ω^c. Since $D(\cdot)$ is quadratic, we have

$$D(v) = D(u + w) = D(u) + \sum_{x,y \in \Omega_1} (\nabla_{xy} u)(\nabla_{xy} w) \mu_{xy} + D(w).$$

Since $w = 0$ in Ω^c and $\mathcal{L}u = 0$ in Ω, we obtain by (2.2) that

$$\frac{1}{2} \sum_{x,y \in \Omega_1} (\nabla_{xy} u)(\nabla_{xy} w) \mu_{xy} = \sum_{x \in \Omega_1} \mathcal{L}u(x) w(x) \mu(x) = 0,$$

whence $D(v) = D(u) + D(w) \ge D(u)$. ■

2.3 Geometric estimates of eigenvalues

Recall that, for any subset Ω of V, the edge boundary $\partial\Omega$ is defined by

$$\partial\Omega = \{\overline{xy} \in E : x \in \Omega, y \in \Omega^c\}.$$

Also, for any subset $S \subset E$, its measure is defined by

$$\mu(S) = \sum_{\xi \in S} \mu_\xi.$$

Definition. For any finite subset $\Omega \subset V$, define its *Cheeger constant* by

$$h(\Omega) = \inf_{U \subset \Omega} \frac{\mu(\partial U)}{\mu(U)},$$

where the infimum is taken over all non-empty subsets U of Ω.

In other words, $h(\Omega)$ is the largest constant such that the following inequality is true

$$\mu(\partial U) \geq h(\Omega)\,\mu(U) \tag{2.12}$$

for any non-empty subset U of Ω.

Theorem 2.6 (Cheeger's inequality) *We have*

$$\lambda_1(\Omega) \geq \frac{1}{2} h(\Omega)^2 .$$

The proof is similar to the case of finite graphs. We start with the following lemma.

Lemma 2.7 *For any non-negative function $f \in \mathcal{F}_\Omega$, the following is true:*

$$\sum_{\xi \in E} |\nabla_\xi f| \, \mu_\xi \geq h(\Omega) \sum_{x \in V} f(x) \, \mu(x) . \tag{2.13}$$

Proof. By the co-area formula of Lemma 1.10, we have

$$\sum_{\xi \in E} |\nabla_\xi f| \, \mu_\xi \geq \int_0^\infty \mu(\partial U_t) \, dt,$$

where $U_t = \{x \in V : f(x) > t\}$. Since $U_t \subset \Omega$ for non-negative t, we obtain by (1.29)

$$\mu(\partial U_t) \geq h(\Omega) \, \mu(U_t)$$

whence

$$\sum_{\xi \in E} |\nabla_\xi f| \, \mu_\xi \geq h(\Omega) \int_0^\infty \mu(U_t) \, dt$$

On the other hand, as in the proof of Lemma 1.11, we have

$$\int_0^\infty \mu(U_t) \, dt = \sum_{x \in V} f(x) \, \mu(x) \, ,$$

which implies (2.13). ■

Proof of Theorem 2.6. Let f be the eigenfunction of $\lambda_1(\Omega)$. Rewrite (2.6) in the form

$$\lambda_1(\Omega) = \frac{\sum_{\xi \in E} |\nabla_\xi f|^2 \, \mu_\xi}{\sum_{x \in V} f^2(x) \, \mu(x)}.$$

Hence, to prove (2.13), it suffices to verify that

$$\sum_{\xi \in E} |\nabla_\xi f|^2 \, \mu_\xi \geq \frac{h(\Omega)^2}{2} \sum_{x \in V} f^2(x) \, \mu(x) \, . \tag{2.14}$$

Applying (2.13) to function f^2, we obtain

$$\sum_{\xi \in E} \left| \nabla_\xi \left(f^2 \right) \right| \mu_\xi \geq h\left(\Omega\right) \sum_{x \in V} f^2\left(x\right) \mu\left(x\right). \tag{2.15}$$

The same computation as in the proof of Theorem 1.9 shows that

$$\sum_{\xi \in E} \left| \nabla_\xi \left(f^2 \right) \right| \mu_\xi \leq \left(2 \sum_{\xi \in E} \left| \nabla_\xi f \right|^2 \mu_\xi \sum_{x \in V} f^2(x) \mu\left(x\right) \right)^{1/2}.$$

Combining this with (2.15) yields

$$h\left(\Omega\right) \sum_{x \in V} f^2\left(x\right) \mu\left(x\right) \leq \left(2 \sum_{\xi \in E} \left| \nabla_\xi f \right|^2 \mu_\xi \right)^{1/2} \left(\sum_{x \in V} f^2(x) \mu\left(x\right) \right)^{1/2}.$$

Dividing by $\left(\sum_{x \in V} f^2\left(x\right) \mu\left(x\right) \right)^{1/2}$ and taking square, we obtain (2.14). ∎

2.4 Isoperimetric inequalities

Definition. We say that a weighted graph (V, μ) satisfies the *isoperimetric inequality* with a function $\Phi(s)$ if, for any finite non-empty subset $\Omega \subset V$,

$$\mu(\partial\Omega) \geq \Phi(\mu(\Omega)). \tag{2.16}$$

We always assume that $\Phi(s)$ is a non-negative function that is defined for all

$$s \geq \inf_{x \in V} \mu(x) \tag{2.17}$$

so that the value $\mu(\Omega)$ is in the domain of Φ for all non-empty subsets $\Omega \subset V$.

Example. A connected infinite graph with a simple weight always satisfies the isoperimetric inequality with function $\Phi(s) \equiv 1$. Indeed, any finite subset Ω has at least one edge connecting Ω with Ω^c (because of the connectedness).

For the lattice graph $\mathbb{Z}$ the sharp isoperimetric function is $\Phi(s) \equiv 2$.

As we will show later on, $\mathbb{Z}^m$ satisfies the isoperimetric inequality with the function $\Phi(s) = c_m s^{\frac{m-1}{m}}$ for some constant $c_m > 0$.

There is a tight relation between isoperimetric inequalities and the Dirichlet eigenvalues.

Definition. We say that (V, μ) satisfies the *Faber-Krahn inequality* with a function $\Lambda(s)$ if

$$\lambda_1(\Omega) \geq \Lambda(\mu(\Omega)) \tag{2.18}$$

for any finite non-empty subset $\Omega \subset V$.

Theorem 2.8 *Let (V, μ) satisfy the isoperimetric inequality with a function $\Phi(s)$ such that $\Phi(s)/s$ is decreasing in s. Then (V, μ) satisfies the Faber-Krahn inequality with the function*

$$\Lambda(s) = \frac{1}{2}\left(\frac{\Phi(s)}{s}\right)^2. \tag{2.19}$$

Example. Any connected infinite graph with a simple weight satisfies the Faber-Krahn inequality with function $\Lambda(s) = \frac{1}{2s^2}$.

The lattice graph $\mathbb{Z}^m$ satisfies the Faber-Krahn inequality with function $\Lambda(s) = c'_m s^{-2/m}$.

Proof. We have

$$h(\Omega) = \inf_{U \subset \Omega} \frac{\mu(\partial U)}{\mu(U)} \geq \inf_{U \subset \Omega} \frac{\Phi(\mu(U))}{\mu(U)} \geq \frac{\Phi(\mu(\Omega))}{\mu(\Omega)},$$

whence, by Theorem 2.6, $\lambda_1(\Omega) \geq \frac{1}{2} h(\Omega)^2 \geq \frac{1}{2}\left(\frac{\Phi(\mu(\Omega))}{\mu(\Omega)}\right)^2 = \Lambda(\mu(\Omega))$. ∎

2.5 Isoperimetric inequalities on Cayley graphs

Let G be an infinite group and S be a finite symmetric generating set of G. Let μ be the simple weight on the Cayley graph (G, S). Recall that $\mu(x) = \deg(x) = |S|$ for any $x \in G$. Let e be the neutral element of G, and define the ball centered at e of radius $r \geq 0$ by

$$B_r = \{x \in V : d(x, e) \leq r\} \tag{2.20}$$

Theorem 2.9 (Coulhon–Saloff-Coste '93) *Assume that, for a Cayley graph* (G, S)*,*

$$\mu(B_r) \geq \mathcal{V}(r) \quad \textit{for all integers } r \geq 0, \tag{2.21}$$

where $\mathcal{V}(r)$ *is a non-negative continuous strictly increasing function on* $[0, \infty)$ *such that* $V(r) \to \infty$ *as* $r \to \infty$*. Then* (G, S) *satisfies the isoperimetric inequality with function*

$$\Phi(u) = c_0 \frac{u}{\mathcal{V}^{-1}(2u)}, \quad \textit{where } c_0 > 0. \tag{2.22}$$

Example. In $\mathbb{Z}^m$ (and on nilpotent groups) we have $\mu(B_r) \simeq r^m$ for $r \geq 1$ so that we can take $\mathcal{V}(r) = cr^m$. Then $\mathcal{V}^{-1}(u) = c' u^{1/m}$, and we conclude that $\mathbb{Z}^m$ satisfies the isoperimetric inequality with function

$$\Phi(u) = c'' \frac{u}{u^{1/m}} = c'' u^{\frac{m-1}{m}}.$$

Example. If $\mathcal{V}(r) = \exp(cr)$ then

$$\Phi(u) = c' \frac{u}{\ln u}.$$

This isoperimetric function is sharp on polycyclic groups.

Combining Theorems 2.8 and 2.9, we obtain the following:

Corollary 2.10 *Under the conditions of Theorem 2.9, the Cayley graph* (G, S) *satisfies the Faber-Krahn inequality with the function*

$$\Lambda(u) = c\left(\frac{1}{\mathcal{V}^{-1}(2u)}\right)^2.$$

Example. In $\mathbb{Z}^m$ we obtain

$$\Lambda(u) = cu^{-2/m}$$

as was mentioned above. On the groups with exponential volume growth, we have

$$\Lambda(u) = c(\ln u)^{-2}.$$

Proof of Theorem 2.9. Denote $(V,E)=(G,S)$. For any function f on V with finite support, set

$$\|f\|:=\sum_{x\in V}|f(x)|$$

and

$$\|\nabla f\|:=\sum_{\xi\in E}|\nabla_\xi f|=\frac{1}{2}\sum_{x,y\in V:\ x\sim y}|f(x)-f(y)|.$$

For example, for $f=\mathbf{1}_\Omega$ we have

$$\|f\|=|\Omega|=\frac{1}{|S|}\mu(\Omega),$$

$$|\nabla_\xi f|=\begin{cases}1, & \xi\in\partial\Omega\\ 0, & \xi\notin\partial\Omega\end{cases}$$

and

$$\|\nabla f\|=|\partial\Omega|=\mu(\Omega). \tag{2.23}$$

For any $z\in G$, define a function f_z on G by

$$f_z(x)=f(xz).$$

Claim 1. *If $s \in S$ then*
$$\|f - f_s\| \leq 2\|\nabla f\|.$$

Recall that $x \sim y$ is equivalent to $y = xs$ for some $s \in S$. Hence, for any $s \in S$, we have

$$\|f - f_s\| = \sum_{x\in V} |f(x) - f(xs)| = \sum_{x,y\in V:\ x\sim y} |f(x) - f(y)| = 2\|\nabla f\|. \tag{2.24}$$

Claim 2. *If $z \in B_n$ then*
$$\|f - f_z\| \leq 2n\|\nabla f\|.$$

Any $z \in B_n$ can be represented in the form $z = s_1 s_2 ... s_k$ where $s_i \in S$ and $k \leq n$. Then

$$\begin{aligned}\|f - f_z\| &= \sum_{x\in V} |f(x) - f(xz)| \\ &\leq \sum_{x\in V} |f(x) - f(xs_1)| + \sum_{x\in V} |f(xs_1) - f(xs_1s_2)| + ... \\ &\quad + \sum_{x\in V} |f(xs_1...s_{k-1}) - f(xs_1...s_{k-1}s_k)| \leq 2k\|\nabla f\| \leq 2n\|\nabla f\|.\end{aligned}$$

Claim 3. *For any $n \in \mathbb{N}$ and any function f on V with finite support, set*

$$A_n f(x) = \frac{1}{|B_n|} \sum_{\{y : d(x,y) \le n\}} f(y).$$

Then the following inequality is true:

$$\|f - A_n f\| \le 2n \|\nabla f\|. \tag{2.25}$$

The condition $d(x,y) \le n$ means that $y = x s_1 \dots s_k$ for some $k \le n$ and $s_1, \dots, s_k \in S$. Setting $z = s_1 \dots s_k$ we obtain that $d(x,y) \le n \iff y = xz$ for some $z \in B_n$. Hence, we have

$$\begin{aligned}
\|f - A_n f\| &= \sum_{x \in V} |f(x) - A_n f(x)| = \sum_{x \in V} \left| f(x) - \frac{1}{|B_n|} \sum_{z \in B_n} f(xz) \right| \\
&= \sum_{x \in V} \left| \frac{1}{|B_n|} \sum_{z \in B_n} (f(x) - f(xz)) \right| \le \frac{1}{|B_n|} \sum_{z \in B_n} \sum_{x \in V} |f(x) - f(xz)| \\
&= \frac{1}{|B_n|} \sum_{z \in B_n} \|f - f_z\| \le 2n \|\nabla f\|.
\end{aligned}$$

