CHAPTER 5

# Estimates of the heat kernel

In this Chapter, $(V, \mu)$ is a locally finite weighted graph such that $\mu(x) > 0$ for all $x \in V$.

## 5.1. The notion and basic properties of the heat kernel

Recall that $P_n(x, y)$ is the $n$-step transition function of the random walk on $(V, \mu)$, that can be determined inductively as follows: $P_1(x, y) = P(x, y)$ and

$$P_n(x, y) = \sum_{z \in V} P_{n-1}(x, z) P(z, y)$$

(cf. Proposition 1.28). Furthermore, $P_n(x, y)$ is reversible with respect to measure $\mu(x)$, that is

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

Definition 5.1. The function

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

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

The reversibility condition clearly implies that $p_n(x, y)$ is symmetric in $x, y$ that is

$$p_n(x, y) = p_n(y, x). \tag{5.1}$$

Other useful properties of the heat kernel that follow from the corresponding properties of the transition function, are as follows:

$$P_n f(x) = \sum_{y \in V} p_n(x, y) f(y) \mu(y),$$

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

$$p_{n+m}(x, y) = \sum_{z \in V} p_n(x, z) p_m(z, y) \mu(z). \tag{5.2}$$

For $n = m$ and $x = y$, the latter identity implies that

$$p_{2n}(x, x) = \sum_{z \in V} p_n^2(x, z) \mu(z). \tag{5.3}$$

Lemma 5.2. *We have for all $x, y \in V$ and $n, m \in \mathbb{N}$:*

$$p_{n+m}(x, y) \le (p_{2n}(x, x) p_{2m}(y, y))^{1/2}. \tag{5.4}$$

PROOF. Indeed, it follows from the symmetry (5.1) and the semigroup identities (5.2), (5.3) that

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

□

LEMMA 5.3. *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, that is,

$$p_n(x,y) = p_n(zx,zy) \tag{5.5}$$

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 $x^{-1}y \in S$. Since

$$(zx)^{-1}(zy) = x^{-1}z^{-1}zy = x^{-1}y$$

we see that $x \sim y$ if and only if $zx \sim zy$.

For $n = 1$ we have

$$p_1(x,y) = \frac{P(x,y)}{\mu(y)} = \frac{\mu_{xy}}{\mu(x)\mu(y)}.$$

If $x,y$ are not neighbors, then $p_1(x,y) = 0$. If $x \sim y$, then it follows that

$$p_1(x,y) = \frac{1}{\deg(x)\deg(y)} = \frac{1}{|S|^2}.$$

Since the right hand side is the same for all couples $x \sim y$, we obtain (5.5) for $n = 1$. Let us make the inductive step from $n-1$ to $n$:

$$\begin{aligned} p_n(zx,zy) &= \sum_{w\in G} p_{n-1}(zx,w)\, p_1(w,zy)\, \mu(w) \\ &= \sum_{u\in G} p_{n-1}(zx,zu)\, p_1(zu,zy)\, \mu(u) \\ &= \sum_{u\in G} p_{n-1}(x,u)\, p_1(u,y)\, \mu(u) \\ &= p_n(x,y). \end{aligned}$$

□

One of the most interesting problems on infinite graphs is the rate of convergence of $p_n(x,y)$ 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 considered in this Chapter.

## 5.2. One-dimensional simple random walk

Let $(V,\mu)$ be $\mathbb{Z}$ with a simple weight. Since $\mu(x)=2$, we have $p_n(x,y)=\frac{1}{2}P_n(x,y)$. Since $\mathbb{Z}$ is shift invariant, $p_n(x,y)$ is also shift invariant, that is, $p_n(x,y)=p_n(x-z,y-z)$ for any integer $z$. In particular, for $z=x$, we obtain $p_n(x,y)=p_n(0,y-x)$.

In this section we investigate $p_n(0,x)$ as a function of $x$ and $n$. A first observation is that

$$p_n(0,x)=0 \quad \text{if } |x|>n,$$

since there is no path of length $n$ from 0 to $x$. It follows from Exercise 17 that

$$p_n(0,x)=\begin{cases}\frac{1}{2^{n+1}}\binom{n}{\frac{x+n}{2}}, & |x|\le n \text{ and } x\equiv n \mod 2,\\ 0, & \text{otherwise,}\end{cases} \tag{5.6}$$

where $\binom{n}{m}$ is the binomial coefficient. Using Stirling's formula

$$n!\sim\sqrt{2\pi n}\left(\frac{n}{e}\right)^n \quad \text{as } n\to\infty, \tag{5.7}$$

and assuming that $n$ is even, we obtain

$$\begin{aligned} p_n(0,0) &= \frac{1}{2^{n+1}}\binom{n}{n/2}\\ &= \frac{1}{2^{n+1}}\frac{n!}{((n/2)!)^2}\\ &\sim \frac{1}{2^{n+1}}\frac{\sqrt{2\pi n}\left(\frac{n}{e}\right)^n}{\sqrt{2\pi\frac{n}{2}}^2\left(\frac{n}{2e}\right)^n}\\ &= \frac{1}{\sqrt{2\pi n}}, \end{aligned}$$

so that

$$p_n(0,0)\sim\frac{1}{\sqrt{2\pi n}} \quad \text{as } n\to\infty,\ n \text{ even.} \tag{5.8}$$

In particular, $p_n(0,0)\to 0$ as $n\to\infty$. Since $p_n(x,x)=p_n(0,0)$ for any $x\in\mathbb{Z}$, it follows from (5.4) that also $p_n(x,y)\to 0$ as $n\to\infty$ for all $x,y\in\mathbb{Z}$. Below we get a more precise information about behavior of $p_n(0,x)$.

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 $C\ge 1$ such that

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

Equivalently, $a_n\simeq b_n$ means that $\ln a_n-\ln b_n$ remains bounded as $n\to\infty$.

Clearly, the equivalence $a_n\sim b_n$ implies $a_n\simeq b_n$. For example, (5.7) implies that, for all $n\ge 1$,

$$n!\simeq n^{n+\frac{1}{2}}e^{-n}. \tag{5.9}$$

In fact, for all integers $n\ge 1$, we have

$$\sqrt{2\pi}n^{n+\frac{1}{2}}e^{-n}\le n!\le C\sqrt{2\pi}n^{n+\frac{1}{2}}e^{-n} \tag{5.10}$$

where $C=e^{1/12}\approx 1.086\,9$. Indeed, it is known that

$$n!=\sqrt{2\pi n}n^ne^{-n}e^{\xi_n}$$

where

$$\frac{1}{12n+1} \le \xi_n \le \frac{1}{12n}$$

whence (5.10) follows.

THEOREM 5.4. *For all positive integers $n$ and for all $x \in \mathbb{Z}$ such that $|x| \le n$ and $x \equiv n \mod 2$, the following inequalities hold:*

$$\frac{C_2}{\sqrt{n}} e^{-(\ln 2)\frac{x^2}{n}} \le p_n(0,x) \le \frac{C_1}{\sqrt{n}} e^{-\frac{x^2}{2n}}, \tag{5.11}$$

*where $C_1, C_2$ are some positive constants.*

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

PROOF. Stirling's formula (5.9) implies, for any integer $n \ge 0$,

$$n! = \frac{(n+1)!}{(n+1)} \simeq (n+1)^{n+\frac{1}{2}} e^{-n}. \tag{5.12}$$

Assuming that $m$ is an even non-negative integer and applying (5.12) 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

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

whence

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

and

$$\left(\frac{m}{2}\right)! \simeq (m+1)^{\frac{m+1}{2}} (2e)^{-m/2}. \tag{5.13}$$

