A geometric approach to on-diagonal heat kernel lower bounds on groups

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Abstract

We introduce a new method for obtaining heat kernel on-diagonal lower bounds on non-compact Lie groups and on infinite discrete groups. By using this method, we are able to recover the previously known results for unimodular amenable Lie groups as well as for certain classes of discrete groups including the polycyclic groups, and to give them a geometric interpretation. We also obtain new results for some discrete groups which admit the structure of a semi-direct product or of a wreath product. These include the two-generators groups of affine transformations of the real line $\langle x \mapsto x+1, x \mapsto \lambda x \rangle$ with λ algebraic, as well as lamplighter groups with nilpotent base.

Contents

1 Introduction

Let G be a finite dimensional connected non-compact unimodular Lie group. One can endow G with a left-invariant Riemannian structure. Denote by M the corresponding Riemannian manifold and by Δ its Laplace-Beltrami operator. The associated heat semigroup $\{\exp(t\Delta)\}_{t>0}$ has a smooth density $p_t(x, y)$ with respect to the Haar measure, which is called the heat kernel. Alternatively, $p_t(x, y)$ is the transition density of the Brownian motion on M.

Because of the left-invariance, the on-diagonal value $p_t(x, x)$ of the heat kernel does not depend on $x \in G$; let us denote

$$\Phi_M(t) = p_t(x, x).$$

Our main interest in the present work is in lower estimates for $\Phi_M(t)$ as $t \to +\infty$, as well as in similar estimates for discrete groups. Note that the behavior of $\Phi_M(t)$ for large t does not depend on the choice of the Riemannian structure up to multiplicative constants (see [47], [34]). Therefore, it can be considered as a property of the sole group G.

Denote by $V(r)$ the volume (=the Haar measure) of a geodesic ball on M of radius r. Again, the behavior of $V(r)$ for large r is an invariant of G. The following dichotomy takes place provided G is amenable:

– either the volume growth is polynomial, that is, for some positive integer D,

$$cr^D \le V(r) \le Cr^D, \quad \forall r \ge 1, \tag{1.1}$$

and then the heat kernel decays also polynomially as follows:

$$ct^{-D/2} \le \Phi_M(t) \le Ct^{-D/2}, \quad \forall t \ge 1; \tag{1.2}$$

– or the volume growth is exponential

$$c\exp(cr) \le V(r) \le C\exp(Cr), \quad \forall r \ge 1, \tag{1.3}$$

in which case

$$c\exp(-Ct^{1/3}) \le \Phi_M(t) \le C\exp(-ct^{1/3}), \quad \forall t \ge 1 \tag{1.4}$$

(here C and c stand for some positive constants, possibly different at different occurrences).

Note that, for non-amenable Lie groups, a third possibility takes place: the volume growth is exponential and the heat kernel decays as $\exp(-Ct)$.

The description of the possible behaviors of the volume growth function is due to Guivarc'h ([21]) and Jenkins ([24]). The estimate (1.2) and the upper bound in (1.4) are due to Varopoulos ([44], [45]). The lower estimate in (1.4) is due to Alexopoulos [1], [2] (see also [22] and [46]).

The situation with discrete groups is much more complicated. Let G be an infinite finitely generated group and let Γ be a Cayley graph of G (see Section 5 for definitions). Denote by $p_k(x, y)$ the transition probability of the simple random walk $\{X_k\}_{k \in \mathbb{N}}$ on Γ. Again, $p_k(x, x)$ does not depend on x; let us denote

$$\varphi_\Gamma(k) = p_k(x, x).$$

We are interested in estimating $\varphi_\Gamma(k)$ from below as $k \to +\infty$. Again, the behaviour of $\varphi_\Gamma(k)$ is, up to multiplicative constants, an invariant of the group G (see [34]). Even if we restrict ourselves to the solvable case, the range of possible decay rates of the heat kernel is richer than in the case of Lie groups.

Denote by $V(r)$ the cardinality of a combinatorial ball on Γ of radius r. First of all, there is no dichotomy in the volume growth. By the results of H.Bass [5] and Gromov [20], if the volume growth $V(r)$ is *at most* polynomial then it does admit the estimate (1.1) with an integer D. However, apart from the case of the exponential growth (1.3), there are examples (which are due to Grigorchuk [19], see also [4]) of groups whose volume growth is strictly between polynomial and exponential. For the heat kernel estimates that are known in that case, see Corollary 7.4 below.

In the polynomial volume growth case (1.1), one can also prove that

$$ck^{-D/2} \leq \varphi_\Gamma(k) \leq Ck^{-D/2}, \tag{1.5}$$

where the upper bound holds for all positive integers k and the lower bound holds for all even k (because of the parity problem on bipartite graphs). The upper bound was proved in [43] whereas the lower bound follows from [23].

If G is non-amenable then, again, by a theorem of Kesten [26], the heat kernel decays exponentially in k. Assume that the group G is amenable and its volume growth is exponential as in (1.3) (excluding the groups of intermediate growth). Then one can claim only the upper bound

$$\varphi_\Gamma(k) \leq \exp(-ck^{1/3}). \tag{1.6}$$

In general, the matching lower bound fails. As was shown in [33, Theorem 7.1], there are solvable groups with exponential volume growth for which the heat kernel decays as $\exp(-ck^\alpha)$ with $\alpha \in (0, 1)$, and α can be taken arbitrarily close to 1. It is an interesting question to characterize those groups of exponential volume growth which admit the lower bound

$$\exp(-Ck^{1/3}) \leq \varphi_\Gamma(k), \tag{1.7}$$

for even k. For example, by the result of Alexopoulos ([1], [2]), the lower bound (1.7) holds for polycyclic groups. Since the volume growth on polycyclic groups is either polynomial or exponential, we see that the above dichotomy holds among polycyclic groups, too.

The upper estimates in (1.2), (1.5), (1.4) and (1.6) have now a simple proof and a clear geometric interpretation. One proves first a universal isoperimetric inequality for groups which takes into account the volume growth function $V(r)$ ([13]). From there, one obtains a Faber-Krahn inequality which is known to be equivalent to the correct upper estimate of the heat kernel ([16]). See Section 2 for detailed explanations.

The proof of the lower bound in (1.2), (1.5) can be obtained via the Gaussian upper bounds for the heat kernel ([14], [39], [23]). A simpler proof follows from [11], Thm. 2.7. The proof in [2] of the lower bound in (1.4) and (1.7) uses structure results for Lie groups and polycyclic groups as well as certain properties of Brownian motion in $\mathbb{R}^D$ and random walks in $\mathbb{Z}^D$.

Our method provides a more direct approach to the lower bounds in (1.4), (1.7) for Lie groups and polycyclic groups, and gives new lower bounds for some other situations; as a by-product, it makes the lower bounds in (1.2) and (1.5) completely transparent. The method relies on the following two ingredients:

(*i*) A technique of [11] for obtaining lower bounds, which is based on the so-called anti-Faber-Krahn inequalities (see Sections 2 and 4 for details).

(*ii*) A technique of constructing families of so-called Følner couples - pairs of sets with certain volume and distance properties, which allow to obtain the anti-Faber-Krahn inequalities. Certain aspects of this technique are reminiscent of the construction of Følner sets on groups in [30], [31].

The main emphasis of the present work is on the case of discrete groups. Although we provide a full proof of the lower bounds in (1.2) and (1.4) for amenable unimodular Lie groups (see Sections 2, 3, and Theorem 3.3), the result itself is not new. In the general case, our proof relies on the geometric constructions of [31], but in a model case (the group Sol), it can be made entirely self-contained (see the end of Section 3).

For the discrete case, ingredient (*i*) is developed in Section 4 in the context of arbitrary graphs (Theorem 4.8). As far as (*ii*) is concerned, for certain typical groups, sequences of Følner couples can be built in a direct and explicit way as we do in Section 5 (Theorems 5.1, 5.2). In the general case, we introduce in Section 6 the notion of contraction of graphs as a convenient setting where one can construct sequences of Følner couples (Theorem 6.1). We apply these techniques in Section 7 to obtain the heat kernel lower bounds for certain classes of groups which are semi-direct products as well as for polycyclic groups (Theorems 7.5, 7.10).

Our approach applies (but is not restricted) to the following situations. Let G be the Baumslag-Solitar group $BS(q) = \langle X, Y : XY = X^q Y \rangle$ where $q > 1$ is an integer. This group has exponential volume growth, is solvable but not polycyclic. The heat kernel on its Cayley graph admits the estimate

$$\exp(-Ck^{1/3}) \leq \varphi_\Gamma(k) \leq \exp(-ck^{1/3}), \tag{1.8}$$

where k is even for the lower bound. The upper bound is a consequence of the general result discussed above whereas the lower bound is proved within the scheme (*i*) − (*ii*) (see Theorems 5.1, 7.9). The lower bound for this group was first obtained in [32] (see also [48, III.15.C]).

Let G be the lamplighter group $\mathbb{Z}_2 \wr \mathbb{Z}^D$. Every element of G is a pair (f, a) where $a \in \mathbb{Z}^D$ and f is a function on $\mathbb{Z}^D$ with finite support taking the values $0, 1 \in \mathbb{Z}_2$. The group law in G is given by

$$(f, a) + (g, b) = (f + g(\cdot - a), a + b)$$

where $g(\cdot - a)$ is the function

$$x \mapsto g(x - a).$$

The random walk on the corresponding Cayley graph corresponds to movements of a lamplighter on $\mathbb{Z}^D$ with a current position at a, who can either switch the value of f at a or move to one of the neighboring elements of $\mathbb{Z}^D$. The heat kernel of this group admits the estimate

$$\exp(-Ck^{\frac{D}{D+2}}) \leq \varphi_\Gamma(k), \tag{1.9}$$

for even k. This estimate was proved in [33], alongside with the matching upper bound (see also [48, III.15.D]; see [25], [42] for earlier results). Our Theorem 5.2 provides the estimate (1.9) for a wider class of wreath products $F \wr A$ where F is a finite group and A is a finitely generated group with polynomial volume growth of degree D as in (1.1).

In Section 7.4, we prove the estimate (1.8) in particular for the group of affine transformations of the real line generated by $x \mapsto x + 1$ and $x \mapsto \lambda x$ where λ is an algebraic number not equal to $0, \pm 1$ (Theorem 7.8). If λ is transcendental then the behavior of $\varphi_\Gamma(k)$ on this group is different (see [35] and Remark 7.2).

With the exception of the lamplighter groups with non-abelian nilpotent base, our lower bounds are sharp in the sense that they match previously known upper bounds. However, we believe that the lower bounds we give are sharp in all cases.

In conclusion, let us mention that an on-diagonal estimate of the heat kernel on a finitely generated group G implies a similar estimate for the large time behavior of the heat kernel on any regular co-compact covering manifold with G as a deck transformation group (see [34]). It also follows from [34] that if a finitely generated group embeds as a co-compact lattice in a Lie group, then the large time behaviour of the heat kernel on both objects is the same. But, as it follows from [29], the finitely generated groups under consideration in the present paper (with the exception of polycyclic groups, which are treated in an appendix) do not embed as lattices in any real or complex Lie group with a finite number of connected components. Therefore a direct approach is needed.

NOTATION

C, c denote positive constants whose values are unimportant. Their values may change even within one formula. Normally (but not necessarily) C is a large constant whereas c is small.

$f(s) \simeq g(s)$ means

$$cf(s) \leq g(s) \leq Cf(s),$$

for s large enough.

$f(s) \asymp g(s)$ means

$$cf(cs) \leq g(s) \leq Cf(Cs),$$

for s large enough.

If f and g have an additional non-numerical argument x then

$$f(x, s) \asymp g(x, s), \quad \forall x \in X$$

means that, for all $x \in X$ and large enough s,

$$cf(x, cs) \leq g(x, s) \leq Cf(x, Cs).$$

The same applies to the relation $\simeq$.

2 Estimating heat kernels on manifolds

Let M be a smooth connected geodesically complete non-compact Riemannian manifold. Denote by $d(x, y)$ the geodesic distance on M and by $B(x, r)$ the (open) geodesic ball of radius r centered at x.

We assume that, alongside with the Riemannian structure, the manifold M is equipped with a measure μ having a smooth positive density σ with respect to the Riemannian measure. In particular, μ may be the Riemannian measure, which will be the case in the applications of this paper. However, we present the results of this section in a more general setting because it may prove useful in the future.

The pair (M, μ) is called a *weighted manifold*. There is a natural *weighted Laplace operator* associated with (M, μ) and defined by

$$\Delta_\mu = \sigma^{-1} \text{div} \left(\sigma \nabla u \right),$$

where div and ∇ are the Riemannian divergence and gradient, respectively. Note that Δ_μ is symmetric, and even essentially self-adjoint in $L^2(M, \mu)$ with domain $C_0^\infty(M)$. It is well-known that, for any precompact open set $\Omega \subset M$, the Dirichlet problem for Δ_μ has a discrete positive spectrum. Let us denote by $\lambda_1(\Omega)$ the smallest eigenvalue of this problem. Alternatively, we have the variational definition of the first eigenvalue, which says

$$\lambda_1(\Omega) = \inf_{f \in Lip_0(\Omega), f \not\equiv 0} \frac{\int |\nabla f|^2 \, d\mu}{\int f^2 d\mu}, \tag{2.1}$$

where $Lip_0(\Omega)$ is the set of all Lipschitz functions in M vanishing outside Ω.

Denote by $p_t(x, y)$ the *heat kernel* associated with Δ_μ. By definition, it is the kernel of the semigroup $\exp(t\Delta_\mu)$ acting on $L^2(M, \mu)$. An equivalent definition is that $p_t(x, y)$ is the positive minimal fundamental solution of the heat equation

$$\frac{\partial u}{\partial t} = \Delta_\mu u.$$

Yet another definition is that $p_t(x, y)$ is the density of the transition probability of the Brownian motion X_t on M generated by Δ_μ.