Claim 4. *Let Ω be a non-empty finite subset of V, and $n \in \mathbb{N}$ be such that $|B_n| \geq 2|\Omega|$. Then we have*

$$\mu(\partial\Omega) \geq \frac{1}{4n|S|}\mu(\Omega).$$

Set $f = \mathbf{1}_\Omega$. Then we have, for any $x \in V$,

$$\begin{aligned} A_n f(x) &= \frac{1}{|B_n|}\sum_{\{y:d(x,y)\leq n\}} f(y) \\ &\leq \frac{1}{|B_n|}\sum_{y\in V} f(y) \\ &= \frac{1}{|B_n|}|\Omega| \leq \frac{1}{2}. \end{aligned}$$

It follows that

$$\|f - A_n f\| \geq \sum_{x\in\Omega} |f(x) - A_n f(x)| \geq \frac{1}{2}|\Omega|.$$

Combining with (2.23) and (2.25), we obtain

$$\mu(\partial\Omega) = \|\nabla f\| \geq \frac{1}{2n}\|f - A_n f\| \geq \frac{1}{4n}|\Omega| = \frac{1}{4n|S|}\mu(\Omega).$$

Claim 5. *For any non-empty finite set* $\Omega \subset V$*, we have* $\mu(\partial\Omega) \geq \Phi(\mu(\Omega))$ *where*

$$\Phi(u) = c_0 \frac{u}{\mathcal{V}^{-1}(2u)}.$$

Choose n to be minimal positive integer with the property that

$$\mathcal{V}(n) \geq 2\mu(\Omega).$$

This implies $\mu(B_n) \geq 2\mu(\Omega)$ which is equivalent to $|B_n| \geq 2|\Omega|$ so that by Claim 4

$$\mu(\partial\Omega) \geq \frac{1}{4n|S|}\mu(\Omega). \tag{2.26}$$

The minimality of n implies that

$$n \leq 1 + \mathcal{V}^{-1}(2\mu(\Omega)) \leq C\mathcal{V}^{-1}(2\mu(\Omega)),$$

because otherwise $n - 1 > \mathcal{V}^{-1}(2\mu(\Omega))$ and $\mathcal{V}(n-1) \geq 2(\Omega)$. Substituting this into (2.26), we obtain

$$\mu(\partial\Omega) \geq \frac{1}{4C|S|}\frac{\mu(\Omega)}{\mathcal{V}^{-1}(2\mu(\Omega))} = c_0\frac{\mu(\Omega)}{\mathcal{V}^{-1}(2\mu(\Omega))} = \Phi(\mu(\Omega)),$$

which was to be proved. ∎

3 Heat kernel on infinite graphs

Everywhere (V, μ) is a connected locally finite weighted graph with $|V| > 1$.

3.1 Transition function and heat kernel

Recall that the Markov kernel on a weighted graph (V, μ) is defined by

$$P(x, y) = \frac{\mu_{xy}}{\mu(x)},$$

and the Markov operator $P : \mathcal{F} \to \mathcal{F}$ by

$$Pf(x) = \sum_{y \sim x} P(x, y) f(y) = \sum_{y \in V} P(x, y) f(y)$$

For any non-negative integer n, consider operator $P^n = \underbrace{P \circ P \circ ... \circ P}_{n}$.

The family $\{P^n\}$ is called the *heat semigroup*. It satisfies

$$P_0 = \text{id} \quad \text{and} \quad P^n P^m = P^{n+m}.$$

It is easy to show that, for any $f : V \to \mathbb{R}$ and all $x \in V$ and $n \geq 1$

$$P^n f(x) = \sum_{y \in} P_n(x, y) f(y),$$

where the kernel $P_n(x, y)$ of the operator P^n can be defined inductively by

$$P_1(x, y) = P(x, y) \quad \text{and } P_{n+1}(x, y) = \sum_{z \in V} P_n(x, z) P(z, y). \tag{3.1}$$

Since $P^n P^m = P^{n+m}$, it follows that for all non-negative integers n, m,

$$P_{n+m}(x, y) = \sum_{z \in V} P_n(x, z) P_m(z, y).$$

By induction one proves that

$$\sum_{y \in V} P_n(x, y) = 1.$$

and

$$P_n(x, y) \mu(x) = P_n(y, x) \mu(y).$$

The Markov kernel $P(x,y)$ determines a *random walk* $\{X_n\}_{n=0}^{\infty}$ on V as follows:

$$\mathbb{P}_{x_0}(X_1 = x_1, X_2 = x_2, ..., X_n = x_n) := P(x_0, x_1) P(x_1, x_2) ... P(x_{n-1}, x_n).$$

It follows $\mathbb{P}_x(X_n = y) = \sum_{x_1,...x_{n-1}\in V} P(x,x_1) P(x_1,x_2) ... P(x_{n-1}, y) = P_n(x,y)$, so that $P_n(x,y)$ is the *n-step transition function* of the random walk.

Definition. The function

$$p_n(x,y) := \frac{P_n(x,y)}{\mu(y)}$$

is called the *heat kernel* of (V,μ) or the *transition density* of the random walk.

The heat kernel is non-negative and satisfies the following identities:

1. $P^n f(x) = \sum_{y\in V} p_n(x,y) f(y) \mu(y)$ (by definition)

2. $p_{n+m}(x,y) = \sum_{z\in V} p_n(x,z) p_m(z,y) \mu(z)$ (the semigroup identity)

3. $\sum_{y\in V} p_n(x,y) \mu(y) \equiv 1$ (stochastic completeness)

4. $p_n(x,y) = p_n(y,x)$ (symmetry, reversibility)

Lemma 3.1 *We have for all $x, y \in V$ and $n, m \in \mathbb{N}$:*

$$p_{n+m}(x,y) \leq \left(p_{2n}(x,x)\, p_{2m}(y,y)\right)^{1/2} \tag{3.2}$$

Proof. It follows from the symmetry and semigroup identity that

$$\begin{aligned} p_{n+m}(x,y) &\leq \left(\sum_{z\in V} p_n(x,z)^2 \mu(z)\right)^{1/2} \left(\sum_{z\in V} p_m(z,y)^2 \mu(z)\right)^{1/2} \\ &= \left(\sum_{z\in V} p_n(x,z)\, p_n(z,x)\, \mu(z)\right)^{1/2} \left(\sum_{z\in V} p_m(y,z)\, p_m(z,y)\, \mu(z)\right)^{1/2} \\ &= \left(p_{2n}(x,x)\, p_{2m}(y,y)\right)^{1/2}. \end{aligned}$$

■

The following question is one of the most interesting problems on infinite graphs:

How quickly $p_n(x,y)$ converges to 0 as $n \to \infty$?

The question amounts to obtaining upper and lower estimates of $p_n(x,y)$ for large n, that will be discussed in this Chapter.

3.2 One-dimensional simple random walk

Let (V,μ) be $\mathbb{Z}$ with a simple weight. Let us determine $P_n(0,x)$. We have, for any $x\in\mathbb{Z}$ and $n\in\mathbb{N}$

$$P_n(0,x)=\mathbb{P}_0(X_n=x)=\sum_{x_1,\dots x_{n-1}\in\mathbb{Z}}P(0,x_1)\,P(x_1,x_2)\dots P(x_{n-1},x)=\left(\frac{1}{2}\right)^n C_n,$$

where C_n is a number of all paths $0\sim x_1\sim x_2\dots\sim x_{n-1}\sim x$, that is, C_n is equal to the number of representations of x in the form

$$z_1+z_2+\dots+z_n=x \ \text{ where } z_k\in\{+1,-1\}. \tag{3.3}$$

If $C_n>0$ then $|x|\le n$ and $x\equiv n \bmod 2$. Assuming that the latter conditions are satisfies, (3.3) is equivalent to

$$u_1+u_2+\dots+u_n=\frac{x+n}{2} \quad \text{where } u_k=\frac{z_k+1}{2}\in\{0,1\},$$

and the number of such representations is $\binom{n}{\frac{x+n}{2}}$. Hence, we conclude that

$$P_n(0,x)=\begin{cases}\frac{1}{2^n}\binom{n}{\frac{x+n}{2}}, & |x|\le n \text{ and } x\equiv n \mod 2,\\ 0, & \text{otherwise},\end{cases} \tag{3.4}$$

Using the Stirling formula

$$n! \sim \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \quad \text{as } n \to \infty, \tag{3.5}$$

and assuming that n is even, we obtain

$$P_n(0,0) = \frac{1}{2^n}\binom{n}{n/2} = \frac{1}{2^n}\frac{n!}{((n/2)!)^2} \sim \frac{1}{2^n}\frac{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n}{\sqrt{2\pi\frac{n}{2}}^2\left(\frac{n}{2e}\right)^n} = \sqrt{\frac{2}{\pi n}},$$

so that

$$P_n(0,0) \sim \sqrt{\frac{2}{\pi n}} \quad \text{as} \quad n \to \infty, \quad n \text{ even}. \tag{3.6}$$

Theorem 3.2 *For all positive integers n and for all $x \in \mathbb{Z}$ such that $|x| \leq n$ and $x \equiv n \mod 2$, the following inequalities hold:*

$$\frac{C_2}{\sqrt{n}}e^{-(\ln 2)\frac{x^2}{n}} \leq P_n(0,x) \leq \frac{C_1}{\sqrt{n}}e^{-\frac{x^2}{2n}}, \tag{3.7}$$

where C_1, C_2 are some positive constants.

Note that $\ln 2 \approx 0.69315 > \frac{1}{2}$.

Proof. Given two sequences $\{a_n\}$ and $\{b_n\}$ of positive numbers, we write $a_n \simeq b_n$ (and say that a_n is *comparable* to b_n) if there exists a constant $C \geq 1$ such that

$$C^{-1} \leq \frac{a_n}{b_n} \leq C \ \text{ for all } n.$$

Stirling's formula (3.5) implies, for any integer $n \geq 0$,

$$n! = \frac{(n+1)!}{(n+1)} \simeq \frac{\sqrt{n+1}}{n+1} \left(\frac{n+1}{e}\right)^{n+1} \simeq (n+1)^{n+\frac{1}{2}} e^{-n}. \tag{3.8}$$

Assuming that m is an even non-negative integer and applying (3.8) to $n = m/2$, we obtain

$$\left(\frac{m}{2}\right)! \simeq \left(\frac{m}{2}+1\right)^{\frac{m+1}{2}} e^{-m/2} \simeq (m+2)^{\frac{m+1}{2}} (2e)^{-m/2}.$$

We would like to replace here $m+2$ my $m+1$. For that observe that

$$\left(\frac{m+2}{m+1}\right)^{m+1} = \left(1+\frac{1}{m+1}\right)^{m+1} \leq e$$

whence

$$(m+2)^{m+1} \simeq (m+1)^{m+1}$$

and

$$\left(\frac{m}{2}\right)! \simeq (m+1)^{\frac{m+1}{2}} (2e)^{-m/2} . \tag{3.9}$$

Using (3.8) to estimate $n!$ and (3.9) with $m = n \pm x$ to estimate $\left(\frac{n\pm x}{2}\right)!$, we obtain from (3.4)

$$\begin{aligned} P_n(0,x) &= \frac{1}{2^n}\binom{n}{\frac{x+n}{2}} = \frac{1}{2^n}\frac{n!}{\left(\frac{n+x}{2}\right)!\left(\frac{n-x}{2}\right)!} \\ &\simeq \frac{1}{2^{n-1}}\frac{(n+1)^{n+\frac{1}{2}}e^{-n}}{(n+x+1)^{\frac{n+x+1}{2}}(2e)^{-\frac{n+x}{2}}(n-x+1)^{\frac{n-x+1}{2}}(2e)^{-\frac{n-x}{2}}} \qquad (3.10) \\ &= \frac{2}{\sqrt{n+1}\left(1+\frac{x}{n+1}\right)^{\frac{n+x+1}{2}}\left(1-\frac{x}{n+1}\right)^{\frac{n-x+1}{2}}} \\ &= \frac{2}{\sqrt{N}}\frac{1}{\left(1+\frac{x}{N}\right)^{\frac{N+x}{2}}\left(1-\frac{x}{N}\right)^{\frac{N-x}{2}}}, \qquad (3.11) \end{aligned}$$

where $N = n+1$.