Using (5.12) to estimate $n!$ and (5.13) with $m = n \pm x$ to estimate $\left(\frac{n\pm x}{2}\right)!$, we obtain from (5.6)

$$\begin{aligned} & p_n(0,x) \\ = & \frac{1}{2^{n+1}} \binom{n}{\frac{x+n}{2}} \\ = & \frac{1}{2^{n+1}} \frac{n!}{\left(\frac{n+x}{2}\right)! \left(\frac{n-x}{2}\right)!} \\ \simeq & \frac{2^{-n}(n+1)^{n+\frac{1}{2}} e^{-n}}{(n+x+1)^{\frac{n+x+1}{2}} (2e)^{-\frac{n+x}{2}} (n-x+1)^{\frac{n-x+1}{2}} (2e)^{-\frac{n-x}{2}}} & (5.14) \\ = & \frac{1}{\sqrt{n+1}\left(1+\frac{x}{n+1}\right)^{\frac{n+x+1}{2}} \left(1-\frac{x}{n+1}\right)^{\frac{n-x+1}{2}}} \\ = & \frac{1}{\sqrt{N}} \frac{1}{\left(1+\frac{x}{N}\right)^{\frac{N+x}{2}} \left(1-\frac{x}{N}\right)^{\frac{N-x}{2}}}, & (5.15) \end{aligned}$$

where $N = n+1$. Using the Taylor formula for logarithm

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

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

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

Changing here $x$ to $-x$, we obtain

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

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

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

Substituting into (5.15), we obtain

$$p_n(0,x) \simeq \frac{1}{\sqrt{N}}\exp\left(-\frac{x^2}{N}\left[\frac{1}{2}+\frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2+\frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4+...\right]\right). \tag{5.16}$$

Clearly, this implies the upper bound

$$p_n(0,x) \leq \frac{C_1}{\sqrt{N}}\exp\left(-\frac{x^2}{2N}\right). \tag{5.17}$$

Let us show that $N=n+1$ can be replaced here by $n$. That $\sqrt{N}\simeq\sqrt{n}$ is obvious, while the comparison

$$\exp\left(-\frac{x^2}{2N}\right) \simeq \exp\left(-\frac{x^2}{2n}\right) \tag{5.18}$$

follows from

$$\frac{x^2}{2n}-\frac{x^2}{2N} = \frac{x^2}{2n(n+1)} \leq \frac{x^2}{2n^2} \leq \frac{1}{2}. \tag{5.19}$$

Hence, (5.17) yields the upper bound in (5.11). To prove the lower bound, observe that by $\frac{|x|}{N} < 1$

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

whence by (5.16)

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

Arguing as above, we can replace here $N$ by $n$, thus proving the lower bound in (5.11). ☐

Corollary 5.5. In the domain where $\frac{|x|}{n^{3/4}}$ is bounded, we have the following estimate

$$p_n(0,x) \simeq \frac{1}{\sqrt{n}} \exp\left(-\frac{x^2}{2n}\right). \tag{5.20}$$

Moreover, if $|x| = o\left(n^{3/4}\right)$ as $n \to \infty$, then

$$p_n(0,x) \sim \frac{1}{\sqrt{2\pi n}} \exp\left(-\frac{x^2}{2n}\right). \tag{5.21}$$

Let us recall for comparison that the fundamental solution $p_t(x,y)$ of the heat equation $\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2}$ in $\mathbb{R}$ admits the following explicit formula

$$p_t(0,x) = \frac{1}{\sqrt{2\pi t}} \exp\left(-\frac{x^2}{2t}\right).$$

The similarity of this formula and (5.21) is obvious and can be explained by the fact that $p_t(x,y)$ is the transition density of Brownian motion in $\mathbb{R}$ that can be obtained as a scaled limit of the simple random walk.

Proof. The upper bound in 5.20) is the same as in (5.11), so that we need only to prove the lower bound. The expression under the exponential function in (5.16) can be estimated from above as follows:

$$\begin{aligned}
&\frac{x^2}{N}\left(\frac{1}{2} + \frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2 + \frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4 + ...\right) \\
= \ &\frac{x^2}{2N} + \frac{x^4}{3\cdot 4N^3} + \frac{x^6}{5\cdot 6N^5} + \frac{x^8}{7\cdot 8N^7} + ... \\
= \ &\frac{x^2}{2N} + \frac{x^4}{N^3}\left(\frac{1}{3\cdot 4} + \frac{1}{5\cdot 6}\frac{x^2}{N^2} + \frac{1}{7\cdot 8}\frac{x^4}{N^4} + ...\right) \\
\leq \ &\frac{x^2}{2N} + c\left(\frac{1}{3\cdot 4} + \frac{1}{5\cdot 6} + \frac{1}{7\cdot 8} + ...\right) \\
< \ &\frac{x^2}{2N} + \frac{c}{3},
\end{aligned} \tag{5.22}$$

where $c$ is a constant that bounds $\frac{x^4}{N^3}$. Substituting this into (5.16) and replacing as before $N$ by $n$, we obtain the lower bound in (5.20).

To prove (5.21), let us trace the proof of Theorem 5.4 and see in which places the comparison $\simeq$ can be replaced by the asymptotic equivalence $\sim$. The condition $|x| = o\left(n^{3/4}\right)$ implies that $n - x \to \infty$ so that in the Stirling formula for $\left(\frac{n-x}{2}\right)!$ we can use the equivalence. The same always applies to $\left(\frac{n+x}{2}\right)!$ and $n!$. Hence, in (5.14) we obtain asymptotic equivalence, provided we use a correct constant multiple in the right hand side. Therefore, we obtain also asymptotic equivalence in (5.16):

$$p_n(0,x) \sim \frac{1}{\sqrt{2\pi n}} \exp\left[-\frac{x^2}{N}\left[\frac{1}{2} + \frac{1}{3\cdot 4}\left(\frac{x}{N}\right)^2 + \frac{1}{5\cdot 6}\left(\frac{x}{N}\right)^4 + \dots\right]\right] \tag{5.23}$$

where we use $\sqrt{N} \sim \sqrt{n}$ and the constant $\frac{1}{\sqrt{2\pi}}$ is chosen to match (5.8) for $x = 0$. Note that this asymptotic expansion takes place whenever $n - x \to \infty$.

As $|x|/n^{3/4} \to 0$, the second term in the right hand side of (5.22) goes to 0. Also from (5.19) we get $\frac{x^2}{n} - \frac{x^2}{N} \to 0$. Substituting these estimates into (5.23), we obtain (5.21). □

The following lemma gives another estimate of $P_n(0,x)$, that we will use in the next section.

LEMMA 5.6. *We have, for all positive integers $r, n$,*

$$\sum_{x \geq r} P_n(0,x) \leq \exp\left(-\frac{r^2}{2n}\right). \tag{5.24}$$

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

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

is a simple random walk on $\mathbb{Z}$ started at 0. Recall that

$$P_n(0,x) = \mathbb{P}(X_n = x),$$

which implies that

$$\sum_{x \geq r} P_n(0,x) = \mathbb{P}(X_n \geq r).$$

We have, for any $\alpha > 0$,

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

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

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

Using also that

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

we obtain

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

Finally, choosing $\alpha$ to minimize the expression under the exponential, that is, $\alpha = \frac{r}{n}$, we obtain

$$\mathbb{P}\left(X_n \geq r\right) \leq \exp\left(-\frac{r^2}{2n}\right), \tag{5.25}$$

which was to be proved. ◻

Let us compare the estimate (5.25) with the central limit theorem. Setting in (5.25) $r = s\sqrt{n}$ where $s$ is a new positive variable, we obtain

$$\mathbb{P}\left(X_n \geq s\sqrt{n}\right) \leq \exp\left(-\frac{s^2}{2}\right).$$

Since $\mathbb{E}Z_k = 0$ and $\operatorname{Var} Z_k = 1$, the central limit theorem yields the following:

$$\lim_{n\to\infty} \mathbb{P}\left(X_n \geq s\sqrt{n}\right) = \int_s^\infty \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx.$$

One can verify that, for large $s$,

$$\int_s^\infty \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) dx \approx \frac{1}{\sqrt{2\pi} s} \exp\left(-\frac{s^2}{2}\right),$$

which shows that (5.25) cannot be essentially improved.