We are interested in the long time on-diagonal estimates of the heat kernel, that is, in the behaviour in $t \to +\infty$ of the quantity

$$\sup_{x \in M} p_t(x, x).$$

It is now well-known [16] that the long time behaviour of the heat kernel is closely related to a *Faber-Krahn inequality*, which provides a lower bound for $\lambda_1(\Omega)$ in terms of the measure $\mu(\Omega)$.

For example, in $\mathbb{R}^D$ with the Lebesgue measure μ, one has

$$\lambda_1(\Omega) \geq c_D \mu(\Omega)^{-2/D},$$

whereas

$$p_t(x, x) = (4\pi t)^{-D/2}.$$

In general, by a *Faber-Krahn inequality* with function Λ we mean the following condition:

(FK) For any open precompact set $\Omega \subset M$, $\lambda_1(\Omega) \geq \Lambda(\mu(\Omega))$.

Proposition 2.1 *([16, Theorem 1.1]) Let Λ be a positive continuous decreasing function on $(0, +\infty)$. Assume that (M, μ) admits the Faber-Krahn inequality (FK) with function Λ. Define the function γ on $(0, +\infty)$ by*

$$t = \int_0^{\gamma(t)} \frac{dv}{v\Lambda(v)} \tag{2.2}$$

assuming that the integral converges at 0. Then, for all $t > 0$,

$$\sup_{x \in M} p_t(x, x) \leq \frac{C}{\gamma(ct)}, \tag{2.3}$$

with some constants $C, c > 0$.

This result admits a converse - see [16].

Remark 2.1 The relation (2.2) can be equivalently stated as follows

$$\frac{\gamma'(t)}{\gamma(t)} = \Lambda(\gamma(t)), \quad \gamma(0) = 0. \tag{2.4}$$

In particular, Λ is uniquely determined by γ. It is also useful to observe that the change of function $\Lambda(v) \longmapsto c\Lambda(Cv)$ induces the change of function: $\gamma(t) \longmapsto C^{-1}\gamma(ct)$.

As was shown in [11], in order to obtain a lower bound for $\sup_x p_t(x,x)$, it suffices to prove a so-called anti-Faber-Krahn inequality. We say that (M, μ) admits the *anti-Faber-Krahn inequality* with function Λ if the following is true:

$$(aFK) \quad \begin{cases} \text{For some } v_0 \geq 0 \text{ and all } v > v_0, \text{ there exists an open} \\ \text{precompact set } \Omega_v \text{ such that } \mu(\Omega_v) \leq v \text{ and } \lambda_1(\Omega_v) \leq \Lambda(v). \end{cases}$$

We need also the following definition. Given $\delta > 0$, let us say that a positive increasing function $f \in C^1(0, +\infty)$ is δ-*regular* if, for all $0 < t \leq s \leq 2t$,

$$\frac{f'(s)}{f(s)} \geq \delta \frac{f'(t)}{f(t)}.$$

Then we have the following result.

Proposition 2.2 *([11, Theorem 3.2]) Let Λ be a positive continuous decreasing function on $(v_0, +\infty)$ and assume that (M, μ) admits the anti-Faber-Krahn inequality (aFK) with function Λ. Define a function γ on $(0, +\infty)$ by*

$$t = \int_{v_0}^{\gamma(t)} \frac{dv}{v\Lambda(v)} \tag{2.5}$$

and assume that γ is δ-regular. Then, for all $t > 0$,

$$\sup_{x \in M} p_t(x,x) \geq \frac{1}{\gamma(Ct)}, \tag{2.6}$$

where $C = 2/\delta$.

Remark 2.2 If $v_0 > 0$, which means that (aFK) contains no information on small sets, the estimate (2.6) is of little value for small time, as one should expect: $\gamma(t)$ does not even tend to zero with t.

Remark 2.3 At the present time, we do not know whether one can get rid of the regularity assumption on γ. We will apply Proposition 2.2 in situations where the regularity of γ can be easily verified. For example, the functions $\gamma(t) = t^\alpha$, $\exp(t^\alpha)$ are obviously regular. Assuming that Λ is twice differentiable, the following condition in terms of the function $f(\xi) := \Lambda(e^\xi)$ is sufficient for γ to be δ-regular:

$$f f'' \geq \varepsilon \left(f'\right)^2 \tag{2.7}$$

where $\varepsilon = (\log_2 \frac{1}{\delta})^{-1}$(see [16, Section 2]). For example, the functions $\Lambda(v) = v^{-\alpha}$ and $(\log v)^{-\alpha}$ satisfy (2.7). See Section 8 for another sufficient condition for δ-regularity.

Example 2.1 If $\Lambda(v) = Cv^{-1/\alpha}$, $\alpha > 0$, then one obtains from (2.5)

$$\gamma(t) \simeq t^{\alpha}.$$

If $\Lambda(v) = C(\log v)^{-\alpha}$, $\alpha > 0$, then

$$\gamma(t) \asymp \exp(t^{\frac{1}{\alpha+1}}).$$

If $\Lambda(v) = C(\log\log v)^{\beta}(\log v)^{-\alpha}$, $\alpha, \beta > 0$, then

$$\gamma(t) \asymp \exp(t^{\frac{1}{\alpha+1}}(\log t)^{\frac{\beta}{\alpha+1}}).$$

In all three cases, one checks that γ is regular, either directly or by using Lemma 8.1.

Propositions 2.1 and 2.2 provide a universal method for estimating $\sup_x p_t(x,x)$. Proving matching upper and lower bounds for $\sup_x p_t(x,x)$ amounts therefore to obtaining an optimal Faber-Krahn inequality. Define the L^2-*isoperimetric profile* of M by

$$\Lambda_{\max}(v) = \inf_{\mu(\Omega) \leq v} \lambda_1(\Omega).$$

One can summarize the above by saying that the on-diagonal heat kernel behaviour is controlled from above and below by $\Lambda_{\max}$ (see [10] for details).

Let us discuss some methods for obtaining the Faber-Krahn and anti-Faber-Krahn inequalities. Let $I(\cdot)$ be a positive function on $(0, +\infty)$. We say that the manifold (M, μ) admits the *isoperimetric inequality* with function I if the following is true:

(Iso) For any precompact open set Ω with smooth boundary, $\mu'(\partial\Omega) \geq I(\mu(\Omega))$

(where μ' is the surface area). If $I(s)/s$ is non-increasing then (Iso) implies the Faber-Krahn inequality (FK) with function

$$\Lambda(v) = \frac{1}{4}\left(\frac{I(v)}{v}\right)^2 \tag{2.8}$$

(this is basically Cheeger's inequality - see [6], [28], [16, Proposition 2.4]).

It is natural to ask whether a kind of anti-isoperimetric inequality could imply an anti-Faber-Krahn inequality in the same way as the isoperimetric inequality implies a Faber-Krahn inequality. This is indeed the case in certain situations (see [11, Sections 3 and 4]) and the results of the present paper together with [31, Section 2.2] show that these situations include Lie groups and some interesting examples of finitely generated groups.

Let us now explain a direct method which allows to obtain anti-Faber-Krahn inequalities. Some ancestors or relatives of this method can be found in [11], Propositions 3.4 and 4.9. The following lemma is a simple consequence of (2.1). For any $\rho > 0$ and $\Omega \subset M$, denote

$$\Omega^{\rho} = \big\{x \in \Omega : d(x, \complement\Omega) > \rho\big\}$$

Lemma 2.3 *For any precompact open set* $\Omega \subset M$ *and any* $\rho > 0$, *we have*

$$\lambda_1(\Omega) \leq \frac{1}{\rho^2}\frac{\mu(\Omega)}{\mu(\Omega^{\rho})}.$$

Proof. Let us define a test function $f \in Lip_0(\Omega)$ by $f(x) = d(x, \complement\Omega)$.
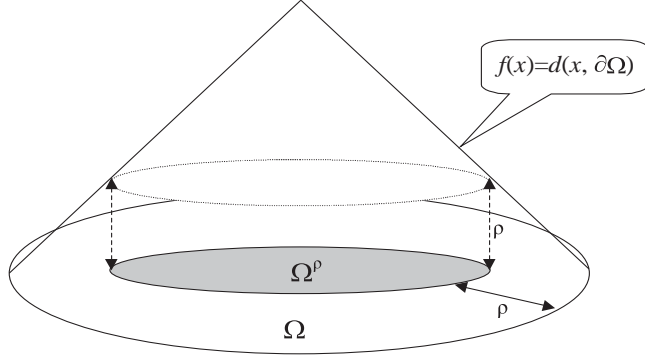
Figure 1 Sets Ω, Ω^ρ and function f.

Then $|\nabla f| \leq 1$, $f = 0$ outside Ω, and $f \geq \rho$ on Ω^ρ, whence we obtain

$$\lambda_1(\Omega) \leq \frac{\int |\nabla f|^2 \, d\mu}{\int f^2 d\mu} \leq \frac{\mu(\Omega)}{\rho^2 \mu(\Omega^\rho)},$$

which was to be proved. ∎

We can now prove our main result for general manifolds.

Proposition 2.4 *Let ρ be a positive increasing continuous function on $(v_0, +\infty)$. Suppose that the manifold (M, μ) satisfies the following property: for any $v > v_0$, there exists a pair of open precompact sets $\Omega_v' \subset \Omega_v$ such that*

$$\mu(\Omega_v) \leq v, \quad \mu\left(\Omega_v'\right) \geq cv, \quad d(\Omega_v', \complement\Omega_v) \geq \rho(v). \tag{2.9}$$

Then M admits the anti-Faber-Krahn inequality (aFK) with function

$$\Lambda(v) = \frac{1}{c\rho^2(v)}.$$

Consequently, the following heat kernel lower bound holds, for all $t > 0$,

$$\sup_{x \in M} p_t(x, x) \geq \frac{1}{\gamma(Ct)},$$

where γ is defined by

$$t = \int_{v_0}^{\gamma(t)} \rho^2(v) \frac{dv}{v},$$

provided γ is δ-regular.

Remark 2.4 By Lemma 8.1 (see Section 8), the function γ is δ-regular provided $v\frac{\rho'(v)}{\rho(v)}$ is non-increasing for large enough v.

Proof. Denote for simplicity $\Omega = \Omega_v$ and $\Omega' = \Omega_v'$. The hypothesis $d(\Omega', \complement\Omega) \geq \rho(v)$ implies $\Omega' \subset \Omega^{\rho(v)}$, whence

$$\mu(\Omega') \leq \mu(\Omega^{\rho(v)}).$$

Now Lemma 2.3 and (2.9) yield

$$\lambda_1(\Omega) \leq \frac{1}{\rho^2(v)} \frac{\mu(\Omega)}{\mu(\Omega^{\rho(v)})} \leq \frac{1}{\rho^2(v)} \frac{\mu(\Omega)}{\mu(\Omega')} \leq \frac{1}{c\rho^2(v)},$$

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which is the first claim. The second claim follows from Proposition 2.2. ∎

The pairs of sets $\Omega'_v \subset \Omega_v$ from the hypothesis (2.9) will be called *Følner couples*, in association with the Følner sets Ω which are fat sets in the sense that the surface area of their boundary $\partial\Omega$ is small compared to their volume $\mu(\Omega)$. Indeed Ω_v is fat in the sense that one can substantially shrink it (with distance $\rho(v)$) while keeping a constant proportion of its volume. Følner sets are used to prove *anti-isoperimetric inequalities* (see for example [30] and [31]). Similarly, Følner couples can be used to prove anti-Faber-Krahn inequalities and, consequently, heat kernel lower bounds.

Remark 2.5 Sometimes it may be convenient to parametrize the Følner couples in a different way. Indeed, assume that the function ρ admits an inverse and denote $\mathcal{V} = \rho^{-1}$. Then, parametrizing Følner couples by a new variable $r = \rho(v)$, we can rewrite (2.9) as follows:

$$\mu(\Omega_r) \le \mathcal{V}(r), \quad \mu(\Omega'_r) \ge c\mathcal{V}(r), \quad d(\Omega'_r, \complement\Omega_r) \ge r. \tag{2.10}$$

The function γ can be found by

$$t = \int_{v_0}^{\gamma(t)} \left[\mathcal{V}^{-1}(v)\right]^2 \frac{dv}{v}.$$

This formula should be compared with formula (3.4) from Corollary 3.2 below, which provides a similar *upper* bound for the heat kernel in terms of the volume growth function

$$V(x, r) = \mu(B(x, r)).$$

If $\mathcal{V}(r) \asymp V(x, r)$ then the Følner sets, though being far from spherical in general (see [30]), still retain something of the behaviour of spheres (as in Example 2.2 below). In this case the lower bound of Proposition 2.4 matches the upper bound of Corollary 3.2.

Proposition 2.4 provides a general approach to heat kernel lower bounds, which will be used in the next section in the case of Lie groups. The following example is a particular case of [11, Theorem 2.7]. However, it demonstrates how the present method works.

Example 2.2 Suppose that the function $V(x, r)$ is polynomial, that is, for some $x \in M$ and $D > 0$,

$$V(x, r) \simeq r^D. \tag{2.11}$$

Define $\Omega_r = B(x, 2r)$ and $\Omega'_r = B(x, r)$. Then $\mu(\Omega'_r) \simeq \mu(\Omega_r) \simeq r^D$ and $d(\Omega'_r, \complement\Omega_r) = r$. Hence, (2.10) holds with the function $\mathcal{V}(r) = Cr^D$, or $\rho(v) = cv^{1/D}$. Consequently, Proposition 2.4 yields the anti-Faber-Krahn inequality with function

$$\Lambda(v) \simeq v^{-2/D} \tag{2.12}$$

and the heat kernel lower bound

$$\sup_{x \in M} p_t(x, x) \ge ct^{-D/2}. \tag{2.13}$$

Note that both (2.12) and (2.13) are sharp in $\mathbb{R}^D$.