Using the Taylor expansion

$$\ln(1+\alpha) = \alpha - \frac{\alpha^2}{2} + \frac{\alpha^3}{3} - ..., \qquad -1 < \alpha \leq 1,$$

and the fact that $\frac{|x|}{N} < 1$, we obtain

$$\begin{aligned}
\ln\left(1+\frac{x}{N}\right)^{N+x} &= (N+x)\ln\left(1+\frac{x}{N}\right) \\
&= (N+x)\left(\frac{x}{N} - \frac{x^2}{2N^2} + \frac{x^3}{3N^3} - \frac{x^4}{4N^4} + \frac{x^5}{5N^5} - \frac{x^6}{6N^6} + ...\right) \\
&= \left(x - \frac{x^2}{2N} + \frac{x^3}{3N^2} - \frac{x^4}{4N^3} + \frac{x^5}{5N^4} - \frac{x^6}{6N^5} + ...\right) \\
&\quad + \left(\frac{x^2}{N} - \frac{x^3}{2N^2} + \frac{x^4}{3N^3} - \frac{x^5}{4N^4} + \frac{x^6}{5N^5} - ...\right) \\
&= x + \frac{1}{2N}x^2 - \frac{1}{2\cdot 3N^2}x^3 + \frac{1}{3\cdot 4N^3}x^4 - \frac{1}{4\cdot 5N^4}x^5 + \frac{1}{5\cdot 6N^5}x^6 - ...
\end{aligned}$$

Changing here x to $-x$, we obtain

$$\ln\left(1-\frac{x}{N}\right)^{N-x} = -x + \frac{1}{2N}x^2 + \frac{1}{2\cdot 3N^2}x^3 + \frac{1}{3\cdot 4N^3}x^4 + \frac{1}{4\cdot 5N^4}x^5 + \frac{1}{5\cdot 6N^5}x^6 - \ldots$$

Adding up the two expressions and observing that all the odd powers of x cancel out, we obtain

$$\begin{aligned}
\ln\left(\left(1+\frac{x}{N}\right)^{\frac{N+x}{2}}\left(1-\frac{x}{N}\right)^{\frac{N-x}{2}}\right) &= \frac{1}{2}\left(\ln\left(1+\frac{x}{N}\right)^{N+x} + \ln\left(1-\frac{x}{N}\right)^{N-x}\right) \\
&= \frac{1}{2N}x^2 + \frac{1}{3\cdot 4N^3}x^4 + \frac{1}{5\cdot 6N^5}x^6 + \ldots \\
&= \sum_{k \text{ even},\, k\geq 0} \frac{x^{k+2}}{(k+1)(k+2)N^{k+1}} \\
&= \frac{x^2}{N}\sum_{k \text{ even},\, k\geq 0} \frac{1}{(k+1)(k+2)}\left(\frac{x}{N}\right)^k .
\end{aligned}$$

Substituting into (3.11), we obtain

$$P_n(0,x) \simeq \frac{1}{\sqrt{N}} \exp\left(-\frac{x^2}{N}\left(\frac{1}{2} + \frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2 + \frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4 + \ldots\right)\right). \tag{3.12}$$

Clearly, this implies the upper bound

$$P_n(0,x) \leq \frac{C_1}{\sqrt{N}} \exp\left(-\frac{x^2}{2N}\right). \tag{3.13}$$

For the lower bound, observe that by $\frac{|x|}{N} < 1$

$$\begin{aligned} \frac{1}{2} + \frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2 + \frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4 + \ldots &< \frac{1}{1\cdot 2} + \frac{1}{3\cdot 4} + \frac{1}{5\cdot 6} + \ldots \\ &= 1 - \frac{1}{2} + \frac{1}{3} - \frac{1}{4} + \frac{1}{5} - \frac{1}{6} + \ldots = \ln 2, \end{aligned}$$

whence by (3.12)

$$P_n(0,x) \geq \frac{C_2}{\sqrt{N}} \exp\left(-(\ln 2)\frac{x^2}{N}\right). \tag{3.14}$$

Finally, $N = n+1$ can be replaced in (3.13) and (3.14) by n since $\sqrt{N} \simeq \sqrt{n}$ and $\frac{x^2}{n} - \frac{x^2}{N} = \frac{x^2}{n(n+1)} \leq \frac{x^2}{n^2} \leq 1$. Hence, (3.13) and (3.14) imply (3.7). ■

Corollary 3.3 *In the domain where $\frac{|x|}{n^{3/4}}$ is bounded, we have the following estimate*

$$P_n(0,x) \simeq \frac{1}{\sqrt{n}} \exp\left(-\frac{x^2}{2n}\right). \tag{3.15}$$

Proof. The upper bound in 3.15) is the same as in (3.7), so that we need only to prove the lower bound. The expression under the exponential function in (3.12) can be estimated from above as follows:

$$\begin{aligned}
\frac{x^2}{N}\left(\frac{1}{2}+\frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2+\frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4+\ldots\right) &= \frac{x^2}{2N}+\frac{x^4}{3\cdot 4N^3}+\frac{x^6}{5\cdot 6N^5}+\frac{x^8}{7\cdot 8N^7}+\ldots \\
&= \frac{x^2}{2N}+\frac{x^4}{N^3}\left(\frac{1}{3\cdot 4}+\frac{1}{5\cdot 6}\frac{x^2}{N^2}+\frac{1}{7\cdot 8}\frac{x^4}{N^4}+\ldots\right) \qquad (3.16) \\
&\le \frac{x^2}{2N}+c\left(\frac{1}{3\cdot 4}+\frac{1}{5\cdot 6}+\frac{1}{7\cdot 8}+\ldots\right) \\
&< \frac{x^2}{2N}+\frac{c}{3},
\end{aligned}$$

where c is a constant that bounds $\frac{x^4}{N^3}$. Substituting this into (3.12) and replacing as before N by n, we obtain the lower bound in (3.15). ■

The following lemma will be used in the next section.

Lemma 3.4 *For a simple random walk in $\mathbb{Z}$, we have, for all positive integers r, n,*

$$\mathbb{P}_0\left(X_n \geq r\right) \leq \exp\left(-\frac{r^2}{2n}\right). \tag{3.17}$$

Proof. Let $\{Z_n\}_{n=1}^{\infty}$ be a sequence of independent random variables each taking values ± 1 with probabilities $1/2$. Then

$$X_n = Z_1 + ... + Z_n$$

is a simple random walk on $\mathbb{Z}$ started at 0. We have, for any $\alpha > 0$,

$$\mathbb{P}\left(X_n \geq r\right) = \mathbb{P}\left(e^{\alpha X_n} \geq e^{\alpha r}\right) \leq e^{-\alpha r}\mathbb{E}e^{\alpha X_n}.$$

Using the independence of Z_k and

$$\mathbb{E}e^{\alpha Z_k} = \frac{1}{2}\left(e^{\alpha} + e^{-\alpha}\right) = \cosh\alpha,$$

we obtain

$$\mathbb{E}e^{\alpha X_n} = \mathbb{E}\left(e^{\alpha Z_1}...e^{\alpha Z_n}\right) = \mathbb{E}e^{\alpha Z_1}...\mathbb{E}e^{\alpha Z_n} = \left(\cosh\alpha\right)^n.$$

Since

$$\cosh \alpha = 1 + \frac{\alpha^2}{2!} + \frac{\alpha^4}{4!} + ... \leq \exp\left(\frac{1}{2}\alpha^2\right),$$

we obtain

$$\mathbb{P}\left(X_n \geq r\right) \leq e^{-\alpha r}\left(\cosh \alpha\right)^n \leq \exp\left(-\alpha r + \frac{1}{2}\alpha^2 n\right).$$

Finally, setting here $\alpha = \frac{r}{n}$ that minimizes $-\alpha r + \frac{1}{2}\alpha^2 n$, we obtain

$$\mathbb{P}\left(X_n \geq r\right) \leq \exp\left(-\frac{r^2}{2n}\right), \tag{3.18}$$

which was to be proved. ■

Set for all $n \in \mathbb{N}$ and $k \in \mathbb{Z}$

$$Q_n(k) = \begin{cases} \frac{1}{2^n}\binom{n}{\frac{k+n}{2}}, & k \equiv n \mod 2 \\ 0, & \text{otherwise.} \end{cases}$$

so that by (3.4) $P_n(0, x) = Q_n(x)$.

Corollary 3.5 *For all positive integers r, n*

$$\sum_{k=r}^{\infty} Q_n(k) \leq \exp\left(-\frac{r^2}{2n}\right). \tag{3.19}$$

Proof. We have

$$\sum_{k=r}^{\infty} Q_n(k) = \sum_{x \geq r} P_n(0, x) = \mathbb{P}_0(X_n \geq r) \leq \exp\left(-\frac{r^2}{2n}\right).$$

■

3.3 Carne-Varopoulos estimate

The main result of this section is the following theorem and its consequences. Consider the Markov operator P as an operator in the Hilbert space

$$L^2(V,\mu) := \left\{ f : V \to \mathbb{R} : \sum_{x\in V} f^2(x)\,\mu(x) < \infty \right\},$$

and observe that P is a symmetric operator and $\|P\| \le 1$.

Theorem 3.6 Carne '85, Varopoulos '85) *Let f, g be two functions from $L^2(V,\mu)$ and let $r = d(\operatorname{supp} f, \operatorname{supp} g)$. Then, for all $n \ge 1$,*

$$|(P^n f, g)| \le 2\,\|f\|\,\|g\| \exp\left(-\frac{r^2}{2n}\right). \tag{3.20}$$

Note that always $|(P^n f, g)| \le \|f\|\,\|g\|$ so that (3.20) is non-trivial only if $r > 1$.

Corollary 3.7 *For all $x, y \in V$ and positive integers n,*

$$p_n(x,y) \le \frac{2}{\sqrt{\mu(x)\,\mu(y)}} \exp\left(-\frac{d^2(x,y)}{2n}\right). \tag{3.21}$$

Proof. Setting in (3.20) $f = \mathbf{1}_{\{x\}}$ and $g = \mathbf{1}_{\{y\}}$ and noticing that $r = d(x, y)$,

$$\|f\| = \sqrt{\mu(x)}, \quad \|g\| = \sqrt{\mu(y)}$$

and

$$(P^n f, g) = \sum_{x,y \in V} p_n(x, y) f(x) g(y) \mu(x) \mu(y) = p_n(x, y) \mu(x) \mu(y),$$

we obtain (3.21). ∎

For the proof of Theorem 3.6 we use the *Chebyshev polynomials* T_k:

$$T_k(\lambda) = \cos(k \arccos \lambda), \quad \lambda \in [-1, 1],$$

where $k \in \mathbb{Z}$ and $\lambda \in [-1, 1]$. Since $T_k \equiv T_{-k}$, we restrict so far our consideration to non-negative k. Setting $\theta = \arccos \lambda$, we obtain

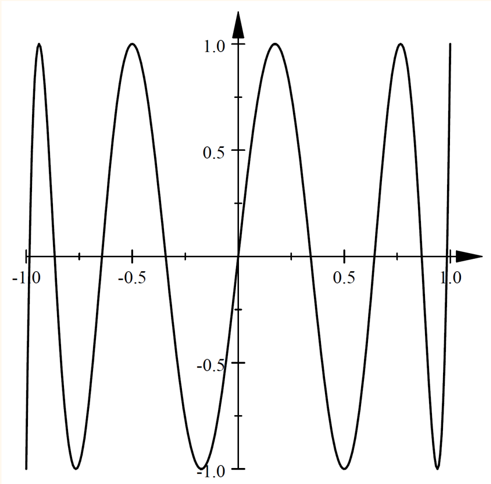
$$\begin{aligned} T_k(\lambda) &= \cos k\theta = \operatorname{Re} e^{ik\theta} = \operatorname{Re}(\cos\theta + i\sin\theta)^k \\ &= \cos^k\theta - \binom{k}{2}\cos^{k-2}\theta \sin^2\theta + \binom{k}{4}\cos^{k-4}\theta\sin^4\theta - \ldots \\ &= \lambda^k - \binom{k}{2}\lambda^{k-2}(1-\lambda^2) + \binom{k}{4}\lambda^{k-4}(1-\lambda^2)^2 - \ldots, \end{aligned}$$

whence we see that $T_k(\lambda)$ is indeed a polynomial of λ of degree k. Note that the leading coefficient in front of λ^k is equal to

$$1+\binom{k}{2}+\binom{k}{4}+\ldots=2^{k-1}.$$

A distinguished property of Chebyshev polynomials is that $|T_k(\lambda)|\leq 1$ for all $\lambda\in[-1,1]$ that is obvious from the definition.