## 5.3. 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

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

and observe that $P$ is a symmetric operator and $\|P\| \leq 1$ (cf. Exercise 18).

THEOREM 5.7. *Let $f, g$ be two functions from $L^2(V,\mu)$ and let $r$ be the distance between* $\operatorname{supp} f$ *and* $\operatorname{supp} g$*. Then*

$$\left|(P^n f, g)\right| \leq 2\,\|f\|\,\|g\| \exp\left(-\frac{r^2}{2n}\right). \tag{5.26}$$

The proof of Theorem 5.7 is based on the technique of Carne [**32**]. It will be given below after Lemma 5.9.

COROLLARY 5.8. *(A Carne-Varopoulos estimate)* For all $x, y \in V$ and positive integers $n$,

$$p_n(x,y) \leq \frac{2}{\sqrt{\mu(x)\,\mu(y)}} \exp\left(-\frac{d^2(x,y)}{2n}\right). \tag{5.27}$$

PROOF. Setting in (5.26) $f = \mathbf{1}_{\{x\}}$ 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 (5.27). ◻

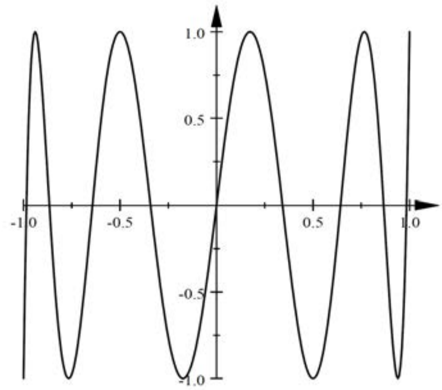


FIGURE 5.1. The Chebyshev polynomial $T_9(\lambda)$

The estimate (5.27) was proved by Varopoulos [**136**] and, by a simpler method, by Carne [**32**]. The comparison with the one-dimensional estimate (5.11) shows that the estimate (5.27) lacks the on-diagonal term that would give the rate of decay of $p_n(x,x)$ as $n \to \infty$. The reason for that is that we do not use in (5.27) any additional information about the graph, without which the decay of $p_n(x,x)$ in $n$ cannot be obtained (cf. Section 5.4). On the contrary, the decay of $p_n(x,y)$ with respect to $d(x,y)$ is a universal phenomenon that takes place on an arbitrary graph.

For the proof of Theorem 5.7 we use the *Chebyshev polynomials* $T_k$ that are defined by the identity

$$T_k(\lambda) = \cos(k \arccos \lambda),$$

where $k$ is an integer parameter 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

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

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

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

A distinguished property of Chebyshev polynomials to be used below is that $|T_k(\lambda)| \leq 1$ for all $\lambda \in [-1,1]$ that is obvious from the definition (see also Figure 5.1).

LEMMA 5.9. *The following identity holds for all $\lambda \in [-1,1]$ and all non-negative integers $n$:*

$$\lambda^n = \sum_{k=-n}^{n} q_n(k)\, T_k(\lambda),$$

*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 $\theta$ be such that $\lambda = \cos\theta$. Setting $z = \cos\theta + i\sin\theta$ and observing that $\overline{z} = \frac{1}{z}$, we obtain, for any $k \in \mathbb{Z}$,

$$T_k(\lambda) = \operatorname{Re} z^k = \frac{1}{2}\left(z^k + z^{-k}\right).$$

On the other hand, $\lambda = \operatorname{Re} z = \frac{1}{2}\left(z + \frac{1}{z}\right)$ whence

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

It follows that also

$$\lambda^n = \frac{1}{2^n}\sum_{k=0}^n \binom{n}{n-k} z^{-(n-2(n-k))} = \frac{1}{2^n}\sum_{l=0}^n \binom{n}{l} z^{-(n-2l)}.$$

Taking the half-sum of the two expressions for $\lambda^n$, we obtain

$$\begin{aligned} \lambda^n &= \frac{1}{2^n}\sum_{k=0}^n \binom{n}{k}\frac{z^{n-2k} + z^{-(n-2k)}}{2} \\ &= \frac{1}{2^n}\sum_{k=0}^n \binom{n}{k} T_{n-2k}(\lambda) \\ &= \frac{1}{2^n}\sum_{l=-n}^n \binom{n}{\frac{n-l}{2}} T_l(\lambda) \\ &= \frac{1}{2^n}\sum_{l=-n}^n \binom{n}{\frac{n+l}{2}} T_l(\lambda), \end{aligned}$$

which was to be proved. □

Proof of Theorem 5.7. Applying the identity of polynomials of Lemma 5.9 to the operator $P$, we obtain

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

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 the above identity that

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

Observe that $(T_k(P) f, g) = 0$ for $|k| < r$, because $T_k$ is a polynomial of degree $|k|$ and $r$ is the distance between the supports of $f$ and $g$ (cf. the proof of Theorem 3.14). On the other hand, for any $k$ we have

$$|(T_k(P) f, g)| \leq \|T_k(P)\|\,\|f\|\,\|g\| \leq \|f\|\,\|g\|.$$

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

$$\mu(U_1(A)) \le MD(D+1)\mu(A).$$

□

The next theorem is the main result of this section.

THEOREM 5.11. *If* $(V,\mu)$ *satisfies* (5.28) *and the Faber-Krahn inequality with function*

$$\Lambda(s) = cs^{-1/\alpha},$$

*for some* $\alpha, c > 0$*, then the the heat kernel satisfies the following estimate*

$$p_n(x,y) \le Cn^{-\alpha}. \tag{5.30}$$

*for all* $x, y \in V$*,* $n \ge 1$ *and some* $C = C(\alpha, c, C_0)$.

Theorem 5.11 was proved in [**81**].

EXAMPLE 5.12. If $(V,\mu)$ is a Cayley graph satisfying the volume growth condition

$$\mu(B_r) \ge ar^m, \tag{5.31}$$

then by Corollary 4.24, $(V,\mu)$ satisfies the Faber-Krahn inequality with the function

$$\Lambda(s) = bs^{-2/m},$$

where $a, b, m > 0$. By Theorem 5.11 we conclude that

$$p_n(x,y) \le Cn^{-m/2}. \tag{5.32}$$

Since (5.31) is satisfied in $\mathbb{Z}^m$, we see that the estimate (5.32) holds in $\mathbb{Z}^m$. As we will see later on, the power $n^{-m/2}$ is sharp here (cf. Example 5.20).

EXAMPLE 5.13. Assume in addition to (5.28) that, for all $x \in V$ and integers $r \ge 1$

$$\mu(B_r(x)) \ge ar^m, \tag{5.33}$$

for some $a, m > 0$. Then, by Corollary 4.17, we have the Faber-Krahn inequality with function

$$\Lambda(s) = bs^{-\frac{m+1}{m}}. \tag{5.34}$$

Theorem 5.11 yields then the heat kernel upper bound

$$p_n(x,y) \le Cn^{-\frac{m}{m+1}}. \tag{5.35}$$

Although this upper bound is not sharp in $\mathbb{Z}^m$ with $m > 1$, in general it cannot be improved under the hypothesis (5.33). Indeed, for the Vicsek tree from Example 4.19, all the conditions (5.33), (5.34) and (5.35) are satisfied with $m = \frac{\ln 5}{\ln 3}$, that is,

$$p_n(x,y) \le Cn^{-\frac{\ln 5}{\ln 15}}. \tag{5.36}$$

As we will see later in Example 5.22, this upper bound is sharp in this case. Further examples of this type can be found in [**13**].

EXAMPLE 5.14. If the weight $\mu$ is simple, then we always have the Faber-Krahn inequality with function $\Lambda(s) = \frac{1}{2}s^{-2}$, that is, with $\alpha = 1/2$ (cf. Example 4.14). Assuming that the degree is uniformly bounded, we obtain by Theorem 5.11 that

$$p_n(x, y) \le Cn^{-1/2}.$$

Note that this estimate is sharp in $\mathbb{Z}$ (up to a constant multiple).