3 Lie groups

Let us first recall how one can obtain heat kernel upper bounds for unimodular amenable Lie groups in a simple and geometric way. Given a connected unimodular Lie group G, fix a left-invariant Riemannian structure on G and denote by M the corresponding Riemannian manifold. Denote by μ the Riemannian measure, which coincides with the Haar measure. By the left-invariance of the metric, $V(x, r) := \mu(B(x, r))$ does not depend on x. We can therefore set $V(r) = V(x, r)$ and call $V(r)$ the volume growth function. Similarly, the heat kernel $p_t(x, x)$ on (M, μ) does not depend on x, and we denote

$$\Phi_M(t) = p_t(x, x).$$

Proposition 3.1 *([13, Theorem 4]) Let G be a connected unimodular Lie group, endowed with a left-invariant Riemannian metric. Then the associated manifold M admits the isoperimetric inequality (Iso) with function*

$$I(v) := \frac{cv}{V^{-1}(Cv)}, \tag{3.1}$$

where V^{-1} is the inverse function of the volume growth function.

Combining with (2.8) and Proposition 2.1, we obtain:

Corollary 3.2 *Under the assumptions of Proposition 3.1, the manifold M admits the Faber-Krahn inequality (FK) with function*

$$\Lambda(v) = \left(\frac{c}{V^{-1}(Cv)}\right)^2. \tag{3.2}$$

Consequently, we have, for all $t > 0$,

$$\Phi_M(t) \leq \frac{C}{\gamma(ct)} \tag{3.3}$$

where γ is defined by

$$t = \int_0^{\gamma(t)} \left[V^{-1}(v)\right]^2 \frac{dv}{v}. \tag{3.4}$$

Example 3.1 If $V(r) \simeq r^D$ then (3.2) and (3.3) yield $\Lambda(v) \simeq v^{-2/D}$ and

$$\Phi_M(t) \leq Ct^{-D/2}, \ t \geq 1. \tag{3.5}$$

If $V(r) \asymp e^r$ then we obtain $\Lambda(v) \simeq (\log v)^{-2}$ and

$$\Phi_M(t) \leq C \exp(-ct^{1/3}), \ t \geq 1. \tag{3.6}$$

Here is our main result for Lie groups. It says that, in the unimodular and amenable case, one can obtain from the volume growth function also a correct lower bound for the heat kernel.

Theorem 3.3 *Let G be a connected non-compact unimodular amenable Lie group, endowed with a left-invariant Riemannian metric. Then the associated Riemannian manifold M admits the anti-Faber-Krahn inequality (aFK) with function*

$$\Lambda(v) := \left(\frac{C}{V^{-1}(cv)}\right)^2, \tag{3.7}$$

and, for all $t > 0$,

$$\Phi_M(t) \geq \frac{c}{\gamma(Ct)}, \qquad (3.8)$$

where γ is defined by

$$t = \int_0^{\gamma(t)} \left[V^{-1}(v)\right]^2 \frac{dv}{v}. \qquad (3.9)$$

Because of the dichotomy for volume growth on Lie groups, one can formulate a combination of Corollary 3.2 and Theorem 3.3 in the following way.

Theorem 3.4 *Under the hypotheses of Theorem 3.3, we have either*

- $V(r) \simeq r^D$ *and* $\Phi_M(t) \simeq t^{-D/2}$,

- *or* $V(r) \asymp e^r$ *and* $\Phi_M(t) \asymp e^{-t^{1/3}}$.

As we already mentioned, this theorem is well-known ([44], [45], [2], [22]). Our contribution here is to give a simple and geometric proof of the lower bounds, which matches somewhat the proof of the upper bounds relying on [13] and [16]. The ideas involved in this new proof will also open the way for the treatment of discrete groups.

Theorem 3.3 will be deduced from Proposition 2.4. The following statement, based on the structure of Lie groups, will be used in order to construct families of Følner couples needed to apply Proposition 2.4.

Given a connected non-compact unimodular amenable Lie group G and an associated Riemannian manifold M, there exists a simply connected solvable Lie group S quasi-isometric to M. Let a be the growth exponent of the commutator group $[S, S]$ of S (which is nilpotent and simply connected). The quotient $S/[S, S]$ is a vector space, let b be its dimension. If the volume growth is exponential then $a, b \geq 1$. For all this, see [31, Sections 2.2, 3.4, 4.4].

Proposition 3.5 *([31, Section 2.2]) Let G be a connected unimodular amenable Lie group with exponential growth, and a, b be defined as above. Then there exists a two-parameter family $\{\Omega_{t,u}\}$ of subsets of G, increasing in t and decreasing in u (where t varies in $[1, +\infty)$ and u varies in $[0, t/2]$), and possessing the following properties:*

(a) *For all t and u in the range,*

$$\mu(\Omega_{t,u}) \simeq \left(\alpha^t - u\beta^t\right)^a (t - u)^b, \qquad (3.10)$$

for some numbers $\alpha > \beta > 1$.

(b) *For all t and u in the range,*

$$d(\Omega_{t,u}, \complement\Omega_{t,0}) \geq \varepsilon u, \qquad (3.11)$$

for some $\varepsilon > 0$.

At the end of this section, we will show a typical example of group G where the family $\{\Omega_{t,u}\}$ can be explicitly constructed. For the general case, see [31].

Proof of Theorem 3.3. If the volume growth $V(r)$ is polynomial then the statement of Theorem 3.3 follows from Example 2.2. An obvious adaptation of the same technique yields the small time estimate in (3.8). Assume now that G has exponential volume growth, i.e. $V(r) \asymp e^r$.

Then we apply Proposition 3.5. It follows from (3.10) and from $a > 0$ that for any v large enough, say $v > v_0 > 0$, there exists $t \simeq \log v$ so that

$$\mu(\Omega_{t,0}) \leq v \quad \text{and} \quad \mu(\Omega_{t,t/2}) \geq cv. \tag{3.12}$$

Using (3.11), we obtain

$$d(\Omega_{t,t/2}, \complement\Omega_{t,0}) \geq \varepsilon t/2 \geq c \log v.$$

Hence, we can apply Proposition 2.4 with the Følner couples $\Omega_v = \Omega_{t,0}$, $\Omega'_v = \Omega_{t,t/2}$ and the function $\rho(v) = \mathcal{V}^{-1}(v) = c \log v$. This yields (aFK) with function $\Lambda_1(v) = \left(\frac{C}{\log v}\right)^2$. Let γ_1 be defined by

$$t = \int_{v_0}^{\gamma_1(t)} \left[\mathcal{V}^{-1}(v)\right]^2 \frac{dv}{v},$$

which yields $\gamma_1(t) = \exp(C'(t + c)^{1/3})$. In particular, γ_1 is regular, and

$$\Phi_M(t) \geq \frac{1}{\gamma_1(Ct)}.$$

Since $V^{-1}(v) \simeq \log v \simeq \mathcal{V}^{-1}(v)$, (3.7) as well as (3.8) for large time are true. ∎

In the rest of this section, we show a simple proof of the crucial Proposition 3.5 for a specific Lie group. Let $G = Sol$, that is, $G = \mathbb{R}^2 \rtimes \mathbb{R}$, where $\mathbb{R}$ (with the coordinate z) acts on $\mathbb{R}^2$ (with the coordinates (x, y)) by the matrix

$$\begin{pmatrix} e^z & 0 \\ 0 & e^{-z} \end{pmatrix}.$$

The commutator group $[G, G]$ is $\mathbb{R}^2$ (with the coordinates (x, y)); the quotient $G/[G, G]$ is isomorphic to $\mathbb{R}$ (with the coordinate z). Thus in that case $a = 2$ and $b = 1$.

As a manifold, Sol is diffeomorphic to $\mathbb{R}^3$, and it can be equipped with the left-invariant Riemannian metric g defined by

$$(g_{ij}) = \begin{pmatrix} e^{-2z} & 0 & 0 \\ 0 & e^{2z} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{3.13}$$

Denote this manifold by M. It is well-known that M has exponential volume growth. Let us define the following two-parameter family of boxes in M

$$\Omega_{t,u} := \left\{(x, y, z) \in \mathbb{R}^3 : |x| < e^{2t} - ue^t, \; |y| < e^{2t} - ue^t, \; |z| < t - u\right\}, \tag{3.14}$$

where $t > 0$ and $0 < u \leq t$, and show that it satisfies the conditions (a) and (b) of Proposition 3.5.

To verify (a), let us observe that $\det(g_{ij}) = 1$. Therefore, the Riemannian volume in M coincides with the Euclidean volume in $\mathbb{R}^3$, whence

$$\mu(\Omega_{t,u}) = 8\left(e^{2t} - ue^t\right)^2 (t - u)$$

matching (3.10).

Let us prove (b). Consider any smooth path $\gamma(s) : [0, l] \to M$ parametrized by the Riemannian arc length s and starting from a point $\gamma(0) \in \Omega_{t,u}$. Assuming that it has length l and that

$$l \leq u, \tag{3.15}$$

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let us prove that $\gamma(l) \in \Omega_{t,0}$ which will then imply

$$d(\Omega_{t,u}, \complement\Omega_{t,0}) \geq u,$$

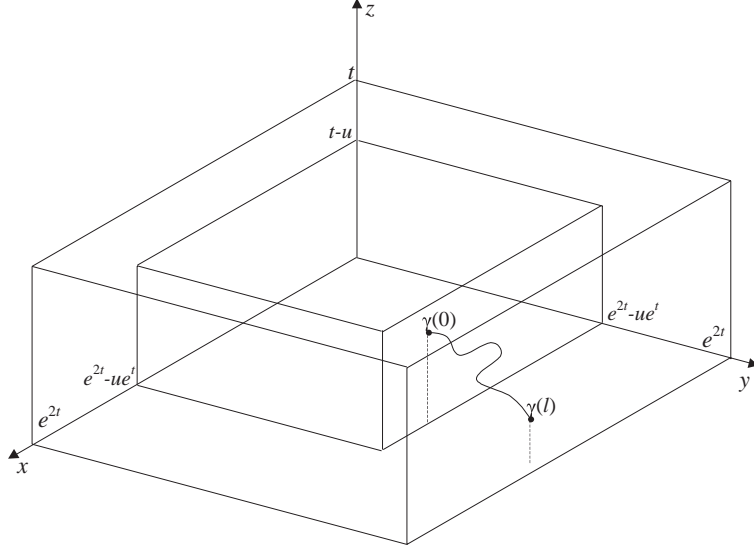that is, (3.11) with $\varepsilon = 1$.

Figure 2 Boxes $\Omega_{t,0}$, $\Omega_{t,u}$ in the first octant and the path $\gamma(s)$.

Let us set

$$\gamma(s) = (x(s), y(s), z(s)).$$

Due to $g_{33} = 1$, the projection of M onto the z-axis does not increase the length. Therefore, for any $s \in [0, l]$, as $\gamma(0) \in \Omega_{t,u}$ and because of (3.15),

$$|z(s)| \leq |z(0)| + s \leq (t - u) + l \leq t. \tag{3.16}$$

Hence, the entire path γ lies between two hyperplanes $z = \pm t$ containing two faces of the box $\Omega_{t,0}$, respectively.

In order to show that $\gamma(l) \in \Omega_{t,0}$, we are left to verify that

$$|\gamma(l) - \gamma(0)|_{Eucl} \leq ue^{t}$$

where the subscript $Eucl$ refers to the Euclidean distance in $\mathbb{R}^3$. As follows from the definition (3.13) of the Riemannian metric of M, for any vector v at the point (x, y, z), we have the following inequality

$$|v|_{Eucl} \leq e^{|z|} |v|_{M}. \tag{3.17}$$

In particular, for the vector $v = \dot{\gamma}$ which has the Riemannian length 1, we obtain from (3.17) and (3.16)

$$|\dot{\gamma}(s)|_{Eucl} \leq e^{|z(s)|} \leq e^{t},$$

whence

$$|\gamma(l) - \gamma(0)|_{Eucl} \leq \int_0^l |\dot{\gamma}(s)|_{Eucl} ds \leq le^{t} \leq ue^{t},$$

which was to be proved.

Note that an easy way to verify that M has exponential growth is to check that, for large t, $B(0, 10t) \supset \Omega_{t,0}$.

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4 Estimating heat kernels on graphs

Let Γ be an infinite (countable) graph, i.e. a set of vertices, some of which are connected by an edge. If two vertices $x, y \in \Gamma$ are neighbors, i.e. are connected by an edge, then we write $x \sim y$ (equivalently, $y \sim x$) and denote the edge by $\overline{xy}$. Assume that Γ is connected, i.e. any two vertices can be joined by an edge path in Γ, and locally finite, i.e. each vertex has a finite number of neighbors called its degree.

Denote by $d(x, y)$ the *graph distance* on Γ: for any $x, y \in \Gamma$, $d(x, y)$ is the minimal number of edges in a path connecting x and y. Let $B(x, r)$ be the ball of radius $r > 0$ centered at $x \in \Gamma$, that is

$$B(x, r) = \{y \in \Gamma : d(x, y) < r\}.$$

Any edge $\overline{xy}$ will be equipped with a *weight* $\mu_{xy} = \mu_{yx} > 0$ (if x and y are not neighbors then we set $\mu_{xy} = 0$). This induces also a weight μ on vertices defined by

$$\mu(x) = \sum_{y \sim x} \mu_{xy}$$

which extends to a *measure* on Γ by

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

for all finite sets $\Omega \subset \Gamma$. We will use also the following notation for the volume of the ball $B(x, r)$:

$$V(x, r) = \mu(B(x, r)).$$

We will call the pair (Γ, μ) a *weighted graph*. For example, we may put $\mu_{xy} = 1$ for all neighboring vertices x and y. This weight is referred to as *the standard weight* on Γ. For the standard weight, $\mu(x)$ is equal to the degree of the vertex x.

There is a natural random walk X_k on the weighted graph (Γ, μ). It is determined by the transition function

$$P(x, y) := \frac{\mu_{xy}}{\mu(x)}. \tag{4.1}$$

If μ is the standard weight then X_k is referred to as the *simple random walk* on Γ.