Graph of T_9:



Lemma 3.8 *For all non-negative integers n we have the identity*

$$\lambda^n = \sum_{k=-n}^{n} Q_n(k)\, T_k(\lambda) \quad \forall \lambda \in [-1, 1], \tag{3.22}$$

where

$$Q_n(k) = \begin{cases} \frac{1}{2^n}\binom{n}{\frac{k+n}{2}}, & k \equiv n \mod 2 \\ 0, & \textit{otherwise.} \end{cases}$$

Proof. As above, let $\theta = \arccos \lambda$ so that $\lambda = \cos\theta$. Setting

$$z = \cos\theta + i \sin\theta$$

and observing that $\overline{z} = \frac{1}{z}$, we obtain, for any $m \in \mathbb{Z}$,

$$T_m(\lambda) = T_m(\cos\theta) = \cos m\theta = \operatorname{Re} z^m = \frac{1}{2}\left(z^m + z^{-m}\right).$$

On the other hand,

$$\lambda = \operatorname{Re} z = \frac{1}{2}\left(z + \frac{1}{z}\right)$$

and

$$\lambda^n = \frac{1}{2^n}\left(z+\frac{1}{z}\right)^n = \frac{1}{2^n}\sum_{m=0}^{n}\binom{n}{m}z^m\left(\frac{1}{z}\right)^{n-m} = \frac{1}{2^n}\sum_{m=0}^{n}\binom{n}{m}z^{n-2m} = \frac{1}{2^n}\sum_{k=-n}^{n}\binom{n}{\frac{n-k}{2}}z^k$$

where $k = n-2m$ and summation is restricted to $k \equiv n \bmod 2$. Changing k to $-k$ we obtain

$$\lambda^n = \frac{1}{2^n}\sum_{k=-n}^{n}\binom{n}{\frac{n+k}{2}}z^{-k}.$$

Taking the half-sum of the two expressions for λ^n and noticing that

$$\binom{n}{\frac{n-k}{2}} = \binom{n}{\frac{n+k}{2}}$$

we obtain

$$\lambda^n = \frac{1}{2^n}\sum_{k=-n}^{n}\binom{n}{\frac{n+k}{2}}\frac{z^k+z^{-k}}{2} = \frac{1}{2^n}\sum_{k=-n}^{n}\binom{n}{\frac{n+k}{2}}T_k(\lambda) = \sum_{m=-n}^{n}Q_n(k)\,T_k(\lambda),$$

which was to be proved. ■

Proof of Theorem 3.6. Applying the identity (3.22) Lemma 3.8 to the operator P, we obtain

$$P^n = \sum_{k=-n}^{n} Q_n(k)\, T_k(P)\,. \tag{3.23}$$

That $\|P\| \leq 1$ implies $\operatorname{spec} P \subset [-1,1]$. Since also $\sup_{[-1,1]} |T_k| \leq 1$, it follows by the spectral mapping theorem that

$$\operatorname{spec} T_k(P) \subset T_k(\operatorname{spec} P) \subset T_k([-1,1]) \subset [-1,1]\,.$$

Hence, we have $\|T_k(P)\| \leq 1$.

It follows from (3.1) that

$$(P^n f, g) = \sum_{k=-n}^{n} Q_n(k)\,(T_k(P)\, f, g)\,.$$

Observe that $(T_k(P)\, f, g) = 0$ provided $|k| < r$, because

$$d(\operatorname{supp} f, \operatorname{supp} g) = r > |k| = \deg T_k$$

(cf. the proof of Theorem 1.6). Therefore, we obtain

$$\begin{aligned}
\left|\left(P^n f, g\right)\right| &= \left|\sum_{r\le|k|\le n} Q_n(k)\left(T_k(P) f, g\right)\right| \\
&\le \sum_{r\le|k|\le n} Q_n(k)\left|\left(T_k(P) f, g\right)\right| \\
&\le \left(\sum_{|k|\ge r} Q_n(k)\right)\|T_k(P)\|\,\|f\|\,\|g\| \\
&\le 2\left(\sum_{k\ge r} Q_n(k)\right)\|f\|\,\|g\| \\
&\le 2\exp\left(-\frac{r^2}{2n}\right)\|f\|\,\|g\|
\end{aligned}$$

where we have used that $\|T_k(P)\| \le 1$ and (3.19). ∎

3.4 On-diagonal lower bound of the heat kernel via volume

Theorem 3.9 (F.Lust-Piquard '95) *Assume that* $\mu_0 := \inf_{x \in V} \mu(x) > 0$. *Fix a vertex* $x_0 \in V$, *set for all* $r > 0$

$$B_r = \{x \in V : d(x, x_0) \leq r\}$$

and $\mathcal{V}(r) = \mu(B_r)$. *Assume that, for all* r *large enough,*

$$\mathcal{V}(r) \leq C r^{\alpha} \tag{3.24}$$

for some constants C *and* α. *Then, for all large enough* n,

$$p_{2n}(x_0, x_0) \geq \frac{1/4}{\mathcal{V}\left(\sqrt{2\alpha n \ln n}\right)} \geq \frac{c'}{(n \ln n)^{\alpha/2}}. \tag{3.25}$$

Example. In $\mathbb{Z}^m$ (3.24) holds with $\alpha = m$ so that for all $x \in \mathbb{Z}^m$

$$p_{2n}(x, x) \geq \frac{c}{(n \ln n)^{m/2}}.$$

In fact, as we will see, in $\mathbb{Z}^m$

$$p_{2n}(x, x) \simeq \frac{1}{n^{m/2}}.$$

Proof. By the semigroup property, we have the identity

$$p_{2n}(x_0, x_0) = \sum_{x \in V} p_n(x_0, x)\, p_n(x, x_0)\, \mu(x) = \sum_{x \in V} p_n^2(x_0, x)\, \mu(x)\,. \tag{3.26}$$

Fix some $r > 0$, restrict the summation to $x \in B_r$ and apply the Cauchy-Schwarz inequality:

$$\begin{aligned} p_{2n}(x_0, x_0) &\geq \sum_{x \in B_r} p_n(x_0, x)^2 \mu(x) \\ &\geq \frac{1}{\mu(B_r)} \left(\sum_{x \in B_r} p_n(x_0, x)\, \mu(x) \right)^2 \\ &= \frac{1}{\mathcal{V}(r)} \left(1 - \sum_{x \in B_r^c} p_n(x_0, x)\, \mu(x) \right)^2. \end{aligned} \tag{3.27}$$

Suppose that, for a given n, we can find $r = r(n)$ so that

$$\sum_{x \in B_r^c} p_n(x_0, x)\, \mu(x) \leq \frac{1}{2}. \tag{3.28}$$

Then (3.27) implies

$$p_{2n}(x_0,x_0) \geq \frac{1/4}{\mathcal{V}(r)},$$

which will yield (3.25) provided $r=\sqrt{2\alpha n \ln n}$.

To prove (3.28) with this r, let us apply Corollary 3.7:

$$p_n(x_0,x) \leq \frac{2}{\sqrt{\mu(x_0)\,\mu(x)}} \exp\left(-\frac{d^2(x_0,x)}{2n}\right) \leq \frac{2}{\mu_0} \exp\left(-\frac{d^2(x_0,x)}{2n}\right),$$

whence, for large enough r,

$$\begin{aligned}
\sum_{x\in B_r^c} p_n(x_0,x)\,\mu(x) &\leq \frac{2}{\mu_0}\sum_{x\in B_r^c} \exp\left(-\frac{d^2(x_0,x)}{2n}\right)\mu(x) \\
&= \frac{2}{\mu_0}\sum_{k=0}^{\infty}\sum_{x\in B_{2^{k+1}r}\setminus B_{2^k r}} \exp\left(-\frac{d^2(x_0,x)}{2n}\right)\mu(x) \\
&\leq \frac{2}{\mu_0}\sum_{k=0}^{\infty}\sum_{x\in B_{2^{k+1}r}\setminus B_{2^k r}} \exp\left(-\frac{\left(2^k r\right)^2}{2n}\right)\mu(x)
\end{aligned}$$

$$
\begin{aligned}
&\le \frac{2}{\mu_0}\sum_{k=0}^{\infty}\exp\left(-\frac{\left(2^k r\right)^2}{2n}\right)\mu\left(B_{2^{k+1}r}\right) \\
&\le \frac{2C}{\mu_0}\sum_{k=0}^{\infty}\exp\left(-\frac{4^k r^2}{2n}\right)\left(2^{k+1}r\right)^{\alpha},
\end{aligned}
$$

where we have used $\mu\left(B_{2^{k+1}r}\right) \le C\left(2^{k+1}r\right)^{\alpha}$. Setting

$$
a_k = \exp\left(-\frac{4^k r^2}{2n}\right)\left(2^{k+1}r\right)^{\alpha},
$$

we see that

$$
\frac{a_{k+1}}{a_k} = \exp\left(-\frac{4^{k+1}-4^k}{2}\frac{r^2}{n}\right)2^{\alpha} \le \exp\left(-\frac{r^2}{n}\right)2^{\alpha}.
$$

If $\frac{r^2}{n} \ge \alpha$ then

$$
\frac{a_{k+1}}{a_k} \le e^{-\alpha}2^{\alpha} =: q < 1,
$$

so that the sequence $\{a_k\}$ decays faster than the geometric sequence with the ratio q, whence

$$
\sum_{k=0}^{\infty} a_k \le \sum_{k=0}^{\infty} a_0 q^k = \frac{a_0}{1-q} = \frac{1}{1-q}\exp\left(-\frac{r^2}{2n}\right)(2r)^{\alpha}.
$$

It follows that

$$\sum_{x\in B_r^c} p_n\left(x_0,x\right)\mu\left(x\right)\leq C'\exp\left(-\frac{r^2}{2n}\right)r^{\alpha}. \tag{3.29}$$

Choose here

$$r=\sqrt{2\alpha n\ln n}$$

so that the condition

$$\frac{r^2}{n}\geq\alpha$$

is satisfied for $n\geq 2$. Then we obtain

$$\begin{aligned}\sum_{x\in B_r^c} p_n\left(x_0,x\right)\mu\left(x\right) &\leq C'\exp\left(-\alpha\ln n\right)\left(2\alpha n\ln n\right)^{\frac{\alpha}{2}}\\ &= C''\frac{\left(\ln n\right)^{\frac{\alpha}{2}}}{n^{\frac{\alpha}{2}}}\\ &< \frac{1}{2},\end{aligned}$$

provided n is large enough, which finishes the proof. ■

3.5 On-diagonal lower bound via the Dirichlet eigenvalues

Theorem 3.10 (AG, Coulhon '97) *For any even integer $n \geq 0$ and for any non-empty finite set $\Omega \subset V$, the following estimate holds:*

$$\sup_{x \in \Omega} p_n(x,x) \geq \frac{(1-\lambda_1(\Omega))^n}{\mu(\Omega)}. \tag{3.30}$$

In particular, if $\lambda_1(\Omega) \leq 1/2$ then

$$\sup_{x \in \Omega} p_n(x,x) \geq \frac{\exp(-2\lambda_1(\Omega)n)}{\mu(\Omega)}. \tag{3.31}$$

Proof. The estimate (3.31) follows from (3.30) using the inequality

$$1-\lambda \geq \exp(-2\lambda)$$

that is true for $0 \leq \lambda \leq 1/2$. Indeed, it is obviously true for $\lambda = 0$ and $\lambda = \frac{1}{2}$ and, hence, is true for $\lambda \in [0, 1/2]$ because the function $1-\lambda$ is linear and $\exp(-2\lambda)$ is convex.

Let us prove (3.30). Fix a non-empty finite set $\Omega \subset V$ and consider in $\mathcal{F}_\Omega$ the operator

$$Q := \mathrm{id} - \mathcal{L}_\Omega,$$

that is, for any $f \in \mathcal{F}_\Omega$,

$$Qf(x) = \sum_{y \in \Omega} P(x, y) f(y) \quad \text{for all } x \in \Omega$$

and $Qf(x) = 0$ for $x \in \Omega^c$. By induction, we have, for any $n \in \mathbb{N}$

$$Q^n f(x) = \sum_{y \in \Omega} Q_n(x, y) f(y), \tag{3.32}$$

where $Q_1(x, y) = P(x, y)$ and

$$Q_{n+1}(x, y) = \sum_{z \in \Omega} Q_n(x, z) P(z, y). \tag{3.33}$$

The function $Q_n(x, y)$ can be regarded as the transition function for a random walk with the killing condition outside Ω. The comparison of (3.1) and (3.33) shows that

$$Q_n(x, y) \leq P_n(x, y).$$

Consider trace Q^n. By (3.32), the matrix of Q^n in the basis $\left\{1_{\{x\}}\right\}_{x \in \Omega}$ has on the diagonal the values $Q_n(x, x)$ so that

$$\operatorname{trace} Q^n = \sum_{x \in \Omega} Q_n(x, x) \leq \sum_{x \in \Omega} P_n(x, x).$$

On the other hand, Q has the eigenvalues $1-\lambda_k(\Omega)$, $k=1,...,N$ where $N=|\Omega|$, and Q^n has the eigenvalues $(1-\lambda_k(\Omega))^n$, whence

$$\operatorname{trace} Q^n = \sum_{k=1}^{N} (1-\lambda_k(\Omega))^n \geq (1-\lambda_1(\Omega))^n .$$

We have used that all the terms in the above sum are non-negative since n is even. Comparing the two estimates of the trace, we obtain

$$\begin{aligned}(1-\lambda_1(\Omega))^n &\leq \operatorname{trace} Q^n \leq \sum_{x\in\Omega} P_n(x,x) \\ &= \sum_{x\in\Omega} p_n(x,x)\mu(x) \\ &\leq \sup_{x\in\Omega} p_n(x,x)\mu(\Omega),\end{aligned}$$

whence (3.30) follows. ■

The following lemma enables us to obtain the lower bounds for $p_n(x,x)$ on Cayley graphs.

Lemma 3.11 *On any Cayley graph (G,S) with a simple weight, the value of $p_n(x,x)$ does not depend on x, that is, $p_n(x,x)=p_n(y,y)$ for all x,y.*

Proof. Let us show that the heat kernel is invariant under the left multiplication:

$$p_n(x,y) = p_n(zx, zy) \tag{3.34}$$

for all $x, y, z \in G$, which will imply for $y = x$ and $z = x^{-1}$ that $p_n(x,x) = p_n(e,e)$.