PROOF OF THEOREM 5.11. We use the notation

$$(f, g) = \sum_{x\in V} f(x)\, g(x)\, \mu(x), \tag{5.37}$$

whenever the right hand side is well-defined. Let $\mathcal{F}$ be the set of all functions $f$ on $V$ with a finite support

$$\operatorname{supp} f = \{x \in V : f(x) \ne 0\}.$$

Clearly, $\mathcal{F}$ is a linear space of infinite dimension. Observe that $f \in \mathcal{F}$ implies that $\mathcal{L}f$ and $Pf$ belong to $\mathcal{F}$, because

$$\operatorname{supp}(Pf) \subset U_1(\operatorname{supp} f).$$

Note that $(f, g)$ is well-defined provided one of the functions $f, g$ belongs to $\mathcal{F}$.

The approach to the proof is as follows. For a fixed $z \in V$, denote $f_n(x) = p_n(x, z)$. We will show that $f_{n+1} = Pf_n$. 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

$$b_n - b_{n+1} = (f_n, f_n) - (Pf_n, Pf_n),$$

which will imply an upper bound for $b_n$ and, hence, for $p_{2n}(z, z)$. Then Lemma 5.2 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 a series of claims.

**Claim 0.** *If $f \in \mathcal{F}$, then $(Pf, 1) = (f, 1)$.*

Note that

$$(f, 1) = \sum_{x\in V} f(x)\, \mu(x).$$

Using Green's formula of Theorem 2.1 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 $f, g \in \mathcal{F}$. Also, we write $Q(f) = Q(f,f)$.

**Claim 1.** *If $\Omega$ is a finite non-empty subset of $V$, $f \in \mathcal{F}$ and $U_1(\operatorname{supp} f) \subset \Omega$, then*

$$Q(f) \geq \lambda_1(\Omega)(f,f). \tag{5.38}$$

*In particular, $Q(f) \geq 0$ for any $f \in \mathcal{F}$.*

Clearly, $\operatorname{supp}(Pf) \subset \Omega$ so that $Pf = P_\Omega f$ where $P_\Omega = \mathrm{id} - \mathcal{L}_\Omega$. Let $\alpha_1 = 1 - \lambda_1(\Omega)$ so that $\operatorname{spec} P_\Omega \subset [-\alpha_1, \alpha_1]$ and $\|P_\Omega\| \leq \alpha_1$. Then

$$\begin{aligned} Q(f) &= (f,f) - (P_\Omega f, P_\Omega f) \\ &\geq \|f\|^2 - \alpha_1^2 \|f\|^2 \\ &= (1-\alpha_1)(1+\alpha_1)\|f\|^2 \\ &\geq \lambda_1(\Omega)\|f\|^2. \end{aligned}$$

**Claim 2.** *For all $f \in \mathcal{F}$ we have*

$$Q(f) = \frac{1}{2}\sum_{x,y\in V} (f(x) - f(y))^2 P_2(x,y)\mu(x). \tag{5.39}$$

Using the symmetry of the Markov operator $P$, we obtain

$$(Pf, Pf) = \left(P^2 f, f\right) = \sum_{x,y\in V} P_2(x,y) f(x) f(y)\mu(x),$$

whence

$$\begin{aligned} Q(f) &= \sum_{x\in V} f^2(x)\mu(x) - \sum_{x,y\in V} P_2(x,y) f(x) f(y)\mu(x) \\ &= \sum_{x,y\in V} P_2(x,y) f^2(x)\mu(x) - \sum_{x,y\in V} P_2(x,y) f(x) f(y)\mu(x) \\ &= \sum_{x,y\in V} P_2(x,y) f(x)(f(x) - f(y))\mu(x). \end{aligned} \tag{5.40}$$

Interchanging $x, y$ we obtain also

$$Q(f) = \sum_{x,y\in V} P_2(x,y) f(y)(f(y) - f(x))\mu(x). \tag{5.41}$$

Adding up (5.40) and (5.41), we obtain (5.39).

**Claim 3.** *If $f \in \mathcal{F}$ and $c$ is a positive constant, then*

$$Q\left((f-c)_+\right) \leq Q(f). \tag{5.42}$$

Define a function $\varphi : \mathbb{R} \to \mathbb{R}$ by

$$\varphi(t) = (t-c)_+.$$

Since $\varphi$ is a Lipschitz function with the Lipschitz constant 1, we obtain by (5.39)

$$\begin{aligned} Q\left((f-c)_+\right) &= Q(\varphi\circ f) \\ &= \frac{1}{2}\sum_{x,y\in V}(\varphi(f(x))-\varphi(f(y)))^2 P_2(x,y)\,\mu(x) \\ &\leq \frac{1}{2}\sum_{x,y\in V}(f(x)-f(y))^2 P_2(x,y)\,\mu(x) = Q(f)\,. \end{aligned}$$

**Claim 4.** *Let $f$ be a non-negative function from $\mathcal{F}$. For any $s\geq 0$ define the set $\Omega_s$ by*

$$\Omega_s = U_1\left(\operatorname{supp}(f-s)_+\right).$$

*Then*[1]

$$Q(f)\geq \lambda_1(\Omega_s)\left((f,f)-2s(f,1)\right). \tag{5.43}$$

*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 (5.38) and (5.42), we have

$$Q(f)\geq Q(g)\geq \lambda_1(\Omega_s)(g,g)\,.$$

On the other hand, we have

$$g^2\geq f^2-2sf. \tag{5.44}$$

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 $f^2-2sf=(f-2s)f\leq 0$. Summing up (5.44) against measure $\mu(x)$, we obtain

$$(g,g)\geq (f,f)-2s(f,1)\,,$$

whence (5.43) follows.

**Claim 5.** *Let $\{f_n\}_{n=0}^{\infty}$ be a sequence of non-negative functions on $V$ such that $f_0\in\mathcal{F}$, $(f_0,1)=1$, and $f_{n+1}=Pf_n$. Set*

$$b_n=(f_n,f_n)\,.$$

*Then*

$$b_n-b_{n+1}\geq c' b_n^{1+1/\alpha}, \tag{5.45}$$

*where $c'=\frac{1}{2}c\,(4C_0)^{-1/\alpha}$.*

By induction, we obtain that $f_n\in\mathcal{F}$ and $(f_n,1)=1$ (by Claim 0). Note that

$$b_n-b_{n+1}=(f_n,f_n)-(Pf_n,Pf_n)=Q(f_n)\,.$$

Estimating $Q(f_n)$ by Claim 4 and choosing

$$s=\frac{1}{4}\frac{(f_n,f_n)}{(f_n,1)}=\frac{1}{4}b_n,$$

[1] Note that, for $s=0$, (5.43) coincides with (5.38).

we obtain

$$b_n - b_{n+1} \geq \frac{1}{2}\lambda_1(\Omega_s)\, b_n, \tag{5.46}$$

where

$$\Omega_s = U_1\left(\operatorname{supp}(f_n - s)_+\right).$$

On the other hand, we have

$$\begin{aligned}\mu\left(\operatorname{supp}(f_n - s)_+\right) &= \mu(x \in V : f_n(x) > s)\\ &\leq \frac{1}{s}\sum_{x\in V} f_n(x)\,\mu(x) = \frac{1}{s}(f_n, 1) = \frac{1}{s}.\end{aligned}$$

By Lemma 5.10, we obtain that

$$\mu(\Omega_s) \leq \frac{C_0}{s} = \frac{4C_0}{b_n}.$$

Hence, by the Faber-Krahn inequality,

$$\lambda_1(\Omega_s) \geq c\mu(\Omega_s)^{-1/\alpha} \geq c(4C_0)^{-1/\alpha} b_n^{1/\alpha}, \tag{5.47}$$

which together with (5.46) yields (5.45).