Denote by $P_k(x, y)$ the transition probability of the random walk X_k, that is,

$$P_k(x, y) = \mathbb{P}_x\{X_k = y\}.$$

It can also be defined inductively by $P_0(x, y) = \delta_{xy}$ and

$$P_k(x, y) = \sum_{z \in \Gamma} P_{k-1}(x, z) P(z, y).$$

The heat kernel $p_k(x, y)$ of (Γ, μ) is defined by

$$p_k(x, y) = \frac{P_k(x, y)}{\mu(y)}.$$

In other words, $p_k(x, y)$ is the density of the transition probability $P_k(x, y)$ with respect to the measure μ. As follows from (4.1) and $\mu_{xy} = \mu_{yx}$, the heat kernel is symmetric in x, y, that is, the random walk X_k is reversible with respect to the measure μ on Γ.

Alternatively, it is possible to construct a weight on Γ assuming that there is a nearest neighbor random walk X_k on Γ reversible with respect to a measure μ. Indeed, the weight μ_{xy} is recovered via the measure μ and the transition function $P(x, y)$ by

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

We shall need the following notions related to analysis on graphs. Let f denote a function on Γ.

1. *The operators.* Define the gradient

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

and the Laplace operator

$$\Delta f(x) := \sum_{y \in \Gamma} P(x, y)f(y) - f(x) = \sum_{y \in \Gamma} P(x, y)\nabla_{xy}f = \frac{1}{\mu(x)} \sum_{y \in \Gamma} (\nabla_{xy}f)\mu_{xy}.$$

2. *The norms and spaces.* The space $\ell^p(\Gamma)$ is the set of all functions f on Γ for which the following norm is finite:

$$\|f\|_p = \left(\sum_{x \in \Gamma} |f(x)|^p \, \mu(x) \right)^{1/p}.$$

If $\Omega \subset \Gamma$, we denote by $\ell^p(\Omega)$ the set of all functions in $\ell^p(\Gamma)$ vanishing outside Ω.

The Dirichlet form is defined by

$$\mathcal{E}(f) := (-\Delta f, f)_{\ell^2(\Gamma)} = \frac{1}{2} \sum_{x,y \in \Gamma} (\nabla_{xy}f)^2 \, \mu_{xy}.$$

3. *The eigenvalues.* Let $\Omega \subset \Gamma$. Denote by Δ_Ω the restriction of the Laplace operator to $\ell^2(\Omega)$ that is, for any $f \in \ell^2(\Omega)$,

$$\Delta_\Omega f(x) = \begin{cases} \Delta f(x), & x \in \Omega, \\ 0, & x \notin \Omega \end{cases}$$

(recall that $f = 0$ outside Ω). If Ω is non-empty and finite, $-\Delta_\Omega$ is a self-adjoint positive definite operator on the finitely dimensional space of all functions on Ω. Denote by $\lambda_1(\Omega)$ the smallest eigenvalue of $-\Delta_\Omega$. Alternatively, it admits the following variational definition

$$\lambda_1(\Omega) = \inf_{\substack{f \in \ell^2(\Omega) \\ f \not\equiv 0}} \frac{\mathcal{E}(f)}{\|f\|_2^2}. \tag{4.2}$$

Similarly to the case of manifolds, heat kernel upper and lower bounds on (Γ, μ) can be obtained via Faber-Krahn and anti-Faber-Krahn inequalities. The following statement is a discrete version of Proposition 2.1 and can be proved in the same way as [9, Proposition V.1], [16].

Proposition 4.1 *Suppose that*

$$v_0 := \inf_{x \in \Gamma} \mu(x) > 0.$$

Assume that, for any finite non-empty set $\Omega \subset \Gamma$,

$$\lambda_1(\Omega) \geq \Lambda(\mu(\Omega)),$$

where Λ is a continuous positive decreasing function on $[v_0, +\infty)$. Define the function γ on $(0, +\infty)$ by

$$t = \int_{v_0}^{\gamma(t)} \frac{dv}{v\Lambda(v)}. \tag{4.3}$$

Then, for all $k \in \mathbb{N}$,

$$\sup_{x \in \Gamma} p_k(x, x) \leq \frac{C}{\gamma(ck)}.$$

The converse statement is also true, provided γ is δ-regular - see [9], [16].

The rest of this section is devoted to obtaining lower bounds for $\sup_{x \in \Gamma} p_k(x, x)$. We will focus around two results: Proposition 4.4, which states a lower bound similar to the upper bound of Proposition 4.1, and Theorem 4.8, which is a discrete analogue of Proposition 2.4.

Let us start with the following elementary lower bound.

Proposition 4.2 *Let (Γ, μ) be a weighted graph. Then, for any non-empty finite set $\Omega \subset \Gamma$, and for all even $k \in \mathbb{N}$,*

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{(1 - \lambda_1(\Omega))^k}{\mu(\Omega)}. \tag{4.4}$$

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

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{\exp\left(-2\lambda_1(\Omega)k\right)}{\mu(\Omega)}. \tag{4.5}$$

Remark 4.1 Since Γ is connected and infinite, the following inequality holds for any non-empty finite set $\Omega \subset \Gamma$:

$$0 < \lambda_1(\Omega) < 1$$

(see [7] or [12, Lemma 3.2]).

Remark 4.2 Note that, in general, one cannot claim any non-trivial lower bound for $p_k(x, x)$ if k is odd. For example, for any bipartite graph (say the Cayley graph associated to the canonical generating set of $\mathbb{Z}^D$), one has $p_k(x, x) = 0$ for all odd k. Note that the estimate (4.5) was obtained in [11, Proposition 4.3] for all k under the additional hypothesis $P(x, x) \geq c > 0$ which is not assumed here.

Proof. Let $\{\lambda_i(\Omega)\}_{i \geq 1}$ be the eigenvalues of the operator $-\Delta_\Omega$ in increasing order. Then $P^\Omega := \mathrm{Id} + \Delta_\Omega$ has the eigenvalues $1 - \lambda_i(\Omega)$. Writing $\mathrm{tr}\left(P^\Omega\right)^k$ in two ways, we obtain

$$\sum_{i \geq 1} (1 - \lambda_i(\Omega))^k = \sum_{x \in \Omega} P_k^\Omega(x, x).$$

Using the fact that $P_k^\Omega(x, x) \leq P_k(x, x)$ for any x, we obtain, for even k,

$$(1 - \lambda_1(\Omega))^k \leq \sum_{x \in \Omega} P_k(x, x) = \sum_{x \in \Omega} p_k(x, x)\mu(x) \leq \mu(\Omega) \sup_{x \in \Omega} p_k(x, x),$$

whence (4.4) follows.

The estimate (4.5) is a consequence of (4.4) and the following elementary inequality:

$$1 - \lambda \geq \exp\left(-2\lambda\right), \quad \forall \lambda \in [0, \frac{1}{2}].$$

∎

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Definition 4.3 *Given a numerical sequence $\{v_n\}_{n\geq 1}$ such that $v_n \uparrow \infty$ and a function Λ defined on $\{v_n\}$, we say that (Γ, μ) admits the discrete anti-Faber-Krahn inequality with Λ and $\{v_n\}$, if the following holds:*

(daFK) *There exists a sequence $\{\Omega_n\}_{n\geq 1}$ of non-empty finite sets in Γ such that*

$$\mu(\Omega_n) \leq v_n, \quad \lambda_1(\Omega_n) \leq \Lambda(v_n). \tag{4.6}$$

The following proposition is a version of [11, Theorem 4.7] adapted to the above formulation of anti-Faber-Krahn inequalities.

Proposition 4.4 *Let Λ be a positive continuous non-increasing function on $(0, +\infty)$. Assume that (Γ, μ) admits (daFK) with Λ and some sequence $\{v_n\}_{n\geq 1}$. Fix some positive $v_0 < v_1$, define the function γ on $(0, +\infty)$ by*

$$t = \int_{v_0}^{\gamma(t)} \frac{dv}{v\Lambda(v)}, \tag{4.7}$$

and assume that γ is δ-regular in the sense of Section 2. Let k be a positive even integer such that

$$\delta_2 \leq \frac{k}{\gamma^{-1}(v_n)} \leq \delta_1, \tag{4.8}$$

for some $n \geq 1$ and some positive $\delta_2 < \delta_1$, where

$$\delta_1 = \frac{1}{2} \min\left(\delta, \frac{1}{-\log(1 - \lambda_1(\Omega_1))}\right).$$

Then, for this k, we have

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{c}{\gamma(Ck)}, \tag{4.9}$$

where $C = 2/\delta_2$ and $c = v_0/v_1$.

Condition (4.8), with a fixed δ_2, may not be satisfied by all integers k unless the sequence of the volumes $\{v_n\}$ is dense enough. The conclusion of Proposition 4.4 can be reformulated as follows: the estimate (4.9) holds for those k which are in the following union of segments:

$$\bigcup_{n\geq 1} [\delta_2 \gamma^{-1}(v_n), \, \delta_1 \gamma^{-1}(v_n)]. \tag{4.10}$$

Hence, we obtain the following consequence.

Corollary 4.5 *Under the hypotheses of Proposition 4.4, assume in addition that there is a constant $K > 1$ such that*

$$\gamma^{-1}(v_{n+1}) \leq K\gamma^{-1}(v_n), \quad \text{for all } n \text{ large enough.} \tag{4.11}$$

*Then the lower bound (4.9), with suitable c and C, holds for **all** large enough even k.*

Proof. Indeed, take $\delta_2 = \delta_1/K$. Then (4.11) implies that the consecutive segments in (4.10) overlap, whence the claim follows by Proposition 4.4. ∎

For example, if $\gamma(t) \simeq t^\alpha$ then (4.11) becomes

$$v_{n+1} \leq K'v_n,$$

which allows v_n to grow at most as a geometric series. If $\gamma(t) \asymp \exp(t^\alpha)$ then (4.11) becomes

$$\log v_{n+1} \leq K' \log v_n$$

which allows v_n to grow as fast as $v_n = e^{e^n}$.

Proof of Proposition 4.4. Given an even k and a positive integer n satisfying (4.8), let us consider first the (main) case when $\Lambda(v_n) \leq 1/2$. By (4.6), this implies $\lambda_1(\Omega_n) \leq 1/2$. By Proposition 4.2 with $\Omega = \Omega_n$ and by (4.6), we obtain

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{\exp(-2\lambda_1(\Omega_n)k)}{\mu(\Omega_n)} \geq \frac{\exp(-2\Lambda(v_n)k)}{v_n}.$$

Let us rewrite this estimate as follows

$$\sup_{x \in \Gamma} p_k(x, x) \geq \exp(-L_n). \tag{4.12}$$

where

$$L_n := \log v_n + 2k\Lambda(v_n). \tag{4.13}$$

Define τ_n by

$$\tau_n := \int_{v_0}^{v_n} \frac{ds}{s\Lambda(s)} = \gamma^{-1}(v_n)$$

so that $v_n = \gamma(\tau_n)$. Using the identity $\Lambda(\gamma(t)) = (\log \gamma(t))'$ which follows from (4.7), we rewrite (4.13) as

$$L_n = \log \gamma(\tau_n) + 2k(\log \gamma)'(\tau_n). \tag{4.14}$$

By the mean-value theorem, there exists $\theta \in (\tau_n, 2\tau_n)$ such that

$$(\log \gamma)'(\theta) = \frac{\log \gamma(2\tau_n) - \log \gamma(\tau_n)}{\tau_n}. \tag{4.15}$$

The δ-regularity of γ yields

$$(\log \gamma)'(\theta) \geq \delta(\log \gamma)'(\tau_n). \tag{4.16}$$

From (4.14), (4.15) and (4.16), we obtain

$$L_n \leq \log \gamma(\tau_n) + 2k\frac{\log \gamma(2\tau_n) - \log \gamma(\tau_n)}{\delta\tau_n}.$$

Hypothesis (4.8) gives

$$2\delta_2 \leq \frac{2k}{\tau_n} \leq 2\delta_1 \leq \delta$$

whence

$$L_n \leq \log \gamma(2\tau_n) \leq \log \gamma(\frac{2k}{\delta_2})$$

Finally, this inequality and (4.12) imply (4.9) with $c = 1$ and $C = 2/\delta_2$.

Consider now the case $\Lambda(v_n) > 1/2$. By the monotonicity of Λ, we have also $\Lambda(v) > 1/2$ for all $v \leq v_n$. Then, as long as $\gamma(t) \leq v_n$, (4.7) yields

$$t \leq \int_{v_0}^{\gamma(t)} \frac{2dv}{v} = 2\log\frac{\gamma(t)}{v_0}.$$

Hence, for all $t \leq \gamma^{-1}(v_n)$, we have

$$\gamma(t) \geq v_0 \exp(t/2). \tag{4.17}$$

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On the other hand, by Proposition 4.2 with $\Omega = \Omega_1$,

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{(1 - \lambda_1(\Omega_1))^k}{\mu(\Omega_1)} \geq \frac{\exp\left(-k/(2\delta_1)\right)}{v_1}, \tag{4.18}$$

where we have used the condition $\log(1 - \lambda_1(\Omega_1)) \geq -(2\delta_1)^{-1}$. By (4.8), we have $k/\delta_1 \leq \gamma^{-1}(v_n)$. Therefore we can apply (4.17) with $t = k/\delta_1$, and comparing with (4.18) yields (4.9) with $c = v_0/v_1$ and $C = 1/\delta_1$. ∎

The following statement provides a simple upper bound for $\lambda_1(\Omega)$ and is a discrete version of Lemma 2.3.