Recall that $x \sim y$ is equivalent to $x^{-1}y \in S$. It follows that $x \sim y$ is equivalent to $zx \sim zy$ because $(zx)^{-1}(zy) = x^{-1}z^{-1}zy = x^{-1}y$.

Inductive basis for $n = 1$:

$$p_1(x,y) = \frac{P(x,y)}{\mu(y)} = \frac{\mu_{xy}}{\mu(x)\mu(y)} = \frac{\mu_{xy}}{\deg(x)\deg(y)} = \frac{\mu_{xy}}{|S|^2}.$$

Since $\mu_{xy} = \mu_{(zx)(zy)}$, we obtain $p_1(x,y) = p_1(zx,zy)$, that is, (3.34) for $n = 1$.

Inductive step from n to $n+1$:

$$\begin{aligned}
p_{n+1}(zx,zy) &= \sum_{w\in G} p_n(zx,w)\,p_1(w,zy)\,\mu(w) \qquad (w = zu) \\
&= \sum_{u\in G} p_n(zx,zu)\,p_1(zu,zy)\,\mu(u) \qquad (p_1(zu,zy) = p_1(u,z)) \\
&= \sum_{u\in G} p_n(x,u)\,p_1(u,y)\,\mu(u) = p_{n+1}(x,y).
\end{aligned}$$

■

Corollary 3.12 *Let (V, μ) be a Cayley graph with a simple weight. Then, for any finite set $\Omega \subset V$ with $\lambda_1(\Omega) \leq 1/2$ we have*

$$p_n(x,x) \geq \frac{\exp(-2\lambda_1(\Omega)n)}{\mu(\Omega)} \tag{3.35}$$

for all $x \in V$ and even $n \geq 0$.

Proof. By Lemma 3.11, we have, for any $x \in V$,

$$p_n(x,x) = \sup_{x \in \Omega} p_n(x,x),$$

so that (3.35) follows from (3.31). ■

Example. Let us show that in $\mathbb{Z}^m$

$$p_n(x,x) \geq cn^{-m/2} \tag{3.36}$$

for all even positive integers n and $x \in \mathbb{Z}^m$. Indeed, fix $r \in \mathbb{N}$ and take $\Omega = B_r$. By considering a tent function in B_r, one can show that

$$\lambda_1(B_r) \leq \frac{C}{r^2}.$$

It follows that, for large enough r,

$$p_n(x,x) \geq \frac{\exp\left(-2\lambda_1(B_r)n\right)}{\mu(B_r)} \geq c' \frac{\exp\left(-\frac{C}{r^2}n\right)}{r^m}.$$

Choosing $r \approx \sqrt{n}$, we obtain (3.36).

3.6 On-diagonal upper bounds of the heat kernel

In this section (V, μ) is an infinite locally finite connected weighted graph that satisfies in addition the conditions

$$\begin{array}{l} 1 \leq \mu_{xy} \leq M \text{ for all } x \sim y, \\ \deg(x) \leq D \text{ for all } x \in V, \end{array} \tag{3.37}$$

for some constants M and D. The first condition is trivially satisfied for a simple weight, the second condition is always satisfied on Cayley graphs.

Lemma 3.13 *The conditions (3.37) imply that, for any non-empty finite set $A \subset V$,*

$$\mu(U_1(A)) \leq C_0 \mu(A), \tag{3.38}$$

where $C_0 = C_0(D, M)$.

Proof. Since $\mu(x) = \sum_{y \sim x} \mu_{xy}$, it follows from (3.37) that

$$1 \leq \mu(x) \leq MD.$$

Therefore, for any finite set A, we have

$$|A| \leq \mu(A) \leq MD|A|.$$

Recall that the the r-neighborhood of A is defined by

$$U_r(A) = \{y \in V : d(x, y) \le r \text{ for some } x \in A\},$$

and the balls of radius r are defined by

$$B_r(x) = \{y \in V : d(x, y) \le r\}.$$

It follows that

$$U_r(A) = \bigcup_{x \in A} B_r(x).$$

The ball $B_1(x)$ consists of the vertex x and of the vertices $y \sim x$ so that $|B_1(x)| \le D + 1$. Hence,

$$|U_1(A)| \le \sum_{x \in A} |B_1(x)| \le (D + 1)|A|,$$

whence it follows that

$$\mu(U_1(A)) \le MD(D + 1)\mu(A).$$

$\blacksquare$

The next theorem is the main result of this section.

Theorem 3.14 (AG, Telcs '01) *If* (V, μ) *satisfies* (3.37) *and the Faber-Krahn inequality with function* $\Lambda(s) = cs^{-1/\alpha}$, *for some* $\alpha, c > 0$, *then the following estimate is true*

$$p_n(x, y) \le Cn^{-\alpha}. \tag{3.39}$$

for all $x, y \in V$, $n \ge 1$ *and some* $C = C(\alpha, c, C_0)$.

Example. If the weight is simple then we always have the Faber-Krahn inequality with function $\Lambda(s) = \frac{1}{2s^2}$, that is, with $\alpha = 1/2$. Assuming that the degree is uniformly bounded, we obtain by Theorem 3.14 that $p_n(x, y) \le Cn^{-1/2}$.

Example. If (V, μ) is a Cayley graphs satisfying the volume growth condition

$$\mu(B_r) \ge cr^m \tag{3.40}$$

then we have the Faber-Krahn inequality with the function $\Lambda(s) = c's^{-2/m}$ whence

$$p_n(x, y) \le Cn^{-m/2}. \tag{3.41}$$

Since (3.40) is satisfied in $\mathbb{Z}^m$, we see that the estimate (3.41) holds in $\mathbb{Z}^m$. Combining with the lower bounds, we obtain that $p_n(x,x) \simeq n^{-m/2}$ for all $x \in \mathbb{Z}^m$ and all even n,

Proof. As before, we use in the space $L^2(V,\mu)$ the inner product.

$$(f,g) = \sum_{x \in V} f(x)\, g(x)\, \mu(x), \tag{3.42}$$

Let $\mathcal{F}_0$ be the set of all functions f on V with a finite support

$$\operatorname{supp} f = \{x \in V : f(x) \neq 0\},$$

so that $\mathcal{F}_0$ is a subspace of L^2. Observe that $f \in \mathcal{F}_0$ implies that $\mathcal{L}f$ and Pf belong to $\mathcal{F}_0$, because

$$\operatorname{supp}(Pf) \subset U_1(\operatorname{supp} f).$$

The approach to the proof is as follows. For a fixed $z \in V$, denote $f_n(x) = p_n(x,z)$ and set

$$b_n := (f_n, f_n) = \sum_{x \in V} p_n(x,z)^2 \mu(x) = p_{2n}(z,z).$$

We will show that $\{b_n\}$ is a decreasing sequence and will estimate the difference $b_n - b_{n+1}$ from below, which will imply an upper bound for b_n and, hence, for $p_{2n}(z,z)$. Then Lemma 3.1 will allow to estimate $p_n(x,y)$ for all $x, y \in V$.

The technical implementation of this approach is quite long and will be split into steps.

Claim 0. *If $f\in\mathcal{F}_0$ then $(Pf,1)=(f,1)$.*

Note that

$$(f,1)=\sum_{x\in V}f(x)\,\mu(x)\,.$$

Using the Green formula of Theorem 1.1 in domain $\Omega=U_1(\operatorname{supp} f)$, we obtain

$$\begin{aligned}(f,1)-(Pf,1)&=(\mathcal{L}f,1)\\&=\sum_{x\in\Omega}\mathcal{L}f(x)\,1(x)\,\mu(x)\\&=\frac{1}{2}\sum_{x,y\in\Omega}(\nabla_{xy}f)(\nabla_{xy}1)\,\mu_{xy}-\sum_{x\in\Omega}\sum_{y\in\Omega^c}(\nabla_{xy}f)\,\mu_{xy}.\end{aligned}$$

The first sum is 0 because $\nabla_{xy}1=0$. In the second sum, $y\notin\Omega$ and $x\sim y$ imply that $x\notin\operatorname{supp} f$ whence $\nabla_{xy}f=0$ so that the second sum is also 0, which proves the claim.

Consider now the following functional

$$Q(f,g)=(f,g)-(Pf,Pg)\,,$$

that is defined for all $f,g\in\mathcal{F}_0$. Also, we write $Q(f)=Q(f,f)$.

Claim 1. *If Ω is a finite non-empty subset of V, $f \in \mathcal{F}_0$ and $U_1(\operatorname{supp} f) \subset \Omega$ then*

$$Q(f) \geq \lambda_1(\Omega)(f,f). \tag{3.43}$$

Clearly, $\operatorname{supp}(Pf) \subset \Omega$ so that $Pf = P_\Omega f$ where

$$P_\Omega = \mathrm{id} - \mathcal{L}_\Omega.$$

Set $\alpha_1 = 1 - \lambda_1(\Omega)$ so that α_1 is the top eigenvalue of P_Ω. Theorem 2.3(b) implies that

$$\operatorname{spec} P_\Omega = 1 - \operatorname{spec} \mathcal{L}_\Omega \subset [1 - (2 - \lambda_1(\Omega)), 1 - \lambda_1(\Omega)] = [-\alpha_1, \alpha_1],$$

whence $\|P_\Omega\| \leq \alpha_1$. Then we have

$$\begin{aligned} Q(f) &= (f,f) - (P_\Omega f, P_\Omega f) \\ &\geq \|f\|^2 - \alpha_1^2 \|f\|^2 \\ &= (1-\alpha_1)(1+\alpha_1)\|f\|^2 \\ &\geq \lambda_1(\Omega)\|f\|^2. \end{aligned}$$

Claim 2. *For all $f \in \mathcal{F}_0$ we have*

$$Q(f) = \frac{1}{2} \sum\nolimits_{x,y \in V} (f(x) - f(y))^2 P_2(x,y)\, \mu(x)\,. \tag{3.44}$$

Using the symmetry of the Markov operator P, we obtain

$$(Pf, Pf) = \left(P^2 f, f\right) = \sum\nolimits_{x,y \in V} P_2(x,y)\, f(x)\, f(y)\, \mu(x)\,,$$

whence

$$\begin{aligned} Q(f) &= \sum\nolimits_{x \in V} f^2(x)\, \mu(x) - \sum\nolimits_{x,y \in V} P_2(x,y)\, f(x)\, f(y)\, \mu(x) \\ &= \sum\nolimits_{x,y \in V} P_2(x,y)\, f^2(x)\, \mu(x) - \sum\nolimits_{x,y \in V} P_2(x,y)\, f(x)\, f(y)\, \mu(x) \\ &= \sum\nolimits_{x,y \in V} P_2(x,y)\, f(x)\, (f(x) - f(y))\, \mu(x)\,. \end{aligned} \tag{3.45}$$

Interchanging x, y we obtain also

$$Q(f) = \sum\nolimits_{x,y \in V} P_2(x,y)\, f(y)\, (f(y) - f(x))\, \mu(x)\,. \tag{3.46}$$

Adding up (3.45) and (3.46), we obtain (3.44).

Claim 3. *If $f \in \mathcal{F}_0$ and s is a positive constant then*

$$Q\left((f-s)_+\right) \leq Q(f). \tag{3.47}$$

Define a function $\varphi : \mathbb{R} \to \mathbb{R}$ by $\varphi(t) = (t-s)_+$. Since φ is a Lipschitz function with the Lipschitz constant 1, we obtain by (3.44)

$$\begin{aligned} Q\left((f-s)_+\right) &= Q(\varphi \circ f) = \frac{1}{2} \sum_{x,y \in V} \left(\varphi(f(x)) - \varphi(f(y))\right)^2 P_2(x,y)\,\mu(x) \\ &\leq \frac{1}{2} \sum_{x,y \in V} \left(f(x) - f(y)\right)^2 P_2(x,y)\,\mu x = Q(f). \end{aligned}$$

Claim 4. *Let f be a non-negative function from $\mathcal{F}_0$. For any $s \geq 0$ define the set Ω_s by*

$$\Omega_s = U_1\left(\operatorname{supp}(f-s)_+\right).$$

Then

$$Q(f) \geq \lambda_1(\Omega_s)\left((f,f) - 2s(f,1)\right). \tag{3.48}$$

In particular, for $s = \frac{1}{4}\frac{(f,f)}{(f,1)}$, we obtain

$$Q(f) \geq \frac{1}{2}\lambda_1(\Omega_s)(f,f).$$

Set $g = (f - s)_+$. By (3.43) and (3.47), we have

$$Q(f) \geq Q(g) \geq \lambda_1(\Omega_s)(g, g).$$

On the other hand, we have

$$g^2 \geq f^2 - 2sf. \tag{3.49}$$

Indeed, if $f \geq s$ then $g = f - s$ and

$$g^2 = f^2 - 2sf + s^2 \geq f^2 - 2sf,$$

and if $f < s$ then $g = 0$ and

$$f^2 - 2sf = (f - 2s) f \leq 0.$$

Integrating (3.49) against measure $\mu(x)$, we obtain

$$(g, g) \geq (f, f) - 2s(f, 1),$$

whence (3.48) follows.