**Claim 6.** *If $\{b_n\}_{n=0}^{\infty}$ is a sequence of positive real numbers satisfying (5.45), then $b_n \leq C' n^{-\alpha}$ where $C' = (\alpha/c')^{\alpha}$.*

We use an elementary inequality

$$y^{-\beta} - x^{-\beta} \geq \frac{\beta(x-y)}{x^{\beta+1}}, \tag{5.48}$$

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 (5.48) follows. Applying (5.48) 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 $f_0 \in \mathcal{F}$ and $(f_0, 1) = 1$. Define the sequence $\{f_n\}$ inductively by $f_{n+1} = Pf_n$ and show that, in fact,

$$f_n(x) = p_n(x, z) \text{ for any } n \geq 1.$$

We have

$$f_1(x) = Pf_0(x) = \sum_{y\in V} P(x, y)\, f_0(y) = \frac{P(x, z)}{\mu(z)} = p_1(x, z)$$

and

$$\begin{aligned}f_{n+1}(x) &= \sum_{y\in V} P(x, y)\, f_n(y)\\ &= \sum_{y\in V} p_1(x, y)\, p_n(y, z)\,\mu(y)\\ &= p_{n+1}(x, z).\end{aligned}$$

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 and 6 that

$$p_{2n}(z, z) \leq C' n^{-\alpha}, \tag{5.49}$$

for all $z \in V$. Using Lemma 5.2 and (5.49), we obtain that

$$p_{k+l}(x, y) \leq (p_{2k}(x, x)\, p_{2l}(y, y))^{1/2} \leq C' (kl)^{-\alpha/2}, \tag{5.50}$$

for all $x, y \in V$ and positive integers $k, l$. Given an integer $n \geq 2$, represent it in the form $n = k + l$ where $l = k$ for even $n$ and $l = k + 1$ for odd $n$. In both cases, we have

$$l \geq k \geq \frac{n-1}{2} \geq \frac{n}{4},$$

whence by (5.50)

$$p_n(x, y) \leq C'' n^{-\alpha}.$$

Finally, for $n = 1$ we obtain $p_1(x, y) = \frac{P(x,y)}{\mu(y)} \leq 1$ because $P(x, y) \leq 1$ and $\mu(y) \geq 1$ by (5.28). □

REMARK 5.15. As we have seen in the last part of the proof, the estimate (5.30) is equivalent to the *on-diagonal estimate*

$$p_n(x, x) \leq C n^{-\alpha}.$$

For that reason, (5.30) 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 (5.30) with the Carne-Varopoulos estimate (5.27), it is easy to show that, for any $0 < \varepsilon < \alpha$,

$$p_n(x, y) \leq \frac{C}{n^{\alpha-\varepsilon}} \exp\left(-c_\varepsilon \frac{d^2(x, y)}{n}\right) \tag{5.51}$$

with some $c_\varepsilon > 0$. Using much more complicated methods, one can show that (5.51) holds also for $\varepsilon = 0$ (see [**10**], [**48**], [**50**], [**56**], [**89**]).

Theorem 5.11 can be extended to a general Faber-Krahn function $\Lambda(s)$ as follows.

THEOREM 5.16. *If* $(V, \mu)$ *satisfies* (5.28) *and the Faber-Krahn inequality with a positive decreasing function* $\Lambda(s)$ *on* $(0, +\infty)$*, then, for all positive integers* $n$ *and all* $x, y \in V$,

$$p_n(x, y) \leq \frac{C}{\gamma^{-1}(n/8)},$$

*where* $C$ *is a constant and the function* $\gamma$ *is defined by*

$$\gamma(s) = \int_1^s \frac{dv}{v\Lambda(v)}.$$

This theorem was proved in [**47**].

EXAMPLE 5.17. In the case $\Lambda(s) = cs^{-1/\alpha}$, we obtain

$$\gamma(s) = \frac{1}{c}\int_1^s v^{1/\alpha - 1} dv = c'\left(s^{1/\alpha} - 1\right) \leq c' s^{1/\alpha}$$

and $\gamma^{-1}(t) \geq c'' t^\alpha$, which gives the previous theorem.

EXAMPLE 5.18. Let $\Lambda(s) = \frac{c}{\ln^2(2s)}$ as it is the case on the Cayley graphs with exponential volume growth. Then

$$\gamma(s) = \frac{1}{c}\int_1^s \ln^2(2v)\frac{dv}{v} = \frac{1}{c}\int_2^{2s} \ln^2 u \frac{du}{u} \leq \frac{1}{3c}\ln^3(2s)$$

whence $\gamma^{-1}(t) \geq \frac{1}{2}\exp\left(-c' t^{1/3}\right)$ and

$$p_n(x,y) \leq C \exp\left(-c'' n^{1/3}\right). \tag{5.52}$$

One can show that, for a large family of Cayley graphs, there is a similar lower bound, with different values of constants $C, c''$ (see Example 5.23).

PROOF. The proof goes the same lines as that of Theorem 5.11. The only place where we have used the Faber-Krahn inequality was the estimate (5.47) in Claim 5, which now becomes

$$\lambda_1(\Omega_s) \geq \Lambda(\mu(\Omega_s)) \geq \Lambda\left(\frac{4C_0}{b_n}\right).$$

Put together with (5.46) and setting $C = 4C_0$, we obtain

$$b_n - b_{n+1} \geq \frac{1}{2}\Lambda\left(\frac{C}{b_n}\right) b_n. \tag{5.53}$$

Using (5.53), we estimate $b_n$ from above as follows. Consider the function

$$\varphi(b) = \frac{1}{\Lambda\left(\frac{C}{b}\right) b},$$

which is monotone decreasing in $b \in (0, +\infty)$. It follows that

$$\int_{b_{n+1}}^{b_n} \varphi(b)\, db \geq (b_n - b_{n+1})\varphi(b_n) = \frac{b_n - b_{n+1}}{\Lambda\left(\frac{C}{b_n}\right) b_n} \geq \frac{1}{2},$$

where in the last inequality we have used (5.53). Summing up this inequality from 0 to $n$, we obtain

$$\int_{b_n}^{b_0} \frac{db}{\Lambda\left(\frac{C}{b}\right) b} \geq \frac{n}{2},$$

which implies by the change $v = \frac{C}{b}$ that

$$\int_{C/b_0}^{C/b_n} \frac{dv}{\Lambda(v)\, v} \geq \frac{n}{2}. \tag{5.54}$$

Recall that

$$b_0 = (f_0, f_0) = \sum_x f_0^2(x)\mu(x).$$

Since

$$\sum_x f_0(x)\mu(x) = (f_0, 1) = 1,$$

it follows that

$$\sum_x f_0^2(x)\mu^2(x) \leq 1.$$

Since $\mu(x) \geq 1$, we obtain that

$$b_0 = \sum_x f_0^2(x)\mu(x) \leq 1 < C,$$

because $C = 4C_0 > 4$. Hence, $\frac{C}{b_0} > 1$, and (5.54) implies that

$$\gamma\left(\frac{C}{b_n}\right) = \int_1^{C/b_n} \frac{dv}{\Lambda(v)\,v} \geq \frac{n}{2},$$

whence

$$\frac{C}{b_n} \geq \gamma^{-1}\left(\frac{n}{2}\right)$$

and

$$b_n \leq \frac{C}{\gamma^{-1}(n/2)}.$$

As in the previous proof, choosing $f_0 = \frac{1}{\mu(z)}\mathbf{1}_{\{z\}}$, we obtain $b_n = p_{2n}(z,z)$ and

$$p_{2n}(z,z) \leq \frac{C}{\gamma^{-1}(n/2)}.$$

For any integer $n \geq 2$, using (5.50) and choosing $k, l$ as in the previous proof, we obtain

$$p_n(x,y) \leq \frac{C}{\left(\gamma^{-1}(k/2)\,\gamma^{-1}(l/2)\right)^{1/2}} \leq \frac{C}{\gamma^{-1}(n/8)}. \tag{5.55}$$