Lemma 4.6 *Let Ω be a finite subset of Γ and let $\Omega' \subset \Omega$. If, for some $\rho \geq 1$,*

$$d(\Omega', \complement\Omega) \geq \rho$$

then

$$\lambda_1(\Omega) \leq \frac{1}{\rho^2} \frac{\mu(\Omega)}{\mu(\Omega')}.$$

Proof. Indeed, define a test function $f \in \ell^2(\Omega)$ by $f(x) = d(x, \complement\Omega)$. Then $|\nabla_{xy} f| \leq 1$ for $x \sim y$ and $f(x) \geq \rho$ on Ω' whence we obtain, by (4.2),

$$\lambda_1(\Omega) \leq \frac{\frac{1}{2} \sum_{x,y \in \Gamma} (\nabla_{xy} f)^2 \mu_{xy}}{\sum_{x \in \Gamma} f^2(x) \mu(x)} \leq \frac{\sum_{x \in \Omega} \sum_{y \sim x} \mu_{xy}}{\rho^2 \mu(\Omega')} = \frac{\mu(\Omega)}{\rho^2 \mu(\Omega')},$$

which was to be proved. ∎

Finally, we can state our main result for graphs. Let $\mathcal{V}$ be a positive continuous increasing function on $[1, +\infty)$ whose inverse $\mathcal{V}^{-1}$ is defined on $[\mathcal{V}(1), +\infty)$.

Definition 4.7 *We say that (Γ, μ) admits a* sequence of Følner couples *adapted to $\mathcal{V}$ if there exists a sequence $\{(\Omega'_n, \Omega_n)\}_{n \geq 1}$ of pairs of non-empty finite sets $\Omega'_n \subset \Omega_n$ in Γ such that $v_n := \mu(\Omega_n) \uparrow \infty$ and*

$$\begin{cases} \mu(\Omega'_n) \simeq v_n, & v_n \leq \mathcal{V}(n), \\ \mathcal{V}^{-1}(v_{n+1}) \leq C\mathcal{V}^{-1}(v_n), & d(\Omega'_n, \complement\Omega_n) \geq cn. \end{cases} \tag{4.19}$$

Any individual pair (Ω_n, Ω'_n) from this sequence is called a Følner couple *(see Fig. 3). The function $\mathcal{V}$ is called a* Følner volume function.
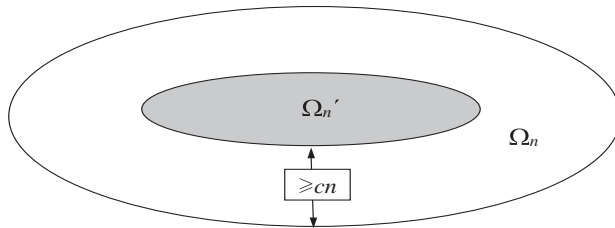

Figure 3 A Følner couple Ω_n, Ω'_n.

Let us introduce some notation for logarithmic derivatives:

$$\mathcal{L}f := \frac{f'}{f} \quad \text{and} \quad \mathcal{L}^2 f := \mathcal{L}(\mathcal{L}f) = \frac{f''}{f'} - \frac{f'}{f}.$$

Theorem 4.8 *Assume that (Γ, μ) admits a sequence of Følner couples adapted to a function $\mathcal{V}$. Assume also that $\mathcal{V} \in C^2(1, +\infty)$, $\mathcal{V}' > 0$, and*

$$-\frac{1}{s} \leq \mathcal{L}^2 \mathcal{V}(s) \leq \frac{C}{s}, \tag{4.20}$$

for all large enough positive s. Define the function γ by

$$t = \int_{\mathcal{V}(1)}^{\gamma(t)} \left[\mathcal{V}^{-1}(v) \right]^2 \frac{dv}{v}. \tag{4.21}$$

Then, for all large enough even integers k,

$$\sup_{x \in \Gamma} p_k(x, x) \geq \frac{c}{\gamma(Ck)}. \tag{4.22}$$

Comparing (4.21) with the formula (7.2) of Corollary 7.2 we see that the Følner volume function $\mathcal{V}(r)$ plays here the same role as the ball volume growth function $V(x, r)$ in the upper bound result (cf. the comments at the end of Remark 2.5). We shall encounter below some situations where the property $\mathcal{V}(r) \asymp V(x, r)$ holds, as well as situations where it does not.

Computation of $\mathcal{L}^2 \mathcal{V}$ for standard functions $\mathcal{V}$ is shown in the table (where α is a positive parameter):

$\mathcal{V}(s) =$	s^α	$\exp(s^\alpha)$	$\exp(\exp(s^\alpha))$	$\log^\alpha s$
$\mathcal{L}^2 \mathcal{V}(s) =$	$-\frac{1}{s}$	$\frac{\alpha-1}{s}$	$\frac{\alpha-1}{s} + \alpha s^{\alpha-1}$	$-\frac{1}{s}\left(1 + \frac{1}{\log s}\right)$
(4.20) holds	for all α	for all α	never	never

For our applications, we will need the functions $\mathcal{V}(s) = Cs^\alpha$ and $\exp(Cs^\alpha)$ for which the hypothesis (4.20) holds.

Example 4.1 If $\mathcal{V}(n) = Cn^D$ then (4.21) yields $\gamma(t) \simeq t^{D/2}$. For example, if the volume growth of (Γ, μ) satisfies $V(x, r) \simeq r^D$ for some $x \in \Gamma$ and all r large enough then we can take $\Omega_n = B(x, 2n)$ and $\Omega'_n = B(x, n)$. Hence, we obtain a sequence of Følner couples adapted to the function $\mathcal{V}(n) = Cn^D$, and the heat kernel satisfies the lower bound (4.22) with $\gamma(t) \simeq t^{D/2}$.

Example 4.2 If $\mathcal{V}(n) = \exp(Cn^\alpha)$, $0 < \alpha \leq 1$, then $\gamma(t) \asymp \exp(t^{\frac{\alpha}{\alpha+2}})$. A particularly important case is $\mathcal{V}(n) = \exp(Cn)$ where we have $\gamma(t) \simeq \exp(t^{1/3})$. Examples of Cayley graphs with such Følner volume functions will be discussed in Section 7.

Proof of Theorem 4.8. We use the notation of Definition 4.7 for the sequence of Følner couples. By Lemma 4.6 and (4.19) we have

$$\lambda_1(\Omega_n) \leq \frac{C}{n^2}. \tag{4.23}$$

By (4.19) we have, if $v_n \geq \mathcal{V}(1)$,

$$n \geq \mathcal{V}^{-1}(v_n) \tag{4.24}$$

whence

$$\lambda_1(\Omega_n) \leq \left(\frac{C}{\mathcal{V}^{-1}(v_n)} \right)^2.$$

Introduce the function

$$\Lambda(v) = \left(\frac{C}{\mathcal{V}^{-1}(v)} \right)^2 \tag{4.25}$$

and observe that the equality (4.7) which defines a function γ on the base of a function Λ can be rewritten as

$$t = \int_{\mathcal{V}(1)}^{\gamma(t)} \frac{dv}{v\Lambda(v)} = c \int_{\mathcal{V}(1)}^{\gamma(t)} \left[\mathcal{V}^{-1}(v)\right]^2 \frac{dv}{v} \qquad (4.26)$$

where we have taken $v_0 = \mathcal{V}(1)$. Therefore, up to a constant multiple of the variable, the function γ we have just defined coincides with the one defined by (4.21), so that it suffices to prove (4.22) with this γ.

The estimate (4.22) will follow from Corollary 4.5 if we show that γ is δ-regular and that

$$\gamma^{-1}(v_{n+1}) \leq C\gamma^{-1}(v_n). \qquad (4.27)$$

We will obtain these properties of γ using the hypothesis (4.20).

The δ-regularity of γ. Denote $\rho = \mathcal{V}^{-1}$. By Lemma 8.1 (see Section 8), γ is δ-regular provided $v\mathcal{L}\rho(v)$ is non-increasing for large v. Taking $v = \mathcal{V}(s)$ we see that

$$v\mathcal{L}\rho(v) = \frac{1}{s\mathcal{L}\mathcal{V}(s)}$$

The hypothesis $\mathcal{L}^2\mathcal{V}(s) \geq -\frac{1}{s}$ implies $(s\mathcal{L}\mathcal{V}(s))' \geq 0$ so that $s\mathcal{L}\mathcal{V}(s)$ increases and hence $v\mathcal{L}\rho(v)$ decreases.

The density condition (4.27). Changing $s = \mathcal{V}^{-1}(v)$ in (4.26) and taking $t = \gamma^{-1}(v_n)$, we obtain

$$\gamma^{-1}(v_n) = c \int_1^{\mathcal{V}^{-1}(v_n)} s^2 \mathcal{L}\mathcal{V}(s)\, ds.$$

Since by (4.19) $\mathcal{V}^{-1}(v_{n+1}) \leq C\mathcal{V}^{-1}(v_n)$, the density condition (4.27) will follow from the following inequality

$$\int_1^{Cr} s^2 \mathcal{L}\mathcal{V}(s)\, ds \leq C' \int_1^r s^2 \mathcal{L}\mathcal{V}(s)\, ds. \qquad (4.28)$$

Observe that if a positive continuous function $f(s)$ satisfies the doubling condition

$$f(2s) \leq Cf(s), \quad \text{for } s \text{ large enough,}$$

then $F(s) = \int_1^s f(u)\, du$ also satisfies this condition. A sufficient condition for f being doubling is:

$$\mathcal{L}f(s) \leq \frac{C}{s},$$

as one can see by integrating between t and $2t$. Since we know by (4.20) that $\mathcal{L}^2\mathcal{V}(s) \leq \frac{C}{s}$, the function $\mathcal{L}\mathcal{V}(s)$ is doubling. This implies that $s^2\mathcal{L}\mathcal{V}(s)$ is also doubling, whence (4.28) follows. $\blacksquare$

We conclude this section by quoting the following result which allows to obtain the heat kernel lower bound directly from the volume growth function.

Proposition 4.9 *Suppose that, for some vertex $x_0 \in \Gamma$ and all r large enough,*

$$V(x_0, r) \leq V(r)$$

where $V(r)$ is a continuous increasing function on $(0, +\infty)$ such that the function

$$r \mapsto \frac{r^2}{\log V(r)} \qquad (4.29)$$

is strictly increasing and going to $+\infty$ as $r \to +\infty$. Denote by $\mathcal{R}(s)$ the inverse function to (4.29). Then, for all large enough even k,

$$p_k(x_0, x_0) \geq \frac{c}{V(\mathcal{R}(Ck))}. \qquad (4.30)$$

The proof of Proposition 4.9 in the setting of manifolds can be found in [11, Theorem 6.1]. Strictly speaking, the proof for the setting of graphs in this form is not written anywhere. For the case of polynomial function $V(r)$, it was proved by Lust-Piquard [27]. Some modification of her method in the spirit of [11] allows to obtain Proposition 4.9 in full generality (see [11, p.160]).

If $V(x_0, r) \leq Cr^D$ then Proposition 4.9 gives $\mathcal{R}(t) \simeq \sqrt{t \log t}$ and

$$p_k(x_0, x_0) \geq c \left(k \log k\right)^{-D/2}.$$

There are examples showing that the factor $\log k$ cannot be eliminated - see [3], [11] and [18]. Let us recall that if $V(x_0, r) \simeq r^D$ then as we have seen in Example 4.1,

$$\sup_x p_k(x, x) \geq ck^{-D/2},$$

which contains no $\log k$.

If $V(x_0, r) \leq \exp(Cr^\alpha)$ where $\alpha \in (0, 1]$ then we obtain $\mathcal{R}(t) \simeq t^{\frac{1}{2-\alpha}}$ and

$$p_k(x_0, x_0) \geq \exp(-Ck^{\frac{\alpha}{2-\alpha}}). \tag{4.31}$$

The exponent $\frac{\alpha}{2-\alpha}$ here is sharp ([11], §8).

5   Discrete groups: some examples

Let G be an infinite finitely generated group and let S be a finite symmetric set of generators of G, not containing the identity element. The couple (G, S) induces a so-called *Cayley graph* Γ. The vertices of Γ are identified with the elements of G, and two vertices $x, y \in \Gamma$ are connected by an edge if $x^{-1}y \in S$ (in particular, G acts simplicially on Γ on the left). Each vertex $x \in \Gamma$ has $|S|$ neighbors in Γ (here $|S|$ is the cardinality of S). Define the weight on Γ by $\mu_{xy} = \frac{1}{|S|}$, for all neighboring vertices x, y. Then the corresponding measure μ on Γ satisfies $\mu(x) \equiv 1$, and $\mu(\Omega) = |\Omega|$.

The random walk associated with μ is the simple random walk on Γ. Clearly, the heat kernel $p_k(x, x)$ *does not depend on x* so that we can set

$$\varphi_\Gamma(k) = p_k(x, x).$$

Hence, lower bounds for $\sup_x p_k(x, x)$ obtained in the previous section, will imply for Cayley graphs lower bounds for $\varphi_\Gamma(k)$.

The purpose of this section is to prove lower estimates for $\varphi_\Gamma(k)$ for Cayley graphs Γ of certain groups G such as Baumslag-Solitar groups and lamplighter groups. We will show how one can directly construct sequences of Følner couples on such groups and hence, obtain the heat kernel lower bounds by Theorem 4.8. More general groups will be treated in Section 7, after introducing tools for constructing sequences of Følner couples.

For the (standard) group theoretic terminology that we use in the sequel we refer for instance to [37].