Claim 5. *Let $\{f_n\}_{n=0}^{\infty}$ be a sequence of non-negative functions on V such that $f_0 \in \mathcal{F}_0$, $(f_0, 1) = 1$, and $f_{n+1} = Pf_n$. Set*
$$b_n = (f_n, f_n) \,.$$
Then
$$b_n - b_{n+1} \geq c' b_n^{1+1/\alpha}, \tag{3.50}$$
where $c' = \frac{1}{2} c \left(4C_0\right)^{-1/\alpha}$.

By induction, we obtain that $f_n \in \mathcal{F}_0$ and $(f_n, 1) = 1$ (by Claim 0). Note that

$$b_n - b_{n+1} = (f_n, f_n) - (Pf_n, Pf_n) = Q\left(f_n\right).$$

Estimating $Q\left(f_n\right)$ by Claim 4 and choosing

$$s = \frac{1}{4}\frac{(f_n, f_n)}{(f_n, 1)} = \frac{1}{4} b_n,$$

we obtain
$$b_n - b_{n+1} \geq \frac{1}{2}\lambda_1\left(\Omega_s\right) b_n, \tag{3.51}$$
where
$$\Omega_s = U_1\left(\operatorname{supp}\left(f_n - s\right)_+\right).$$

On the other hand, we have

$$\begin{aligned}\mu\left(\operatorname{supp}\left(f_n-s\right)_+\right) &= \mu\left(x\in V : f_n\left(x\right)>s\right)\\ &\leq \frac{1}{s}\sum_{x\in V} f_n\left(x\right)\mu\left(x\right)=\frac{1}{s}\left(f_n,1\right)=\frac{1}{s}.\end{aligned}$$

By Lemma 3.13, we obtain that

$$\mu\left(\Omega_s\right)\leq\frac{C_0}{s}=\frac{4C_0}{b_n}.$$

Hence, by the Faber-Krahn inequality,

$$\lambda_1\left(\Omega_s\right)\geq c\mu\left(\Omega_s\right)^{-1/\alpha}\geq c\left(4C_0\right)^{-1/\alpha}b_n^{1/\alpha}, \tag{3.52}$$

which together with (3.51) yields (3.50).

Claim 6. *If* $\{b_n\}_{n=0}^{\infty}$ *is a sequence of positive real numbers satisfying (3.50) then* $b_n\leq C'n^{-\alpha}$ *where* $C'=\left(\alpha/c'\right)^{\alpha}$.

We use an elementary inequality

$$y^{-\beta}-x^{-\beta}\geq\frac{\beta\left(x-y\right)}{x^{\beta+1}}, \tag{3.53}$$

that is true for all $\beta > 0$ and $x > y > 0$. Indeed, by the mean-value theorem, we have

$$\frac{y^{-\beta} - x^{-\beta}}{x - y} = -\frac{y^{-\beta} - x^{-\beta}}{y - x} = \beta \xi^{-\beta - 1}$$

where $\xi \in (y, x)$, whence (3.53) follows. Applying (3.53) with $\beta = \frac{1}{\alpha}$, we obtain

$$b_{n+1}^{-1/\alpha} - b_n^{-1/\alpha} \geq \frac{b_n - b_{n+1}}{\alpha b_n^{1+1/\alpha}} \geq \frac{c' b_n^{1+1/\alpha}}{\alpha b_n^{1+1/\alpha}} = \frac{c'}{\alpha}.$$

Summing up this inequality from 0 to n, we conclude that $b_n^{-1/\alpha} \geq \frac{c'}{\alpha} n$ and $b_n \leq C' n^{-\alpha}$.

Now we can finish the proof as follows. Fix a vertex $z \in V$ and set $f_0 = \frac{1}{\mu(z)} \mathbf{1}_{\{z\}}$. Then $f_0 \in \mathcal{F}_0$ and $(f_0, 1) = 1$. Define the sequence $\{f_n\}$ inductively by

$$f_{n+1} = P f_n$$

and show that, in fact,

$$f_n(x) = p_n(x, z) \text{ for any } n \geq 1.$$

We have

$$f_1(x) = P f_0(x) = \sum_{y \in V} P(x, y) f_0(y) = \frac{P(x, z)}{\mu(z)} = p_1(x, z)$$

and

$$f_{n+1}(x) = \sum_{y \in V} P(x,y) f_n(y) = \sum_{y \in V} p_1(x,y) p_n(y,z) \mu(y) = p_{n+1}(x,z).$$

The sequence $\{f_n\}$ satisfies the hypotheses of Claim 5. Setting

$$b_n = (f_n, f_n) = p_{2n}(z,z),$$

we obtain by Claims 5,6 that

$$p_{2n}(z,z) \le C' n^{-\alpha}, \tag{3.54}$$

for all $z \in V$. Using Lemma 3.1 and (3.54), we obtain that

$$p_{k+l}(x,y) \le \left(p_{2k}(x,x) p_{2l}(y,y)\right)^{1/2} \le C' (kl)^{-\alpha/2}, \tag{3.55}$$

for all $x, y \in V$ and positive integers k, l. Given an integer $n \ge 2$, represent it in the form $n = k + l$ where $l = k$ for even n and $l = k + 1$ for odd n. In the both cases, we have

$$l \ge k \ge \frac{n-1}{2} \ge \frac{n}{4},$$

whence by (3.55)

$$p_n(x,y) \le C'' n^{-\alpha}.$$

Finally, for $n = 1$ we obtain $p_1(x,y) = \frac{P(x,y)}{\mu(y)} \le 1$ because $P(x,y) \le 1$ and $\mu(y) \ge 1$ by (3.37). $\blacksquare$

Remark. As we have seen in the last part of the proof, the estimate (3.39) is equivalent to the *on-diagonal estimate*

$$p_n(x,x) \le Cn^{-\alpha}.$$

For that reason, (3.39) is also frequently referred to as an on-diagonal estimate of the heat kernel. The point is that this estimate does not take into account the distance between points x, y, which could improve the estimate. Indeed, if $d(x,y) > n$ then obviously $p_n(x,y) = 0$. Combining the on-diagonal estimate (3.39) with the Carne-Varopoulos estimate (3.21), it is easy to show that, for any $0 < \varepsilon < \alpha$,

$$p_n(x,y) \le \frac{C}{n^{\alpha-\varepsilon}} \exp\left(-c_\varepsilon \frac{d^2(x,y)}{n}\right) \tag{3.56}$$

with some $c_\varepsilon > 0$. Using much more complicated method, one can show that (3.56) holds also for $\varepsilon = 0$ (Hebisch–Saloff-Coste).

4 The type problem

4.1 Recurrence of the random walk via the heat kernel

We say that an event $A_n, n \in \mathbb{N}$, occurs *infinitely often* if there is a sequence $n_k \to \infty$ of indices such that A_{n_k} takes place for all k.

Definition. We say that the random walk $\{X_n\}$ on (V, μ) is *recurrent* if, for any $x \in V$,

$$\mathbb{P}_x \left(X_n = x \text{ infinitely often}\right) = 1,$$

and *transient* otherwise, that is, if there is $x \in V$ such that

$$\mathbb{P}_x \left(X_n = x \text{ infinitely often}\right) < 1.$$

The *type problem* is the problem of deciding whether the random walk is recurrent or transient.

Theorem 4.1 (Khas'minski '60) *$\{X_n\}$ is transient if and only if for some/all $x \in V$*

$$\sum_{n=1}^{\infty} p_n \left(x, x\right) < \infty. \tag{4.1}$$

Corollary 4.2 (Polya '21) *In $\mathbb{Z}^m$ the random walk is transient if and only if $m > 2$.*

Proof. Indeed, in $\mathbb{Z}^m$ we have

$$\sum_n p_n(x,x) \simeq \sum_n \frac{1}{n^{m/2}}$$

and the latter series converges if and only if $m > 2$. ■

We start the proof of Theorem 4.1 with the following lemma.

Lemma 4.3 *If the condition*

$$\sum_{n=1}^{\infty} p_n(x,y) < \infty \tag{4.2}$$

holds for some $x, y \in V$ then it holds for all $x, y \in V$. In particular, if (4.1) holds for some $x \in V$ then it holds for all $x \in V$ and, moreover, (4.2) holds for all $x, y \in V$.

Proof. Let us show that if (4.2) holds for some $x, y \in V$ then the vertex x can be replaced by any of its neighbors, and (4.2) will be still true. Since the graph (V, μ) is connected, in a finite number of steps the initial point x can be then replaced by any other point. By the symmetry, the same applies to y so that in the end both x and y can take arbitrary values.

Fix a vertex $x' \sim x$ and prove that

$$\sum_{n=1}^{\infty} p_n\left(x', y\right) < \infty.$$

We have

$$P_{n+1}\left(x, y\right) = \sum_z P\left(x, z\right) P_n\left(z, y\right) \geq P\left(x, x'\right) P_n\left(x', y\right),$$

whence

$$p_n\left(x', y\right) = \frac{P_n\left(x', y\right)}{\mu\left(y\right)} \leq \frac{P_{n+1}\left(x, y\right)}{P\left(x, x'\right) \mu\left(y\right)} = \frac{p_{n+1}\left(x, y\right)}{P\left(x, x'\right)}.$$

It follows that

$$\sum_{n=1}^{\infty} p_n\left(x', y\right) \leq \frac{1}{P\left(x, x'\right)} \sum_{n=1}^{\infty} p_{n+1}\left(x, y\right) < \infty,$$

which was to be proved. ■

Proof of Theorem 4.1: the sufficiency of (4.1). Fix a vertex $x_0 \in V$ and denote by A_n the event $\{X_n = x_0\}$ so that, for any $x \in V$,

$$\mathbb{P}_x (A_n) = \mathbb{P}_x (X_n = x_0) = P_n (x, x_0) = p_n (x, x_0) \mu (x_0) .$$

By Lemma 4.3, the condition (4.1) implies $\sum_n p_n (x, x_0) < \infty$ whence

$$\sum_n P_x (A_n) < \infty. \tag{4.3}$$

By the Borel-Cantelli lemma, the probability that the events A_n occur infinitely often, is equal to 0 that is,

$$\mathbb{P}_x (X_n = x_0 \text{ infinitely often}) = 0, \tag{4.4}$$

and the random walk is transient. ■

Note that the condition (4.4) is in fact stronger than the definition of the transience as the latter is

$$\mathbb{P}_{x_0} (X_n = x_0 \text{ infinitely often}) < 1$$

for some $x_0 \in V$. We will take advantage of (4.4) later on.

The proof of the necessity of condition (4.1) in Theorem 4.1 will be preceded by some lemmas.

Definition. A function $u : V \to \mathbb{R}$ is called *subharmonic* in Ω if $\mathcal{L}u\,(x) \leq 0$ for all $x \in \Omega$, and *superharmonic* in Ω if $\mathcal{L}u\,(x) \geq 0$ for all $x \in \Omega$. A function u is called harmonic in Ω if it is both subharmonic and superharmonic, that is, if it satisfies the Laplace equation $\mathcal{L}u = 0$.

For example, the constant function is harmonic on all sets.

Lemma 4.4 (A maximum/minimum principle) *Let Ω be a non-empty finite subset of V such that Ω^c is non-empty. Then, for any function $u : V \to \mathbb{R}$, that is subharmonic in Ω, we have*

$$\max_{\Omega} u \leq \sup_{\Omega^c} u,$$

and for any function $u : V \to \mathbb{R}$, that is superharmonic in Ω, we have

$$\min_{\Omega} u \geq \inf_{\Omega^c} u.$$

Proof. It suffices to prove the first claim. If $\sup_{\Omega^c} u = +\infty$ then there is nothing to prove. If $\sup_{\Omega^c} u < \infty$ then, by replacing u by $u + \mathrm{const}$, we can assume that $\sup_{\Omega^c} u = 0$. Set

$$M = \max_{\Omega} u$$

and show that $M \leq 0$, which will settle the claim. Assume from the contrary that $M > 0$ and consider the set

$$S := \{x \in V : u(x) = M\}. \tag{4.5}$$

Clearly, $S \subset \Omega$ and S is non-empty.

Claim 1. *If $x \in S$ then all neighbors of x also belong to S.*

Indeed, we have $\mathcal{L}u(x) \leq 0$ which can be rewritten in the form

$$u(x) \leq \sum_{y \sim x} P(x,y)\, u(y).$$

Since $u(y) \leq M$ for all $y \in V$, we have

$$\sum_{y \sim x} P(x,y)\, u(y) \leq M \sum_{y \sim x} P(x,y) = M.$$

Since $u(x) = M$, all inequalities in the above two lines must be equalities, whence it follows that $u(y) = M$ for all $y \sim x$. This implies that all such y belong to S.