For $n = 1$ we have $p_1(x,y) \leq 1$. By increasing if necessary the value of $C$, we can have $\frac{C}{\gamma^{-1}(1/8)} \geq 1$ so that (5.55) is satisfied also for $n = 1$. □

## 5.5. On-diagonal lower bound via the Dirichlet eigenvalues

THEOREM 5.19. *For any even positive integer $n$ and for any non-empty finite set $\Omega \subset V$, the heat kernel satisfies the following estimate :*

$$\sup_{x\in V} p_n(x,x) \geq \frac{(1-\lambda_1(\Omega))^n}{\mu(\Omega)}. \tag{5.56}$$

*In particular, if $\lambda_1(\Omega) \leq 1/2$, then*

$$\sup_{x\in V} p_n(x,x) \geq \frac{\exp(-2\lambda_1(\Omega)n)}{\mu(\Omega)}. \tag{5.57}$$

*On a Cayley graph with a simple weight $\mu$, we have instead of (5.57)*

$$p_n(x,x) \geq \frac{\exp(-2\lambda_1(\Omega)n)}{\mu(\Omega)} \tag{5.58}$$

*for all $x \in V$ and even $n$.*

This theorem was proved in [**47**] and [**49**]. Since the set $\Omega$ is arbitrary, one can rewrite (5.57) in the form

$$\sup_{x\in V} p_n(x,x) \geq \sup_{\Omega\subset V} \frac{\exp(-2\lambda_1(\Omega)n)}{\mu(\Omega)},$$

where sup is taken over all non-empty finite subsets $\Omega$. In this form, it appears as an inequality between two functions of $n$.

PROOF. The estimate (5.57) follows from (5.56) using the inequality

$$1-\lambda \geq \exp(-2\lambda) \tag{5.59}$$

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 (5.56). We use again the Markov operator $P = \mathrm{id} - \mathcal{L}$, that acts on functions $f \in \mathcal{F}$ as follows:

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

Recall that the powers $P^n$ of the Markov operators are given by

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

where $P_n(x,y)$ is the transition function that can be defined inductively by $P_1(x,y) = P(x,y)$ and

$$P_n(x,y) = \sum_{z \in V} P_{n-1}(x,z) P(z,y). \tag{5.60}$$

Fix a non-empty finite set $\Omega \subset V$ and consider the operator $Q = P_\Omega = \mathrm{id} - \mathcal{L}_\Omega$ in $\mathcal{F}_\Omega$, that is,

$$Qf(x) = \sum_{y \in \Omega} P(x,y) f(y).$$

The distinction between $Q$ and $P$ is that the range of the summation of the former is restricted to $y \in \Omega$. For any positive integer $n$, consider the powers $Q^n$. By induction, one obtains

$$Q^n f(x) = \sum_{y \in \Omega} Q_n(x,y) f(y), \tag{5.61}$$

where $Q_1(x,y) = P(x,y)$ and

$$Q_n(x,y) = \sum_{z \in \Omega} Q_{n-1}(x,z) P(z,y). \tag{5.62}$$

The function $Q_n(x,y)$ can be regarded as the transition function for a random walk with the killing condition outside $\Omega$. The comparison of (5.60) and (5.62) shows that

$$Q_n(x,y) \le P_n(x,y).$$

Consider $\operatorname{trace} Q^n$. On the one hand, (5.61) means that the matrix of this operator in the basis $\left\{1_{\{x\}}\right\}_{x \in \Omega}$ has on the diagonal the values $Q_n(x,x)$ so that

$$\operatorname{trace} Q^n = \sum_{x \in \Omega} Q_n(x,x) \le \sum_{x \in \Omega} P_n(x,x).$$

On the other hand, the operator $Q$ has the eigenvalues $1 - \lambda_k(\Omega)$, $k = 1, ..., N$ where $N = |\Omega|$. The operator $Q^n$ has the eigenvalues $(1 - \lambda_k(\Omega))^n$ whence

$$\operatorname{trace} Q^n = \sum_{k=1}^N (1 - \lambda_k(\Omega))^n \ge (1 - \lambda_1(\Omega))^n.$$

We have used that all the terms in the above sum are non-negative, which is true because $n$ is even. Comparing the two expressions for the trace, we obtain

$$\begin{aligned}
(1 - \lambda_1(\Omega))^n &\le \sum_{x \in \Omega} P_n(x,x) \\
&= \sum_{x \in \Omega} p_n(x,x) \mu(x) \\
&\le \sup_{x \in \Omega} p_n(x,x) \mu(\Omega),
\end{aligned}$$

whence (5.56) follows.

In the case of a Cayley graph, we have by Lemma 5.3 that, for any $x \in V$,

$$p_n(x, x) = \sup_{x \in V} p_n(x, x)$$

so that (5.58) follows from (5.57). $\square$

EXAMPLE 5.20. We claim that in $\mathbb{Z}^m$

$$p_n(x, x) \geq c n^{-m/2}, \tag{5.63}$$

for all even positive integers $n$ and $x \in \mathbb{Z}^m$. Indeed, fix $r \in \mathbb{N}$ and take $\Omega = B_r$. One can show that

$$\lambda_1(B_r) \leq \frac{C}{r^2}$$

(see Exercise 44). Since $\mathbb{Z}^m$ is a Cayley graph, we obtain by Theorem 5.19 that, for large enough $r$,

$$p_n(x, x) \geq \frac{\exp(-2\lambda_1(B_r) n)}{\mu(B_r)} \geq c' \frac{\exp\left(-\frac{C}{r^2} n\right)}{r^m}.$$

Choosing $r \simeq \sqrt{n}$, we obtain (5.63). Combining (5.63) with the on-diagonal upper bound (5.32) for the heat kernel in $\mathbb{Z}^m$, we obtain that, for all $x \in \mathbb{Z}^m$ and all even $n$,

$$p_n(x, x) \simeq n^{-m/2}.$$

Note that, for odd $n$, $p_n(x, x) = 0$.

COROLLARY 5.21. Assume that there exists a sequence $\{\Omega_k\}_{k=1}^{\infty}$ of subsets of $V$ such that

$$\mu(\Omega_k) \leq C a^k \quad \text{and} \quad \lambda_1(\Omega_k) \leq C b^{-k}$$

for some $a, b, C > 1$. Then, for all even $n$,

$$\sup_{x \in V} p_n(x, x) \geq c n^{-\alpha} \tag{5.64}$$

where $c > 0$ and

$$\alpha = \frac{\ln a}{\ln b}.$$

PROOF. Applying Theorem 5.19 with $\Omega = \Omega_k$, we obtain, for any even $n$ and all large enough $k$,

$$\sup_{x \in V} p_n(x, x) \geq \frac{\exp\left(-2Cb^{-k} n\right)}{C a^k}.$$

If $n$ is large enough, then we can choose $k$ so that $n \simeq b^k$. Then

$$a^k = b^{k \frac{\ln a}{\ln b}} \simeq n^{\alpha},$$

and we obtain (5.64) for large enough $n$. For a bounded range of $n$ this estimate is trivial. $\square$

EXAMPLE 5.22. Let $(V, \mu)$ be the Vicsek tree from Example 4.19, with a simple weight $\mu$. Denote by $\Omega_k$ the finite graph at the step $k$ of construction of the Vicsek tree, considered as a subgraph of $(V, \mu)$ (see Figure 4.2). It is easy to see that

$$|\Omega_k| = 5 |\Omega_{k-1}| - 4,$$

which implies that

$$\mu(\Omega_k) \simeq |\Omega_k| \simeq 5^k.$$

Let us show that

$$\lambda_1(\Omega_k) \le C\,15^{-k}.$$

Denote by $z_0$ the center of $\Omega_k$ and by $z_1, ..., z_4$ its corners. Define a function $f$ on $\Omega_k$ as follows. First set

$$f(z_0) = 1 \text{ and } f(z_i) = 0 \text{ for } i = 1, ..., 4,$$

then extend $f$ linearly on each path of length $3^k$ connecting $z_0$ with $z_i$, and by constant on any transversal path (see Figure 5.2). Since $f \ge \frac{2}{3}$ on $\Omega_{k-1}$, it follows