5.1   Baumslag-Solitar groups

Fix a positive integer q and let $\mathbb{Z}[\frac{1}{q}]$ be the smallest additive subgroup of $\mathbb{Q}$ containing all rational numbers k/q^m with $k, m \in \mathbb{Z}$. Then $\mathbb{Z}$ acts on $\mathbb{Z}[\frac{1}{q}]$ as follows: $a(u) = q^a u$. Hence, the semi-direct product $G = \mathbb{Z}[\frac{1}{q}] \rtimes \mathbb{Z}$ is defined with the group law

$$(u, a)(v, b) = (u + q^a v, a + b) \tag{5.1}$$

(we use here the multiplicative notation for G and the additive notation for $\mathbb{Z}[\frac{1}{q}]$ and $\mathbb{Z}$). The group G is solvable (in fact it is metabelian), but not polycyclic as it contains the non-finitely generated subgroup $\mathbb{Z}[\frac{1}{q}]$. It is generated by the set $S = \left\{X, X^{-1}, Y, Y^{-1}\right\}$ where $X = (0, 1)$ and $Y = (1, 0)$. This can be easily seen from the identities

$$\begin{aligned}
(u, a)X &= (u, a + 1), & (u, a)X^{-1} &= (u, a - 1), \\
(u, a)Y &= (u + q^a, a), & (u, a)Y^{-1} &= (u - q^a, a).
\end{aligned}$$

The group $\mathbb{Z}[\frac{1}{q}] \rtimes \mathbb{Z}$ is isomorphic to the *Baumslag-Solitar group*

$$BS(q) := \langle X, Y : XY = Y^q X \rangle ,$$

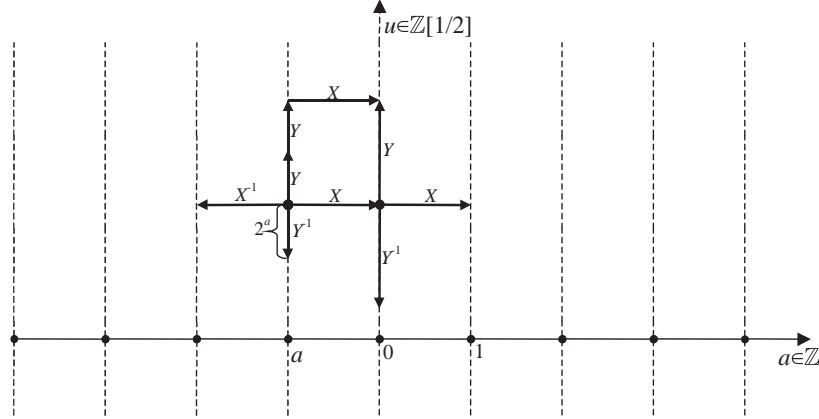and it has exponential volume growth (see [32], chap.8).

Figure 4 The Cayley graph of the group $\mathbb{Z}[\frac{1}{2}] \rtimes \mathbb{Z}$.

The Cayley graph Γ of $BS(2)$ is illustrated by Fig. 4. Each vertical dotted line contains a countable dense set of vertices of Γ. Any vertex on Γ has two horizontal and two vertical edges which correspond to acting by the generators X, X^{-1} and Y, Y^{-1}, respectively.

Theorem 5.1 *The heat kernel on the Cayley graph* $\Gamma = (\mathbb{Z}[\frac{1}{q}] \rtimes \mathbb{Z}, S)$ *admits the estimate*

$$\varphi_\Gamma(k) \asymp \exp(-k^{1/3}) \tag{5.2}$$

for even k.

Credits for this result were given in the introduction.

Proof. The upper bound in (5.2) follows from the fact that G has exponential volume growth and from Corollary 7.4 in Section 7 below. The lower bound will be derived from Theorem 4.8. For all positive integers n and for non-negative $m \le n/2$, define the set $\Omega_{n,m}$ by

$$\Omega_{n,m} = \{(u, a) \in G : m < a < n - m, \ u \text{ is integer and } |u| < (2q)^n - mq^n\}$$
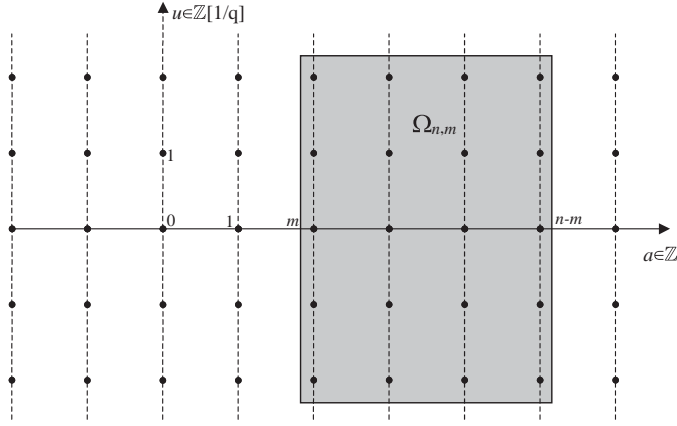
(see Fig. 5).

Figure 5 The set $\Omega_{n,m}$ consists of the integer nodes which fall into the shaded box.

First observe that if $x \in \Omega_{n,m}$ and $y \sim x$ in Γ then $y \in \Omega_{n,m-1}$ provided $m \geq 1$. Indeed, $y = xs$ where s is a generator. If $x = (u, a)$ and $s = (0, \pm 1)$ then

$$y = (u, a \pm 1) \in \Omega_{n,m-1}.$$

If $s = (\pm 1, 0)$ then

$$y = (u \pm q^a, a).$$

Since $u \pm q^a$ is an integer and

$$\left| u \pm q^a \right| \leq |u| + q^a < \left((2q)^n - mq^n \right) + q^n = (2q)^n - (m-1) \, q^n,$$

we see that $y \in \Omega_{n,m-1}$.

Let us take $\Omega_n = \Omega_{n,0}$ and $\Omega'_n = \Omega_{n,n/3}$. As a consequence of the above argument, we obtain

$$d(\Omega'_n, \complement \Omega_n) \geq n/3.$$

On the other hand, it is obvious that

$$|\Omega_n| \simeq n \, (2q)^n, \quad \left| \Omega'_n \right| \simeq n \left((2q)^n - \frac{n}{3} q^n \right)$$

(where $|\Omega|$ is the cardinality of the set Ω). If n is large enough, this implies

$$|\Omega_n| \simeq \left| \Omega'_n \right| \leq Cn \, (2q)^n.$$

Let $\mathcal{V}(s) = Cs \, (2q)^s$. Note that $\mathcal{V}^{-1}(v) \simeq \log v$. One checks easily that $\mathcal{V}$ satisfies conditions (4.19) and (4.20), therefore Theorem 4.8 applies. Hence, computing the function $\gamma(t)$ by (4.21), we obtain $\gamma(t) \asymp \exp(t^{1/3})$, whence the claim follows. ∎

5.2 Lamplighter groups

Let F and A be two groups. Denote by U the set of all functions $u : A \to F$ having finite support[1]. Then U has a natural group structure induced by that of F. The group A acts by left translations on the group U as follows:

$$u^a(x) := u(a^{-1}x).$$

---

[1] The support of a function $u : A \to F$ is defined by $\operatorname{supp} u := \{ x \in A : u(x) \neq \operatorname{Id}_F \}$.

The semi-direct product $G = U \rtimes A$ is defined with the group law

$$(u, a)(v, b) = (uv^a, ab).$$

The group $U \rtimes A$ is called *the wreath product* of F with A and is denoted by $F \wr A$.

Assume now that F and A are finitely generated. Fix some symmetric sets of generators $S_F = \{f_1, f_2, ..., f_n\}$ and $S_A = \{a_1, a_2, ..., a_m\}$ for the groups F and A, respectively. A natural set S of generators of the group $\Gamma = F \wr A$ consists of the following two sequences

$$(\mathrm{Id}_U, a_1),\ (\mathrm{Id}_U, a_2), ..., \ (\mathrm{Id}_U, a_m) \tag{5.3}$$

(where Id_U is the function on A identically equal to Id_F) and

$$(v_1, \mathrm{Id}_A),\ (v_2, \mathrm{Id}_A), ..., \ (v_n, \mathrm{Id}_A), \tag{5.4}$$

where the functions $v_i \in U$ are defined by

$$v_i(x) = \begin{cases} f_i, & x = \mathrm{Id}_A, \\ \mathrm{Id}_F, & x \neq \mathrm{Id}_A. \end{cases} \tag{5.5}$$

The group $G = U \rtimes A$ is called *a lamplighter group*, for the following reason. A vertex a on the Cayley graph $\mathcal{A} = (A, S_A)$ is regarded as the current position of the lamplighter moving on $\mathcal{A}$, whereas the value $u(x) \in F$ describes the current status of a lamp at the point $x \in \mathcal{A}$. Acting by the generators (5.3) corresponds to a move of the lamplighter to a neighboring vertex on $\mathcal{A}$, whereas acting by the generators (5.4) means switching a lamp at the current position a to a neighboring status.

A typical example of a wreath product is $\mathbb{Z}_2 \wr \mathbb{Z}^D$. The group law of $G = \mathbb{Z}_2 \wr \mathbb{Z}^D$ is given by

$$(u, a)(v, b) = (u + v(\cdot - a),\ a + b).$$

The generating set S consists of the $2D + 1$ elements

$$(0, \pm e_1), (0, \pm e_2), ..., (0, \pm e_D), (\delta(x), 0),$$

where $\{e_i\}$ is the canonical basis in $\mathbb{Z}^D$ and $\delta(x)$ is the $\mathbb{Z}_2$-valued delta-function on $\mathbb{Z}^D$ taking the value 1 at $0 \in \mathbb{Z}^D$, and 0 otherwise. In this case, the lamplighter moves on the nodes of $\mathbb{Z}^D$, and a lamp at each node may be either ON or OFF (see Fig. 6).
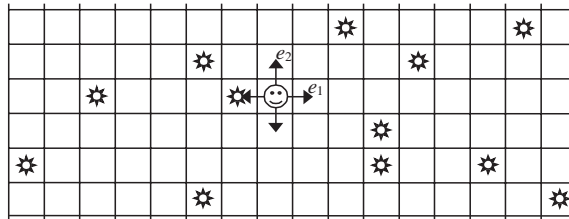

Figure 6 Lamplighter group $\mathbb{Z}_2 \wr \mathbb{Z}^2$.

The next theorem is our main result for wreath products.

Theorem 5.2 *Let F be a finite group and A be a finitely generated group with polynomial volume growth of degree $D > 0$. Then the heat kernel on the Cayley graph $\Gamma = (F \wr A, S)$ admits the following lower bound*

$$\varphi_\Gamma(k) \geq \exp(-Ck^{\frac{D}{D+2}}), \tag{5.6}$$

for all even k.

For the case $A = \mathbb{Z}^D$, the estimate (5.6) was proved in [33, Theorem 7.1] as well as a matching upper bound for $\varphi_\Gamma(k)$ (see also [25], [42] for earlier results). In the setting of Theorem 5.2, the base A may be nilpotent, in which case no matching upper bound for $\varphi_\Gamma(k)$ seems to be known.

Proof. The proof is similar to the one of Theorem 5.1. Denote by $B_A(r)$ the ball in $\mathcal{A}$ of radius r centered at Id_A, and define the sets $\Omega_{n,m}$ by

$$\Omega_{n,m} = \{(u,a) \in G : a \in B_A(n-m) \text{ and } \operatorname{supp} u \subset B_A(n)\}$$
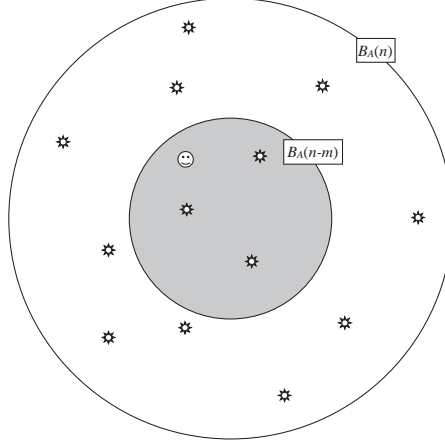
(see Fig. 7).

Figure 7 The set $\Omega_{n,m}$: the lamplighter is inside the ball $B_A(n-m)$, and the lamps may be "ON" only inside the ball $B_A(n)$.

We claim that if $x \in \Omega_{n,m}$ and $y \sim x$ then $y \in \Omega_{n,m-1}$. Indeed, let $y = xs$ where s is a generator. If $x = (u,a)$ and $s = (\mathrm{Id}_U, a_i)$ then

$$y = (u,a)(\mathrm{Id}_U, a_i) = (u, aa_i).$$

Since $aa_i \in B(n-m+1)$, we see that $y \in \Omega_{n,m-1}$. If $s = (v_i, \mathrm{Id}_A)$ then we have

$$y = (u,a)(v_i, \mathrm{Id}_A) = (uv_i^a, a).$$

Note that v_i has support at a single point Id_A. Hence, $\operatorname{supp} v_i^a$ is a single point a. Since $\operatorname{supp} u \subset B_A(n)$ and $a \in B_A(n)$, we see that

$$\operatorname{supp} uv_i^a \subset B_A(n)$$

whence $y \in \Omega_{n,m-1}$.