Claim 2. *Let S be a non-empty set of vertices of a connected graph such that $x \in S$ implies that all neighbors of x belong to S. Then $S = V$.*

Indeed, let $x \in S$ and y be any other vertex. Then there is a path $\{x_k\}_{k=0}^n$ between x and y, that is,

$$x = x_0 \sim x_1 \sim x_2 \sim \ldots \sim x_n = y.$$

Since $x_0 \in S$ and $x_1 \sim x_0$, we obtain $x_1 \in S$. Since $x_2 \sim x_1$, we obtain $x_2 \in S$. By induction, we conclude that all $x_k \in S$, whence $y \in S$.

It follows from the two claims that the set (4.5) must coincide with V, which is not possible since $u(x) \leq 0$ in Ω^c. This contradiction shows that $M \leq 0$. ■

Lemma 4.5 (Strong maximum principle) *Let u be a subharmonic function on V, that is, such that $\mathcal{L}u \leq 0$ on V. If, for some point $x \in V$,*

$$u(x) = \sup u,$$

then $u \equiv \text{const}$. In other words, a subharmonic function on V cannot attain its supremum unless it is a constant.

Proof. Set $M = \sup u$ and let x be a vertex where $u(x) = M$. Since $\mathcal{L}u(x) \leq 0$, it follows that

$$M = u(x) \leq Pu(x) = \sum_{y \sim x} P(x,y)\, u(y).$$

The right hand side here is bounded by M because $u(y) \leq M$ for all y. If $u(y) < M$ for some $y \sim x$, then we obtain that the right hand side $< M$, which is a contradiction. Hence, $u(y) = M$ for all $y \sim x$. Hence, the set

$$S = \{x \in V : u(x) = M\}$$

has the property that if $x \in S$ then all neighbors of x also belong to S. Since S is non-empty and the graph V is connected, it follows that $S = V$, that is, $u \equiv M$. ∎

Definition. Fix a finite non-empty set $K \subset V$ and consider the function

$$v_K(x) = \mathbb{P}_x(\exists n \geq 0 \; X_n \in K).$$

The function $v_K(x)$ is called the *hitting (or visiting) probability* of K. Consider also the function

$$h_K(x) = \mathbb{P}_x(X_n = x_0 \text{ infinitely often}),$$

that is called the *recurring probability* of K.

Clearly, we have $v \equiv 1$ on K and $0 \leq h_K(x) \leq v_K(x) \leq 1$ for all $x \in V$.

In the next two lemmas, the set K will be fixed so that we write $v(x)$ and $h(x)$ instead of $v_K(x)$ and $h_K(x)$, respectively.

Lemma 4.6 *We have $\mathcal{L}v(x) = 0$ if $x \notin K$ (that is, v is harmonic outside K), and $\mathcal{L}v(x) \geq 0$ for any $x \in K$.*

Proof. If $x \notin K$ then we have by the Markov property

$$\begin{aligned}
v(x) &= \mathbb{P}_x(\exists n \geq 0\ X_n \in K) \\
&= \mathbb{P}_x(\exists n \geq 1\ X_n \in K) \\
&= \sum_y P(x,y)\,\mathbb{P}_y(\exists n \geq 1\ X_{n-1} \in K) \\
&= \sum_y P(x,y)\,\mathbb{P}_y(\exists n \geq 0\ X_n \in K) \\
&= \sum_y P(x,y)\,v(y)
\end{aligned}$$

so that $v(x) = Pv(x)$ and $\mathcal{L}v(x) = 0$. If $x \in K$ then

$$\mathcal{L}v(x) = v(x) - Pv(x) = 1 - Pv(x) \geq 0$$

because $Pv(x) \leq P1(x) = 1$. ■

Lemma 4.7 *The sequence of functions $\{P^n v\}$ is decreasing in n and*

$$\lim_{n\to\infty} P^n v(x) = h(x) \tag{4.6}$$

for any $x \in V$.

Proof. Since $\mathcal{L}v \geq 0$, we obtain

$$P^n v - P^{n+1} v = P^n (v - Pv) = P^n (\mathcal{L}v) \geq 0$$

so that $\{P^n v\}$ is decreasing. Hence, the limit in (4.6) exists.

Consider the events

$$B_m = \{\exists n \geq m \ \ X_n \in K\}.$$

Obviously, the sequence $\{B_m\}$ is decreasing and the event

$$\bigcap_m B_m = \{\forall m \ \exists n \geq m \ \ X_n \in K\}$$

is identical to the event that $X_n \in K$ infinitely often. Hence, we have

$$h(x) = \mathbb{P}_x\left(\bigcap_m B_m\right) = \lim_{m\to\infty} \mathbb{P}_x(B_m). \tag{4.7}$$

We claim that

$$\mathbb{P}_x(B_m) = P^m v(x). \tag{4.8}$$

Indeed, for $m = 0$ this is the definition of $v(x)$. Here is the inductive step from $m-1$ to m using the Markov property:

$$\begin{aligned}
\mathbb{P}_x(\exists n \geq m \quad X_n \in K) &= \sum_y P(x,y)\,\mathbb{P}_y(\exists n \geq m \quad X_{n-1} \in K) \\
&= \sum_y P(x,y)\,\mathbb{P}_y(\exists n \geq m-1 \; X_n \in K) \\
&= \sum_y P(x,y)\,P^{m-1} v(y) \\
&= P^m v(x).
\end{aligned}$$

Combining (4.7) with (4.8), we obtain (4.6). ■

Proof of Theorem 4.1: the necessity of (4.1). Assume that the random walk is transient and show that (4.1) is true. Let $x_0 \in V$ be a point where

$$\mathbb{P}_{x_0}(X_n = x_0 \text{ infinitely often}) < 1.$$

Consider the hitting and recurring probabilities $v(x)$ and $h(x)$ with respect to the set $K = \{x_0\}$. The above condition means that $h(x_0) < 1$. It follows that $v \not\equiv 1$ because otherwise

$P^n v \equiv 1$ for all n and by Lemma 4.7 $h \equiv 1$. As we know, $\mathcal{L}v(x) = 0$ for $x \neq x_0$ and $\mathcal{L}v(x_0) \geq 0$.

Claim 1. $\mathcal{L}v(x_0) > 0$.

Assume from the contrary that $\mathcal{L}v(x_0) = 0$, that is, $\mathcal{L}v(x) = 0$ for all $x \in V$. Since v takes its maximal value 1 at some point (namely, at x_0), we obtain by the strong maximum principle that $v \equiv 1$, which contradicts the assumption of the transience.

Denote $f = \mathcal{L}v$ so that $f(x) = 0$ for $x \neq x_0$ and $f(x_0) > 0$.

Claim 2. *We have for all $x \in V$*

$$\sum_{n=0}^{\infty} P^n f(x) \leq v(x). \tag{4.9}$$

Fix a positive integer m and observe that

$$(\mathrm{id} - P)\left(\mathrm{id} + P + P^2 + ... + P^{m-1}\right) = \mathrm{id} - P^m$$

whence it follows that

$$\mathcal{L}\left(\sum_{n=0}^{m-1} P^n f\right) = (\mathrm{id} - P^m) f = f - P^m f \leq f.$$

Set

$$v_m = \sum_{n=0}^{m-1} P^n f.$$

Obviously, v_m has a finite support and $\mathcal{L} v_m \leq f$. For comparison, we have $\mathcal{L} v = f$ and $v \geq 0$ everywhere. We claim that $v_m \leq v$ in V. Indeed, let $\Omega = \operatorname{supp} v_m$ so that outside Ω_m the inequality $v_m \leq v$ is trivially satisfied. In Ω we have $\mathcal{L}(v - v_m) \geq 0$. By the minimum principle of Lemma 4.4, we have

$$\min_{\Omega} (v - v_m) = \inf_{\Omega^c} (v - v_m).$$

Since the right hand side is ≥ 0, it follows that $v - v_m \geq 0$ in Ω, which was claimed. Hence, we have

$$\sum_{n=0}^{m-1} P^n f \leq v,$$

whence (4.9) follows by letting $m \to \infty$.

Using that $\operatorname{supp} f = \{x_0\}$, rewrite (4.9) in the form

$$\sum_{n=0}^{\infty} p_n(x, x_0) f(x_0) \mu(x_0) \leq v(x)$$

whence it follows that $\sum_{n=0}^{\infty} p_n(x, x_0) < \infty$. Setting here $x = x_0$ we finish the proof. $\blacksquare$

Corollary 4.8 *Let K be a non-empty finite subset of V. If the random walk is recurrent then $v_K \equiv h_K \equiv 1$. If the random walk is transient then $v_K \not\equiv 1$ and $h_K \equiv 0$.*

Hence, we obtain a 0-1 law for the recurring probability: either $h_k \equiv 1$ or $h_K \equiv 0$.

Proof. Let x_0 be a vertex from K. Obviously, we have

$$v_{\{x_0\}}(x) \leq v_K(x).$$

Therefore, if the random walk is recurrence and, hence, $v_{\{x_0\}} \equiv 1$ then also $v_K(x) \equiv 1$. Since

$$h_K = \lim_{m \to \infty} P^m v_K, \tag{4.10}$$

it follows that $h_K \equiv 1$.

Let the random walk be transient. Then by Theorem 4.1 and Lemma 4.3, we have

$$\sum_{n=1}^{\infty} p_n(x_0, x) < \infty$$

for all $x_0, x \in V$. It follows from the proof of Theorem 4.1 that $h_{\{x_0\}}(x) = 0$ (cf. (4.4)). If $\{X_n\}$ visits K infinitely often then $\{X_n\}$ visits infinitely often at least one of the vertices in K. Hence, we have

$$h_K \le \sum_{x_0 \in K} h_{\{x_0\}}.$$

Since $h_{\{x_0\}} \equiv 0$, we conclude that $h_K \equiv 0$. Finally, (4.10) implies that $v_K \not\equiv 1$. ■

4.2 The type problem on Cayley graphs

Now we can completely solve the type problem for Cayley graphs.

Theorem 4.9 (Varopoulos '83) *Let (V, E) be a Cayley graph and μ be a simple weight on it. Let $B_r = \{x \in V : d(x, e) \le r\}$.*

(a) If $\mu(B_r) \le Cr^2$ for large enough r with some constant C then (V, μ) is recurrent.

(b) If $\mu(B_r) \ge cr^\alpha$ for large enough r with some constants $\alpha > 2$ and $c > 0$ then (V, μ) is transient.

Remark. It is known from Group Theory (H.Bass) that for Cayley graphs the following two alternatives take places:

1. either $\mu(B_r) \simeq r^m$ for some positive integer m (the power volume growth),

2. or, for any C, N, we have $\mu(B_r) \geq Cr^N$ for large enough r (the superpolynomial volume growth).

It follows from Theorem 4.9 that, in the first case, the random walk is recurrent if and only if $m \leq 2$, while in the second case the random walk is always transient.

Proof. (a) This part is true for an arbitrary weighted graph since by Theorem 3.9 we have

$$p_{2n}(e,e) \geq \frac{\text{const}}{n \ln n}, \quad \text{for large } n,$$

and, hence, $\sum_n p_{2n}(e,e) = \infty$, so that the recurrence follows by Theorem 4.1.

(b) By Corollary 2.10, the graph (V, μ) has the Faber-Krahn function $\Lambda(s) = cs^{-2/\alpha}$ and by Theorem 3.14, we obtain

$$p_n(x,x) \leq \frac{C}{n^{\alpha/2}}.$$

Since $\alpha > 2$, it follows that

$$\sum_n p_n(x,x) < \infty,$$

so that the graph is transient by Theorem 4.1. ■

4.3 Volume test for recurrence

In this section, let us fix an integer-valued function $\rho(x)$ on V with the following two properties:

- For any non-negative integer r, the set
$$B_r = \{x \in V : \rho(x) \leq r\}$$
is finite and non-empty.
- If $x \sim y$ then $|\nabla_{xy}\rho| \leq 1$.

For example, $\rho(x)$ can be the distance function to any finite non-empty subset of V.

Theorem 4.10 (Nash-Williams '59) *If*

$$\sum_{r=0}^{\infty} \frac{1}{\mu(\partial B_r)} = \infty, \tag{4.11}$$

then the random walk on (V, μ) is recurrent.

Note that ∂B_r is non-empty because otherwise the graph (V, μ) would be disconnected.

An alternative way of stating this theorem is the following. Assume that V is a disjoint union of a sequence $\{A_k\}_{k=0}^{\infty}$ of non-empty finite subsets with the following property: if $x \in A_k$ and $y \in A_m$ with $|k-m| \geq 2$ then x and y are not neighbors. Denote by E_k the set of edges between A_k and A_{k+1} and assume that

$$\sum_{k=0}^{\infty} \frac{1}{\mu(E_k)} = \infty. \tag{4.12}$$

Then the random walk on (V, μ) is recurrent. Indeed, defining $\rho(x) = k$ if $x \in A_k$ we obtain that $B_r = \bigcup_{k=0}^{r} A_k$ and $\partial B_r = E_r$. Hence, (4.12) is equivalent to (4.11).

Let us give two simple examples when (4.12) is satisfied:

1. if $\mu(E_k) \leq Ck$ for all large enough k;
2. if $\mu\left(E_{k_j}\right) \leq C$ for a sequence $k_j \to \infty$ (in this case, $\mu(E_k)$ for $k \neq k_j$ may take arbitrarily big values).