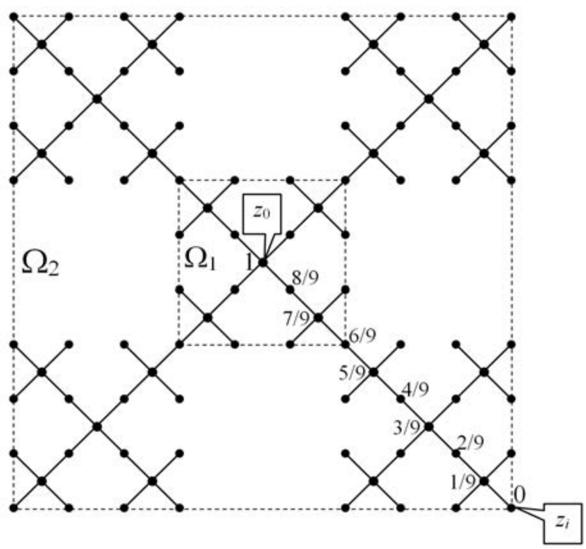


FIGURE 5.2. The values of $f$ on the diagonal $z_0 z_i$ of $\Omega_2$. The function $f$ remains constant on all paths transversal to this diagonal (except for the other diagonals $z_0 z_j$, $j \ne i$).

that

$$(f, f) \simeq \mu(\Omega_k) \simeq 5^k.$$

Also, since $|\nabla_{xy} f| = 3^{-k}$ for any two neighboring points $x, y$ on each of the diagonals connecting $z_0$ and $z_i$, and $|\nabla_{xy} f| = 0$ otherwise, we obtain

$$(\mathcal{L}_{\Omega_k} f, f) = \sum_{x,y\in\Omega_k} |\nabla_{xy} f|^2 \mu_{xy} = \sum_{i=1}^{4} 3^{-2k} d(z_0, z_i) = 4 \cdot 3^{-k}.$$

It follows that

$$\lambda_1(\Omega_k) \le \mathcal{R}(f) = \frac{(\mathcal{L}_{\Omega_k} f, f)}{(f, f)} \le C\,15^{-k},$$

as was claimed. Applying Corollary 5.21, we obtain the lower bound

$$\sup_x p_n(x, x) \ge c n^{-\frac{\ln 5}{\ln 15}},$$

which matches the upper bound (5.36) of Example 5.13. In fact, it is possible to prove that, for all even $n$ and all $x \in V$,

$$p_n(x, x) \simeq n^{-\frac{\ln 5}{\ln 15}}$$

(cf. [**8**], [**82**]).

EXAMPLE 5.23. The method of the proof of Corollary 5.21 can be extended to a more general setting covering a superpolynomial decay of the heat kernel (see [**49**]). In this way one can prove the following lower bound on the Cayley graphs of *polycyclic groups* with exponential volume growth:

$$p_n(x,x) \geq c\exp\left(-Cn^{1/3}\right),$$

for even $n$, which matches the upper bound (5.52) of Example 5.18. In this case, construction of a sequence $\{\Omega_k\}$ is more complicated and requires the use of the group structure (see [**1**], [**49**], [**117**]).

As an example, consider a semi-direct product $\mathbb{Z}^2 \rtimes \mathbb{Z}$ that consists of couples $(x,a)$ where $x \in \mathbb{Z}^2$ and $a \in \mathbb{Z}$, and the group operation is defined by

$$(x,a) * (y,b) = (x + M^a y, a+b),$$

where $M$ is a $2\times 2$ matrix with integer coefficients and with $\det M = 1$ (then also $M^{-1}$ has integer coefficients). If $M = \mathrm{id}$, then we obtain just $\mathbb{Z}^3$. For a less trivial $M$, for example, for $M = \binom{2\ \ 1}{1\ \ 1}$, the group $\mathbb{Z}^2 \rtimes \mathbb{Z}$ has an exponential volume growth, and its heat kernel satisfies the estimates

$$c_2\exp\left(-C_2n^{1/3}\right) \leq p_n(x,x) \leq C_1\exp\left(-c_1n^{1/3}\right),$$

for even $n$, where $c_1, c_2, C_1, C_2 > 0$.

Using Theorem 5.19, we can now prove a converse to Theorem 5.11.

COROLLARY 5.24. Assume that

$$\inf_{x\in V} \mu(x) > 0 \tag{5.65}$$

and that the heat kernel on $(V,\mu)$ satisfies the upper bound

$$p_n(x,x) \leq Cn^{-\alpha} \tag{5.66}$$

for all $x \in V$ and $n \geq 1$. Then $(V,\mu)$ satisfies the Faber-Krahn inequality with the function

$$\Lambda(s) = cs^{-1/\alpha}, \tag{5.67}$$

with some $c > 0$.

Of course, the hypothesis (5.65) can be replaced by a stronger condition (5.28). Hence, under (5.28), the heat kernel bound (5.66) and the Faber-Krahn inequality with the function (5.67) are equivalent.

PROOF. Fix a finite non-empty subset $\Omega$ of $V$ and prove that

$$\lambda_1(\Omega) \geq c\mu(\Omega)^{-1/\alpha}.$$

If $\lambda_1(\Omega) \geq \frac{1}{2}$, then this is true by (5.65).

Assume that $\lambda_1(\Omega) \leq \frac{1}{2}$. Then, by Theorem 5.19 and (5.66), we obtain, for all even integers $n > 0$,

$$\exp(-2\lambda_1(\Omega)n) \leq Cn^{-\alpha}\mu(\Omega). \tag{5.68}$$

Let $n$ be the minimal positive even integer such that

$$Cn^{-\alpha}\mu(\Omega) \leq e^{-2},$$

that is,

$$n^{\alpha} \geq Ce^{-2}\mu(\Omega).$$

Since by (5.65) $\mu(\Omega)$ is separated from 0 and $C$ can be chosen large enough, it follows that

$$n^{\alpha} \simeq \mu(\Omega).$$

Then we obtain from (5.68) that

$$\lambda_1(\Omega)\, n \geq 1,$$

whence

$$\lambda_1(\Omega) \geq n^{-1} \simeq \mu(\Omega)^{-1/\alpha},$$

which was to be proved. □

We will not cover off-diagonal Gaussian and sub-Gaussian estimates of the heat kernel on graphs in this volume. Such results can be found in [**9**], [**10**], [**14**], [**20**], [**48**], [**50**], [**41**], [**56**], [**81**], [**82**] and in many other sources.

## 5.6. On-diagonal lower bound via volume growth

Here we obtain another lower bound for the heat kernel. On Cayley graphs it may be not as sharp as the one of Theorem 5.19, but on general graphs it may be satisfactory.

THEOREM 5.25. *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,*

$$\mathcal{V}(r) \leq Cr^{\alpha} \tag{5.69}$$

*for some constants* $C$ *and* $\alpha$*. Then, for any* $c > \frac{\alpha}{2}$ *and for all large enough positive even integers* $n$*, the heat kernel satisfies the following estimate*

$$p_n(x_0, x_0) \geq \frac{1/4}{\mathcal{V}\left(\sqrt{cn \ln n}\right)}. \tag{5.70}$$

This theorem was proved in [**113**] (see also [**47**]). In general, the term $\sqrt{n \ln n}$ cannot be replaced by $\sqrt{n}$ – see [**74**].