As in Theorem 5.1, we set $\Omega_n = \Omega_{n,0}$ and $\Omega'_n = \Omega_{n,n/2}$, which yields $d(\Omega'_n, \complement\Omega_n) \geq n/2$. We are left to compute $|\Omega_n|$ and $|\Omega'_n|$. Denote by $V_A(r)$ the cardinality of the ball $B_A(r)$ and observe that the number of distinct functions u supported in $B_A(r)$ is equal to $|F|^{V_A(r)}$. Therefore,

$$|\Omega_{n,m}| = V_A(n-m) \, |F|^{V_A(n)}.$$

Since the function $V_A(r)$ is polynomial, we obtain for some $C, D > 0$

$$|\Omega_n| \simeq |\Omega'_n| \simeq V_A(n) \, |F|^{V_A(n)} \simeq n^D \exp\left(Cn^D\right) \leq \exp\left(C'n^D\right).$$

Clearly, the function $\mathcal{V}(s) = \exp\left(C's^D\right)$ satisfies the conditions of Theorem 4.8. Since $\mathcal{V}^{-1}(v) \simeq (\log v)^{1/D}$, we compute by (4.21) $\gamma(t) \asymp \exp(t^{\frac{D}{D+2}})$ whence (5.6) follows. ∎

6 Contractions of graphs

Let Γ and $\mathcal{A}$ be two graphs. We say that $\mathcal{A}$ is a *contraction* of Γ if there is a surjection $\pi : \Gamma \to \mathcal{A}$ such that if $x, y \in \Gamma$ and $x \sim y$ then either $\pi(x) = \pi(y)$ or $\pi(x) \sim \pi(y)$. For each $a \in \mathcal{A}$, denote $\Gamma_a = \pi^{-1}(a)$. Then Γ is the union of all *fibres* Γ_a as a runs over $\mathcal{A}$. If two vertices x, y are neighbors in Γ then they either lie in the same fibre or in neighboring fibres (see Fig. 8).
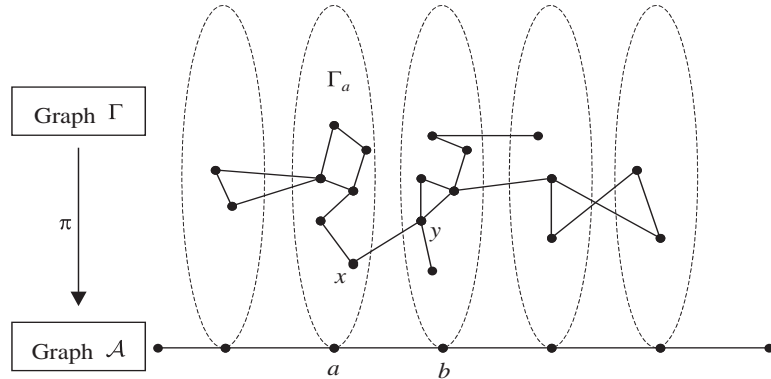

Figure 8 A contraction $\mathcal{A}$ of the graph Γ

Given a graph, we call a *norm* any function on this graph taking values in $[0, +\infty]$. Suppose that two graphs $\mathcal{A}$ and Γ as above are endowed with norms $|\cdot|$ and $\|\cdot\|$, respectively. Assume that the norm on $\mathcal{A}$ satisfies the following property:

(LT) The local triangle inequality: if $a, b \in \mathcal{A}$ and $a \sim b$ then

$$|b| \leq |a| + 1. \tag{6.1}$$

In the applications below, $|\cdot|$ will be defined as a graph distance to a fixed vertex or a subset of $\mathcal{A}$ so that (6.1) will be automatically true.

The following hypothesis relates the norm in Γ to the one in $\mathcal{A}$. Fix a subset $\mathcal{A}_* \subset \mathcal{A}$.

(DT) There exists a positive number β with the following property: for all $x, y \in \Gamma$ such that $x \sim y$,

$$\|y\| \leq \|x\| + \beta^{|\pi(x)|}, \tag{6.2}$$

provided $\pi(x) \in \mathcal{A}_*$.

Here (DT) stands for "Distortion" and "Triangle" because in the setting of groups in Section 7, (DT) will be deduced from a distortion condition for semi-direct products and from a triangle inequality. In most applications, the set $\mathcal{A}_*$ coincides with $\mathcal{A}$, in which case the condition $\pi(x) \in \mathcal{A}_*$ may be discarded. Of course, (DT) is always valid if $\mathcal{A}_*$ is empty but no interesting result can be obtained in this case. Examples with a non-trivial $\mathcal{A}_*$ will be considered in Section 7.4.

Let us introduce another norm on $\mathcal{A}$ by

$$|a|_* = d_{\mathcal{A}}(a, \complement \mathcal{A}_*)$$

where $d_{\mathcal{A}}$ is the graph distance on $\mathcal{A}$. If $\mathcal{A}_* = \mathcal{A}$ then $\complement \mathcal{A}_*$ is empty and $|a|_* \equiv +\infty$. Note that $|a|_* > 0$ is equivalent to $a \in \mathcal{A}_*$.

Let us define the balls $B_a(r)$ in Γ_a and the truncated balls $B_A(r, \rho)$ in $\mathcal{A}$ as follows:

$$B_a(r) = \{x \in \Gamma_a : \|x\| < r\} \quad \text{and} \quad B_A(r, \rho) = \{a \in \mathcal{A} : \rho < |a|_*, \ |a| < r\}. \tag{6.3}$$
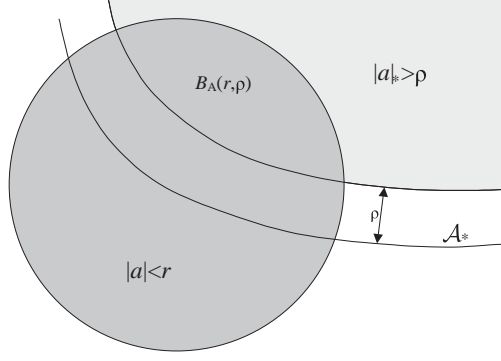
Figure 9 The truncated ball $B_A(r, \rho)$ on $\mathcal{A}$ is the intersection of the sets $\{|a| < r\}$ and $\{|a|_* > \rho\}$.

If $\mathcal{A}_* = \mathcal{A}$ then $B_A(r, \rho)$ is independent of ρ:

$$B_A(r, \rho) = B_A(r) = \{a \in \mathcal{A} : |a| < r\}. \tag{6.4}$$

We say that a function $f(r)$ is *doubling* if, for all r large enough,

$$f(r/2) \geq cf(r). \tag{6.5}$$

Let us introduce the following volume hypothesis.

(W) There exist positive increasing functions $V_A(r)$ and $V_\perp(r)$ on $(0, +\infty)$, such that, for r large enough,

$$V_A(r) \simeq \#B_A(r, 0) \simeq \#B_A(r, \varepsilon r), \tag{6.6}$$

for some $\varepsilon > 0$, and

$$V_\perp(r) \simeq \#B_a(r) \quad \forall a \in \mathcal{A}. \tag{6.7}$$

Moreover, both $V_\perp(r)$ and $V_A(r)$ are doubling.

If $\mathcal{A}_* = \mathcal{A}$ then the condition (6.6) simplifies as follows:

$$V_A(r) \simeq \#B_A(r).$$

The next theorem is our main result for graphs which admit a contraction.

Theorem 6.1 *Let Γ be an infinite connected locally finite graph, and let $\mathcal{A}$ be a contraction of Γ. Suppose that there are norms on Γ and $\mathcal{A}$ satisfying (LT), (DT) and (W). Assume also that the graph Γ is equipped with a weight μ such that, for all $x \in \Gamma$,*

$$\mu(x) \simeq 1. \tag{6.8}$$

Then the heat kernel of the weighted graph (Γ, μ) satisfies the estimate

$$\sup_{x \in \Gamma} p_k(x, x) \geq \exp(-Ck^{1/3}), \tag{6.9}$$

for all large enough even k.

Examples of applications of Theorem 6.1 will be given in Section 7. The proof of Theorem 6.1 uses Theorem 4.8, for which we need to construct on Γ a sequence of Følner couples Ω'_n, Ω_n satisfying (4.19). The contraction procedure will enable us to construct them as certain cylindrical sets in Γ.

Let us define the following two-parameter family of sets

$$\Omega_{n,m} = \{x \in \Gamma : m < |\pi(x)|_*, \ |\pi(x)| < n - m \text{ and } \|x\| < \alpha^n - m\beta^n\}, \qquad (6.10)$$

where $n \in \mathbb{N}$ and $0 \le m < n$. Here we choose $\alpha > \beta > 1$ so that, for all $n \in \mathbb{N}$,

$$\alpha^n \ge 2n\beta^n. \qquad (6.11)$$

The set $\Omega_{n,m}$ can be regarded as a cylinder in Γ with base $B_A(n-m,m)$ and "height" $\alpha^n - m\beta^n$ (see Fig. 10).
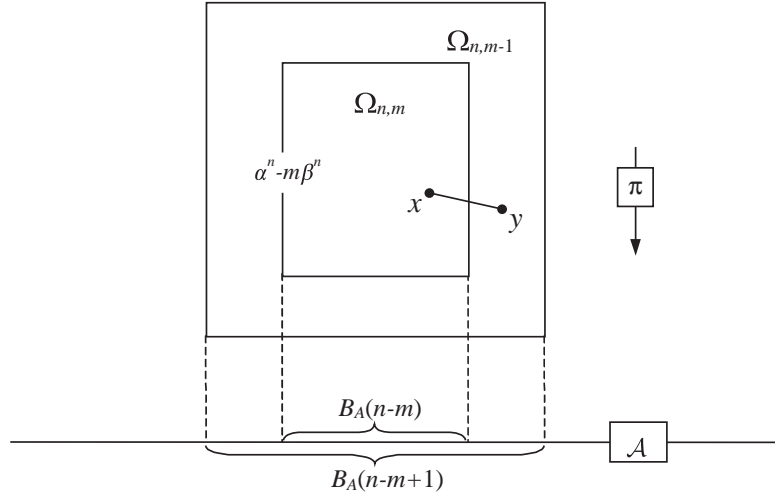

Figure 10 The sets $\Omega_{n,m}$ and $\Omega_{n,m-1}$ in Γ.

Lemma 6.2 *If* $x \in \Omega_{n,m}$ *and* $y \sim x$ *then* $y \in \Omega_{n,m-1}$ *provided* $1 \le m < n$.

Proof. Since $y \sim x$, we have either $\pi(y) = \pi(x)$ or $\pi(y) \sim \pi(x)$. As follows from the hypothesis (LT) and definition (6.10) of $\Omega_{n,m}$,

$$|\pi(y)| \le |\pi(x)| + 1 < n - (m - 1)$$

and

$$|\pi(y)|_* \ge |\pi(x)|_* - 1 > m - 1.$$

Observe that $|\pi(x)|_* > m > 0$ implies $\pi(x) \in \mathcal{A}_*$. Hence, we can apply (DT) and obtain

$$\|y\| \le \|x\| + \beta^{|\pi(x)|} < (\alpha^n - m\beta^n) + \beta^n = \alpha^n - (m-1)\beta^n,$$

whence $y \in \Omega_{n,m-1}$. ∎

Lemma 6.3 *There exists* $\varepsilon > 0$ *such that, for all* n *large enough and* $0 \le m \le \varepsilon n$,

$$\#\Omega_{n,m} \simeq V_\perp(\alpha^n)V_A(n). \qquad (6.12)$$

Consequently,

$$\#\Omega_{n,\varepsilon n} \simeq \#\Omega_{n,0}. \qquad (6.13)$$

Proof. As follows from definitions (6.10) of $\Omega_{n,m}$ and (6.3) of B_a,

$$\#\Omega_{n,m} = \sum_{m<|a|_*,\,|a|<n-m} \#B_a(\alpha^n - m\beta^n).$$

Together with (6.7), this implies

$$\#\Omega_{n,m} \simeq V_\perp(\alpha^n - m\beta^n)\#B_A(n-m,m).$$

If n is large enough and $m \leq \varepsilon n$ for small enough $\varepsilon > 0$, then we obtain, by (6.6) and the doubling property of V_A,

$$\#B_A(n-m,m) \simeq V_A(n-m) \simeq V_A(n)$$

whence

$$\#\Omega_{n,m} \simeq V_\perp(\alpha^n - m\beta^n)V_A(n). \tag{6.14}$$

Finally, we have by (6.11)

$$\alpha^n - m\beta^n \geq \alpha^n - n\beta^n \geq \frac{\alpha^n}{2},$$

so that (6.12) follows from (6.14) by the doubling property of $V_\perp$. ∎

Lemma 6.4 *If n is large enough and $0 \leq m \leq \varepsilon n$ then*

$$d(\Omega_{n,m}, \complement\Omega_{n,0}) > m.$$

Proof. As follows from Lemma 6.3, if n is large enough and $0 \leq m \leq \varepsilon n$ then $\Omega_{n,m}$ is non-empty and finite. Since Γ is infinite and $\Omega_{n,0}$ is finite, $\complement\Omega_{n,0}$ is non-empty. Choose points x and y so that $x \in \Omega_{n,m}$ and $y \notin \Omega_{n,0}$. Then it suffices to show that $d(x,y) > m$. Let x and y be connected by a path of length k

$$x = x_0 \sim x_1 \sim ... \sim x_k = y.$$

Suppose that $k \leq m$. By Lemma 6.2, we obtain $x_1 \in \Omega_{n,m-1}$, $x_2 \in \Omega_{n,m-2}$, ..., and $y \in \Omega_{n,m-k}$. Hence $y \in \Omega_{n,0}$, which contradicts the choice of y. Therefore, $k > m$ and $d(x,y) > m$. ∎

Proof of Theorem 6.1. As Theorem 4.8 says, in order to estimate the heat kernel on Γ from below, it suffices to construct a sequence of Følner couples $\{\Omega'_n, \Omega_n\}$, that is, sets $\Omega'_n \subset \Omega_n$ such that $v_n := \mu(\Omega_n) \uparrow +\infty$ and

$$\mu(\Omega'_n) \simeq v_n, \quad v_n \leq \mathcal{V}(n), \quad \mathcal{V}^{-1}(v_{n+1}) \leq C\mathcal{V}^{-1}(v_n), \quad d(\Omega'_n, \complement\Omega_n) \geq cn, \tag{6.15}$$

with a function $\mathcal{V}$, which is C^2 and with C^1 inverse, satisfying the regularity condition (4.20Then the function $\mathcal{V}(n)$ determines the lower bound for $\sup_x p_k(x,x)$.

Let us take

$$\Omega_n = \Omega_{n,0} \quad \text{and} \quad \Omega'_n = \Omega_{n,\varepsilon n},$$

where ε is determined by Lemma 6.3. By Lemma 6.4, we have $d(\Omega'_n, \complement\Omega_n) \geq \varepsilon n$. By Lemma 6.3 and hypothesis (6.8),

$$\mu(\Omega'_n) \simeq \mu(\Omega_n) \simeq V_\perp(\alpha^n)V_A(n).$$

The doubling hypothesis in condition (W) imply that, for r large enough, $V_\perp(r) \leq Cr^C$ and $V_A(r) \leq Cr^C$ whence, for C large enough,

$$\mu(\Omega_n) \leq \exp(Cn) := \mathcal{V}(n).$$

We are left to verify the third condition in (6.15) which amounts to

$$\log v_{n+1} \leq C \log v_n. \tag{6.16}$$

Since $v_n \simeq V_\perp(\alpha^n)V_A(n)$, (6.16) follows from the doubling property of $V_\perp$ and V_A.