Proof of Theorem 4.10. Consider the hitting probability of B_0:

$$v(x) = v_{B_0}(x) = \mathbb{P}_x(\exists n \geq 0 : \ X_n \in B_0).$$

Recall that $0 \leq v \leq 1$, $v = 1$ on B_0, and $\mathcal{L}v = 0$ outside B_0 (cf. Lemma 4.6). Our purpose is to show that $v \equiv 1$, which will imply the recurrence by Corollary 4.8.

We will compare $v(x)$ to the sequence of functions $\{u_k\}_{k=1}^{\infty}$ that is constructed as follows. Define $u_k(x)$ as the solution to the following Dirichlet problem in $\Omega_k = B_k \setminus B_0$:

$$\begin{cases} \mathcal{L}u_k = 0 & \text{in } \Omega_k \\ u_k = f & \text{in } \Omega_k^c \end{cases} \tag{4.13}$$

where $f = \mathbf{1}_{B_0}$. In other words, $u_k = 1$ on B_0 and $u_k = 0$ outside B_k, while u_k is harmonic in Ω_k. By Theorem 2.4, the problem (4.13) has a unique solution. By the maximum/minimum principle of Lemma 4.4, we have $0 \leq u_k \leq 1$.

Since $u_{k+1} = u_k$ on B_0 and $u_{k+1} \geq 0 = u_k$ in B_k^c, we obtain by the maximum principle that $u_{k+1} \geq u_k$ in Ω_k. Therefore, the sequence $\{u_k\}$ increases and converges to a function u_∞ as $k \to \infty$. The function u_∞ has the following properties: $0 \leq u_\infty \leq 1$, $u_\infty = 1$ on B_0, and $\mathcal{L}u_\infty = 0$ outside B_0 (note that $\mathcal{L}u_k \to \mathcal{L}u_\infty$ as $k \to \infty$). Comparing v with u_k in Ω_k and using the maximum principle, we obtain that $v \geq u_k$, whence it follows that $v \geq u_\infty$. Hence, in order to prove that $v \equiv 1$, it suffices to prove that $u_\infty \equiv 1$, which will be done in the rest of the proof.

By the Dirichlet principle of Theorem 2.5, the solution u_k of the Dirichlet problem (4.13) it minimizes the energy

$$D(u) := \frac{1}{2} \sum_{x,y \in U_1(\Omega_k)} (\nabla_{xy} u)^2 \mu_{xy}$$

among all functions u such that $u = f$ in Ω_k^c. Since $u \equiv 1$ in B_0, $u \equiv 0$ in B_k^c, and $U_1(B_k) \subset B_{k+1}$, we have

$$D(u) = \frac{1}{2} \sum_{x,y \in B_{k+1}} (\nabla_{xy} u)^2 \mu_{xy}.$$

Choose a function u with the above boundary condition in the form

$$u(x) = \varphi(\rho(x)),$$

where $\varphi(s)$ is a function on $\mathbb{Z}$ such that $\varphi(s) = 1$ for $s \le 0$ and $\varphi(s) = 0$ for $s \ge k+1$. Set $S_0 = B_0$ and

$$S_r = \{x \in V : \rho(x) = r\}$$

for positive integers r. Clearly, B_r is a disjoint union of $S_0, S_1, ..., S_r$. Observe also that if $x \sim y$ then x, y belong either to the same S_r (and in this case $\nabla_{xy} u = 0$) or the one to S_r

and the other to S_{r+1}, because $|\rho(x) - \rho(y)| \leq 1$. Having this in mind, we obtain

$$\begin{aligned} D(u) &= \sum_{r=0}^{k} \sum_{x \in S_r, y \in S_{r+1}} (\nabla_{xy} u)^2 \mu_{xy} \\ &= \sum_{r=0}^{k} \sum_{x \in S_r, y \in S_{r+1}} (\varphi(r) - \varphi(r+1))^2 \mu_{xy} \\ &= \sum_{r=0}^{k} (\varphi(r) - \varphi(r+1))^2 \mu(\partial B_r). \end{aligned}$$

Denote

$$m(r) := \mu(\partial B_r)$$

and define $\varphi(r)$ for $r = 0, ..., k$ from the following conditions: $\varphi(0) = 1$ and

$$\varphi(r) - \varphi(r+1) = \frac{c_k}{m(r)}, \ \ r = 0, ..., k \tag{4.14}$$

where the constant c_k is to be found. Indeed, we have still the condition $\varphi(k+1)=0$ to be satisfied. Summing up (4.14), we obtain

$$\varphi(0)-\varphi(k+1)=c_k\sum_{r=0}^{k}\frac{1}{m(r)}$$

so that $\varphi(k+1)=0$ is equivalent to

$$c_k=\left(\sum_{r=0}^{k}\frac{1}{m(r)}\right)^{-1}. \tag{4.15}$$

Hence, assuming (4.15), we obtain

$$D(u)=\sum_{r=0}^{k}\frac{c_k^2}{m(r)^2}m(r)=c_k^2\sum_{r=0}^{k}\frac{1}{m(r)}=c_k.$$

By the Dirichlet principle, we have $D(u_k)\le D(u)$ whence

$$D(u_k)\le c_k. \tag{4.16}$$

On the other hand, by the Green formula

$$\sum_{B_{k+1}} \mathcal{L}u_k(x)\,u_k(x)\,\mu(x) = \frac{1}{2}\sum_{x,y\in B_{k+1}} (\nabla_{xy}u_k)^2\,\mu_{xy} - \sum_{x\in B_{k+1}}\sum_{y\in B_{k+1}^c} (\nabla_{xy}u_k)\,u_k(x)\mu_{xy}.$$

The last sum vanishes because if $y \in B_{k+1}^c$ and $x \sim y$ then $x \in B_k^c$ and $u_k(x) = 0$. The range of summation in the first sum can be reduced to B_k because $u_k = 0$ outside B_k, and then further to B_0 because $\mathcal{L}u_k = 0$ in $B_k \setminus B_0$. Finally, since $u_k \equiv 1$ in B_0, we obtain the identity

$$\sum_{B_0} \mathcal{L}u_k(x)\,\mu(x) = \frac{1}{2}\sum_{x,y\in B_{k+1}} (\nabla_{xy}u_k)^2\,\mu_{xy} = D(u_k).$$

It follows from (4.16) that

$$\sum_{B_0} \mathcal{L}u_k(x)\,\mu(x) \le c_k.$$

Since u takes the maximal value 1 at any point of B_0, we have at any point $x \in B_0$ that $Pu_k(x) \le 1$ and

$$\mathcal{L}u_k(x) = u_k(x) - Pu_k(x) \ge 0.$$

Hence, at any point $x \in B_0$, we have

$$0 \le \mathcal{L}u_k(x)\,\mu(x) \le c_k.$$

By (4.11) and (4.15), we have $c_k \to 0$ as $k \to \infty$, whence it follows that

$$\mathcal{L}u_k(x) \to 0 \text{ for all } x \in B_0.$$

Hence, $\mathcal{L}u_\infty(x) = 0$ for all $x \in B_0$. Since $\mathcal{L}u_\infty(x) = 0$ also for all $x \notin B_0$, we see that u_∞ is harmonic on the whole graph V. Since u_∞ takes its supremum value 1 at any point of B_0, we conclude by the strong maximum principle that $u_\infty \equiv 1$, which finishes the proof. ∎

The following theorem provides a convenient volume test for the recurrence.

Theorem 4.11 *If*

$$\sum_{r=0}^{\infty} \frac{r}{\mu(B_r)} = \infty \tag{4.17}$$

then the random walk is recurrent. In particular, this is the case when

$$\mu(B_{r_k}) \leq C r_k^2 \tag{4.18}$$

for a sequence $r_k \to \infty$.

The condition (4.18) holds in $\mathbb{Z}^m$ with $m \leq 2$ for the function $\rho(x) = d(x, 0)$. Hence, we obtain one more proof of the recurrence of $\mathbb{Z}^m$ for $m \leq 2$ (cf. Corollary 4.2).

We need the following lemma for the proof of Theorem 4.11.

Lemma 4.12 *Let* $\{\sigma_r\}_{r=0}^n$ *be a sequence of positive reals and let*

$$v_r = \sum_{i=0}^{r} \sigma_i. \tag{4.19}$$

Then

$$\sum_{r=0}^{n} \frac{1}{\sigma_r} \geq \frac{1}{4} \sum_{r=0}^{n} \frac{r}{v_r}.$$

Proof. Assume first that the sequence $\{\sigma_r\}$ is monotone increasing. If $0 \leq k \leq \frac{n-1}{2}$ then

$$v_{2k+1} \geq \sum_{i=k+1}^{2k+1} \sigma_i \geq (k+1)\,\sigma_k$$

whence

$$\frac{1}{\sigma_k} \geq \frac{k+1}{v_{2k+1}} \geq \frac{1}{2}\frac{2k+1}{v_{2k+1}}.$$

Similarly, if $0 \leq k \leq \frac{n}{2}$ then

$$v_{2k} \geq \sum_{i=k+1}^{2k} \sigma_i \geq k\sigma_k$$

and
$$\frac{1}{\sigma_k} \geq \frac{k}{v_{2k}} = \frac{1}{2}\frac{2k}{v_{2k}}.$$
It follows that
$$4\sum_{k=0}^{n}\frac{1}{\sigma_k} \geq \sum_{k=0}^{\left[\frac{n-1}{2}\right]}\frac{2k+1}{v_{2k+1}} + \sum_{k=0}^{\left[\frac{n}{2}\right]}\frac{2k}{v_{2k}} = \sum_{r=0}^{n}\frac{r}{v_r},$$
which was claimed. Now consider the general case when the sequence $\{\sigma_r\}$ is not necessarily increasing. Let $\{\widetilde{\sigma}_r\}_{r=0}^{n}$ be an increasing permutation of $\{\sigma_r\}_{r=0}^{n}$ and set
$$\widetilde{v}_r = \sum_{i=0}^{r}\widetilde{\sigma}_i.$$
Note that $\widetilde{v}_r \leq v_r$ because $\widetilde{v}_r$ is the sum of r smallest terms of the sequence $\{\sigma_i\}$ whereas v_r is the sum of some r terms of the same sequence. By the first part of the proof,
$$\sum_{r=0}^{n}\frac{1}{\sigma_r} = \sum_{r=0}^{n}\frac{1}{\widetilde{\sigma}_r} \geq \frac{1}{4}\sum_{r=0}^{n}\frac{r}{\widetilde{v}_r} \geq \frac{1}{4}\sum_{r=0}^{n}\frac{r}{v_r},$$
which finishes the proof. ■

Proof of Theorem 4.11. Set for any $r \geq 1$

$$S_r = \{x \in V : \rho(x) = r\} = B_r \setminus B_{r-1}$$

and $S_0 = B_0$. Then we have

$$\mu(\partial B_r) = \sum_{x \in B_r, y \notin B_r} \mu_{xy} = \sum_{x \in S_r, y \in S_{r+1}} \mu_{xy} \leq \sum_{x \in S_r, y \in V} \mu_{xy} = \sum_{x \in S_r} \mu(x) = \mu(S_r).$$

Denoting $v_r = \mu(B_r)$ and $\sigma_r = \mu(S_r)$ and observing that the sequences $\{v_r\}$ and $\{\sigma_r\}$ satisfy (4.19), we obtain by Lemma 4.12 and (4.17) that

$$\sum_{r=0}^{\infty} \frac{1}{\mu(\partial B_r)} \geq \sum_{r=0}^{\infty} \frac{1}{\sigma_r} \geq \frac{1}{4} \sum_{r=0}^{\infty} \frac{r}{v_r} = \infty.$$

Hence, (4.11) is satisfied, and we conclude by Theorem 4.10 that the random walk on (V, μ) is recurrent.

We are left to show that (4.18) implies (4.17). Given positive integers $a < b$, we have

$$\sum_{r=a+1}^{b} r = \sum_{r=1}^{b} r - \sum_{r=1}^{a} r = \frac{b(b+1)}{2} - \frac{a(a+1)}{2} \geq \frac{b^2 - a^2}{2},$$

whence it follows that

$$\sum_{r=a+1}^{b} \frac{r}{v_r} \geq \frac{1}{v_b} \frac{b^2 - a^2}{2}.$$

By choosing a subsequence of $\{r_k\}$, we can assume that $r_k \geq 2r_{k-1}$. Then we have, using (4.18),

$$\begin{aligned}
\sum_{r=0}^{\infty} \frac{r}{v_r} &\geq \sum_k \sum_{r=r_{k-1}+1}^{r_k} \frac{r}{v_r} \\
&\geq \sum_k \frac{1}{v_{r_k}} \frac{r_k^2 - r_{k-1}^2}{2} \\
&\geq \frac{1}{2C} \sum_k \frac{r_k^2 - r_{k-1}^2}{r_k^2} \\
&= \frac{1}{2C} \sum_k \left(1 - \frac{r_{k-1}^2}{r_k^2}\right) \geq \frac{1}{2C} \sum_k \frac{3}{4} = \infty,
\end{aligned}$$

which was to be proved. ■