PROOF. In fact, we will prove the following inequality

$$p_{2n}(x_0, x_0) \geq \frac{1/4}{\mathcal{V}\left(\sqrt{cn \ln n}\right)}, \tag{5.71}$$

that holds for any $c > \alpha$ and for all large enough positive integers $n$. Clearly, (5.71) implies

$$p_{2n}(x_0, x_0) \geq \frac{1/4}{\mathcal{V}\left(\sqrt{\frac{c}{2} 2n \ln(2n)}\right)},$$

whence (5.70) follows upon renaming $2n$ by $n$ and $\frac{c}{2}$ by $c$.

To prove (5.71) we use (5.3) and the Cauchy-Schwarz inequality in a ball $B_r$ as follows:

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

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

$$\sum_{x\in B_r^c} p_n(x_0,x)\mu(x)\leq\frac{1}{2}. \tag{5.72}$$

Then the previous estimate implies

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

which will allow us to obtain (5.71), if $r=\sqrt{cn\ln n}$.

To prove (5.72) with this $r$, let us apply Theorem 5.7. By (5.27) we have

$$p_n(x_0,x)\leq\frac{2}{\sqrt{\mu(x_0)\mu(x)}}\exp\left(-\frac{d^2(x_0,x)}{2n}\right)\leq\frac{2}{\mu_0}\exp\left(-\frac{d^2(x_0,x)}{2n}\right),$$

whence, for large enough $r$,

$$\begin{aligned} \sum_{x\in B_r^c} p_n(x_0,x)\mu(x) &\leq \frac{2}{\mu_0}\sum_{x\in B_r^c}\exp\left(-\frac{d^2(x_0,x)}{2n}\right)\mu(x) \\ &= \frac{2}{\mu_0}\sum_{k=0}^{\infty}\sum_{x\in B_{2^{k+1}r}\setminus B_{2^k r}}\exp\left(-\frac{d^2(x_0,x)}{2n}\right)\mu(x) \\ &\leq \frac{2}{\mu_0}\sum_{k=0}^{\infty}\sum_{x\in B_{2^{k+1}r}\setminus B_{2^k r}}\exp\left(-\frac{\left(2^k r\right)^2}{2n}\right)\mu(x) \\ &\leq \frac{2}{\mu_0}\sum_{k=0}^{\infty}\exp\left(-\frac{\left(2^k r\right)^2}{2n}\right)\mu\left(B_{2^{k+1}r}\right) \\ &\leq \frac{2C}{\mu_0}\sum_{k=0}^{\infty}\exp\left(-\frac{4^k r^2}{2n}\right)\left(2^{k+1}r\right)^{\alpha}, \end{aligned}$$

where we have used $\mu\left(B_{2^{k+1}r}\right)\leq C\left(2^{k+1}r\right)^{\alpha}$. Setting

$$a_k=\exp\left(-\frac{4^k r^2}{2n}\right)\left(2^{k+1}r\right)^{\alpha},$$

we see that

$$\frac{a_{k+1}}{a_k} = \exp\left(-\frac{4^{k+1}-4^k}{2}\frac{r^2}{n}\right)2^\alpha \leq \exp\left(-\frac{r^2}{n}\right)2^\alpha.$$

If $\frac{r^2}{n} \geq \alpha$, then

$$\frac{a_{k+1}}{a_k} \leq e^{-\alpha}2^\alpha =: q < 1,$$

so that the sequence $\{a_k\}$ decays faster than the decreasing geometric sequence with the ratio $q$, whence

$$\sum_{k=0}^{\infty} a_k \leq \sum_{k=0}^{\infty} a_0 q^k = \frac{a_0}{1-q}.$$

It follows that

$$\sum_{x\in B_r^c} p_n(x_0,x)\,\mu(x) \leq C' \exp\left(-\frac{r^2}{2n}\right) r^\alpha \tag{5.73}$$

where $C' = \frac{2^{\alpha+1}C}{\mu_0(1-q)}$. Choose here $r = \sqrt{cn\ln n}$ with $c > \alpha$ so that the condition $\frac{r^2}{n} \geq \alpha$ is satisfied, at least for large $n$. Then we obtain

$$\sum_{x\in B_r^c} p_n(x_0,x)\,\mu(x) \leq C' e^{-\frac{c}{2}\ln n}(cn\ln n)^{\frac{\alpha}{2}} = C' c^{\frac{\alpha}{2}} \frac{(\ln n)^{\frac{\alpha}{2}}}{n^{\frac{c}{2}-\frac{\alpha}{2}}}. \tag{5.74}$$

Since $c/2 - \alpha/2 > 0$, the right hand side here goes to 0 as $n \to \infty$. In particular, it becomes $< \frac{1}{2}$ provided $n$ is large enough, which finishes the proof. □

## 5.7. Escape rate of random walk

Using the computations from the proof of Theorem 5.25, we can prove the following property of the random walk.

THEOREM 5.26. *Let $\{X_n\}$ be the random walk on $(V,\mu)$. Under the hypothesis of Theorem* 5.25*, we have*

$$\mathbb{P}_{x_0}\left(d(X_0,X_n) \leq \sqrt{cn\ln n} \text{ for all large enough } n\right) = 1,$$

*where $c$ is any constant that is larger that $\alpha + 2$.*

This theorem was proved in [**15**].

PROOF. Let $\{r_n\}$ be an increasing sequence of positive real numbers such that $r_n \to \infty$ as $n \to \infty$. Let us investigate the conditions under which

$$\mathbb{P}_{x_0}(d(X_0,X_n) \leq r_n \text{ for all large enough } n) = 1. \tag{5.75}$$

For that, consider the events

$$A_n = \{d(X_0,X_n) > r_n\}$$

and observe that, by the lemma of Borel and Cantelli, if

$$\sum_n \mathbb{P}_{x_0}(A_n) < \infty, \tag{5.76}$$

the events $A_n$ occur finitely often with probability 1. In other words, the probability that $A_n$ does not occur for large enough $n$ is equal to 1, which is exactly what we need for (5.75). We are left to verify (5.76), more precisely, to see, under what conditions on $r_n$, (5.76) is satisfied. Observe that

$$\mathbb{P}_{x_0}(A_n) = \mathbb{P}_{x_0}\left(X_n \in B^c_{r_n}\right) = \sum_{x \in B^c_{r_n}} P_n(x_0, x) = \sum_{x \in B^c_{r_n}} p_n(x_0, x)\,\mu(x).$$

Assuming that $n$ is large enough and $r_n = \sqrt{cn \ln n}$ with $c \geq \alpha$, we obtain by (5.74)

$$P_{x_0}(A_n) = \sum_{x \in B^c_{r_n}} p_n(x_0, x)\,\mu(x) \leq C' c^{\frac{\alpha}{2}} \frac{(\ln n)^{\frac{\alpha}{2}}}{n^{\frac{c}{2} - \frac{\alpha}{2}}}.$$

Clearly, if $c > \alpha + 2$, then $\frac{c}{2} - \frac{\alpha}{2} > 1$ whence it follows that the series (5.76) converges, which finishes the proof. $\square$

REMARK 5.27. Any function $f(n)$ such that

$$\mathbb{P}_{x_0}\left(d(X_0, X_n) \leq f(n) \text{ for all large enough } n\right) = 1,$$

is called an *upper rate function* (or escape rate) for the random walk. Corollary 5.26 can be then restated as follows: the function $f_1(n) = \sqrt{cn \ln n}$ is an upper rate function. For a simple random walk in $\mathbb{Z}^m$ the Khinchin's law of iterated logarithm says that

$$\limsup_{n \to \infty} \frac{|X_n - X_0|}{\sqrt{2n \ln \ln n}} = 1.$$

It follows that a function $f_2(n) = \sqrt{Cn \ln \ln n}$ with any constant $C > 2$ is an upper rate function, too. Clearly, $f_2$ is a sharper upper rate function than $f_1$. However, in the general context of Theorem 5.26, function $f_1$ is optimal and cannot be replaced by $f_2$, as was shown in [**15**] (see also [**74**]).