Finally, with the function $\mathcal{V}(n) = \exp(Cn)$, Theorem 4.8 yields the lower bound (6.9). ∎

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7 Discrete groups: a general method

The main result of this section is Theorem 7.5 which generalizes the heat kernel estimates obtained in Section 5. While in Section 5 we directly constructed Følner couples on certain groups and applied Theorem 4.8, in the present section we will use the machinery of graph contraction based on Theorem 6.1. Applications of Theorem 7.5 for concrete groups are presented in Theorems 7.9 and 7.8.

We use the same notation as in Section 5.

7.1 Heat kernel and volume growth on groups

Let us first recall how one obtains heat kernel upper bounds on a Cayley graph Γ via its volume growth. We say that the graph (Γ, μ) admits the *isoperimetric inequality* with function I if, for all finite sets Ω,

(Iso) $\mu(\partial\Omega) \geq I(\mu(\Omega))$,

where

$$\partial\Omega = \{x \in \Omega : x \sim y \text{ for some } y \notin \Omega\}.$$

Recall that $B(x, r)$ denotes balls on Γ and that $V(x, r) = \mu(B(x, r))$. Since $V(x, r)$ does not depend on x, we denote

$$V(k) = V(x, k)$$

for $k \in \mathbb{N}$, and extend V to $\mathbb{R}_+^*$ by linearity. In this way V is a continuous strictly increasing function.

Proposition 7.1 *([13, Theorem 4]) Let Γ be the Cayley graph of a an infinite finitely generated group G. Then Γ admits the isoperimetric inequality (Iso) with function*

$$I(v) := \frac{cv}{V^{-1}(Cv)}.$$

Combining Propositions 7.1 and 4.1 with a discrete version of Cheeger's inequality (see [7], [8, Proposition 7.1], [15]), we obtain the following.

Corollary 7.2 *Under the assumptions of Proposition 7.1, the Cayley graph Γ admits the Faber-Krahn inequality (FK) with function*

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

Consequently, we have, for all $k \in \mathbb{N}$,

$$\varphi_\Gamma(k) \leq \frac{C}{\gamma(ck)} \tag{7.1}$$

where γ is defined by

$$t = \int_1^{\gamma(t)} \left[V^{-1}(v)\right]^2 \frac{dv}{v}. \tag{7.2}$$

Corollary 7.3 *Assume that the volume growth on a Cayley graph Γ is polynomial:*

$$V(r) \simeq r^D. \tag{7.3}$$

Then, for even k,

$$\varphi_\Gamma(k) \simeq k^{-D/2}. \tag{7.4}$$

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Proof. The upper bound in (7.4) is implied by Corollary 7.2 whereas the lower bound follows from Theorem 4.8. Indeed, as was explained in Example 4.1, (7.3) implies, for arbitrary weighted graphs,

$$\sup_{x \in \Gamma} p_k(x,x) \geq ck^{-D/2}.$$

Since for Cayley graphs $\varphi_\Gamma(k) = \sup_{x \in \Gamma} p_k(x,x)$, the lower bound in (7.4) follows. ■

Recall that by a theorem of Gromov, among finitely generated groups, the class of those with polynomial growth coincides with the class of virtually nilpotent groups. It seems that the above argument is the simplest known method to obtain the on-diagonal estimates (7.4) of the heat kernel on such groups. Recall that the upper bound is originally due to Varopoulos (see [47]). The lower bound is stated with hints in [41]. One can find a complete proof in [23].

As a consequence of Corollary 7.3 and Corollary 7.2 we see that the simple random walk on a Cayley graph Γ is recurrent if and only if it has polynomial volume growth with exponent $D \leq 2$ (see [42] and the discussion in [17, p.199]). This is a way to obtain very easily the crucial step of the proof of Kesten's conjecture (see [48, I.3.B] for more information).

Corollary 7.4 *Let $\alpha, \beta \in (0,1]$. If a Cayley graph Γ satisfies, for all r large enough,*

$$V(r) \leq \exp\left(Cr^\alpha\right)$$

then, for all even $k \in \mathbb{N}$,

$$\varphi_\Gamma(k) \geq \exp(-Ck^{\frac{\alpha}{2-\alpha}}). \tag{7.5}$$

If, for all large enough r,

$$V(r) \geq \exp\left(cr^\beta\right),$$

then, for all $k \in \mathbb{N}$,

$$\varphi_\Gamma(k) \leq \exp(-ck^{\frac{\beta}{2+\beta}}). \tag{7.6}$$

Indeed, the upper bound (7.6) follows from Corollary 7.2 and the lower bound (7.5) from Proposition 4.9. [2]

Note, that the lower and upper bounds (7.5) and (7.6) *do not match* even if $\alpha = \beta$. For example, if $\alpha = \beta = 1$ then

$$\exp\left(-Ck\right) \leq \varphi_\Gamma(k) \leq \exp(-ck^{1/3}). \tag{7.7}$$

Both upper and lower bounds here are sharp in the sense that information about the volume growth of balls cannot imply more. Indeed, the lower bound in (7.7) is attained for non-amenable groups whereas the upper bound is attained for polycyclic groups with exponential growth. The lower bound is also sharp for amenable groups, since, as we already mentioned, there are groups with exponential volume growth for which the heat kernel decays as $\exp(-ck^\alpha)$ with $\alpha \in (0,1)$, and α can be taken arbitrarily close to 1 ([33, Theorem 7.1]).

It is not surprising that one does not get in general sharp information about the heat kernel from the volume growth function. The point is that on amenable groups with exponential growth balls are far from being the level sets of the heat kernel, and one needs to look at different sets, too.

We will apply Theorem 6.1 to obtain sharp lower bounds of the heat kernel on certain Cayley graphs. Theorem 6.1 is particularly well-adapted to the case when the group G is a semi-direct product. Indeed, this structure allows to define in a natural way a contraction of the Cayley graph Γ of G.

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[2]If we knew that $V(r) \simeq \exp\left(Cr^\alpha\right)$ then the lower bound (7.5) could also be obtained by Theorem 4.8 similarly to Corollary 7.3 and Example 4.1. However, normally for groups and graphs one cannot have such a sharp information about the volume growth.

7.2 Semi-direct products

Suppose that G is a semi-direct product of two groups A and U, which we denote by $G = U \rtimes A$. This means that there is a group morphism from A to the group of automorphisms of U, called the action. The action of $a \in A$ on $u \in U$ is denoted by $a(u)$ or u^a. Then G is defined as the set of pairs (u, a), $u \in U$, $a \in A$, the group law being given by

$$(u, a)(v, b) = (uv^a, ab).$$

Both U and A can be identified with subgroups of G in an obvious way, and U is a normal subgroup.

Assume that G is finitely generated, and let $S = \{(v_i, a_i)\}$ be a finite symmetric set of generators of G, not containing the identity element of G. Denote

$$S_U = \{v_i\} \setminus \{\mathrm{Id}_U\} \quad \text{and} \quad S_A = \{a_i\} \setminus \{\mathrm{Id}_A\}.$$

Then S_A is a finite symmetric set of generators of A.

In general, S_U does not generate U. In fact, U need not be finitely generated. However, if U is finitely generated, then one may choose some finite symmetric sets of generators S_U in U and S_A in A, and define a generating set S in G by

$$S = (S_U \times \{\mathrm{Id}_A\}) \cup (\{\mathrm{Id}_U\} \times S_A).$$

Denote by Γ the Cayley graph (G, S) and by $\mathcal{A}$ the Cayley graph (A, S_A). Then $\mathcal{A}$ can be considered as a contraction of Γ (see Section 6) with the projection $\pi : \Gamma \to \mathcal{A}$ defined by

$$\pi(u, a) = a. \tag{7.8}$$

The projection π is a homomorphism, and the fibres Γ_a of π are the classes aU.

Suppose that we are given norms $|\cdot|$ on A and $\|\cdot\|$ on U. By a norm we simply mean a function on a group with values in $[0, +\infty]$, with no a priori assumptions. Let us introduce some further hypotheses.

(A) The norm $|\cdot|$ on A satisfies the *local triangle inequality*: if $a \sim b$ then

$$|b| \le |a| + 1.$$

(T) The norm $\|\cdot\|$ on U satisfies the *triangle inequality:* for all $u, v \in U$,

$$\|uv\| \le \|u\| + \|v\|. \tag{7.9}$$

(D) The *distortion* condition: there is a positive number β and a subset $A_* \subset A$ such that

$$\|v^a\| \le \beta^{|a|}, \tag{7.10}$$

for all $v \in S_U$ and $a \in A_*$.

A typical example of a norm $|\cdot|$ on A is the *distance norm*, that is the distance in the Cayley graph $\mathcal{A}$ to the identity element. If the group U is finitely generated then $\|\cdot\|$ can also be defined as a distance norm, which obviously satisfies (T). If U is not finitely generated, one still can choose a finitely generated subgroup $U_* \subset U$, define a distance norm on U_* and extend it by $+\infty$ outside U_*. The resulting norm satisfies (T) as well.

Condition (D) relates the norms in A and U to the structure of the semi-direct product $U \rtimes A$. To some extent, the number β says how "distorted" is $U \rtimes A$ compared to the direct product $U \times A$. In most applications we have $A_* = A$ in which case (7.10) should be true for all $a \in A$.

Example 7.1 Consider the following class of (polycyclic) groups. Let $U = \mathbb{Z}^D$ and $A = \mathbb{Z}$. Define the action of $a \in A$ on $u \in U$ by

$$u^a = T^a u,$$

where T is any $D \times D$ matrix with integer entries such that T^{-1} also has integer entries. Here we regard u as a vector in $\mathbb{R}^D$.

Define $|\cdot|$ and $\|\cdot\|$ as the Euclidean norms in $\mathbb{Z}$ and $\mathbb{Z}^D$, and let S_A and S_U be canonical generating sets in $\mathbb{Z}$ and $\mathbb{Z}^D$, respectively. Conditions (A) and (T) are obviously true. For all $v \in \mathbb{Z}^D$ and $a \in \mathbb{Z}$, we have

$$\|v^a\| = \|T^a v\| \le \beta^{|a|} \|v\|,$$

where β^2 is the maximal eigenvalue of the matrix T^*T, whence (D) follows (with $A_* = A$).

Returning to the general case, define another norm on A by

$$|a|_* = d_{\mathcal{A}}(a, \complement A_*)$$

where $d_{\mathcal{A}}$ is the graph distance on $\mathcal{A}$; if $A_* = A$, set $|a|_* = +\infty$. Obviously, $|\cdot|_*$ satisfies the local triangle inequality.

Let us introduce notation for balls and truncated balls associated with the norms in U and A, respectively:

$$B_U(r) := \{u \in U : \|u\| < r\} \quad \text{and} \quad B_A(r, \rho) := \{a \in A : \rho < |a|_*, \, |a| < r\}. \tag{7.11}$$

Consider the following hypothesis.

(V) There exist increasing functions $V_A(r)$ and $V_U(r)$ on $(0, +\infty)$, which are positive for large enough r and satisfy the conditions

$$V_A(r) \simeq \#B_A(r, 0) \simeq \#B_A(r, \varepsilon r), \tag{7.12}$$

for some $\varepsilon > 0$, and

$$V_U(r) \simeq \#B_U(r). \tag{7.13}$$

Moreover, both functions V_A and V_U are doubling (cf. (6.5)).

If $A_* = A$ then (7.12) can be simplified so as to match (7.13):

$$V_A(r) \simeq \#B_A(r)$$

where

$$B_A(r) = \{a \in A : |a| < r\}. \tag{7.14}$$

The main result of this section is the following theorem.

Theorem 7.5 *Let $G = U \rtimes A$ be an infinite finitely generated group and let Γ be its Cayley graph. Assume that A and U admit norms which satisfy the hypotheses (A), (T), (D), (V). Then the heat kernel on Γ admits the following lower bound*

$$\varphi_\Gamma(k) \ge \exp(-Ck^{1/3}), \tag{7.15}$$

for all even k.

Remark 7.1 If the volume growth of Γ is exponential, then the matching upper bound for the heat kernel is given by Corollary 7.4 so that we obtain

$$\varphi_\Gamma(k) \asymp \exp(-k^{1/3}).$$

Proof. We deduce the claim from Theorem 6.1. The hypothesis (LT) of Theorem 6.1 follows from (A). Extend the norm on U to one on G as follows:

$$|||(u,a)|||_G = \|u\|. \tag{7.16}$$

Let us show that Γ and its contraction $\mathcal{A}$ satisfy the hypothesis (DT) of Theorem 6.1. If $x, y \in \Gamma$ and $x \sim y$ then $s := x^{-1}y \in S$. Let $x = (u, a)$ and $s = (v, b)$ where $v \in S_U$ or $v = \mathrm{Id}_U$. Assuming that $\pi(x) \in \mathcal{A}_* := A_*$, we have $a \in A_*$. Since $y = xs = (uv^a, ab)$, we obtain, by (T) and (D),

$$|||y||| = \|uv^a\| \leq \|u\| + \|v^a\| \leq |||x||| + \beta^{|a|},$$

which settles (DT) for the case $v \in S_U$. If $v = \mathrm{Id}_U$ then we have

$$|||y||| = \|uv^a\| = \|u\| = |||x|||$$

so that (DT) holds again.

Finally, (V) implies the hypothesis (W) of Theorem 6.1. Therefore, Theorem 6.1 applies and yields the claim. ∎

7.3 Constructing norms using subgroups

Let (A, S_A) be a Cayley graph of a group A. Assume that there is a semigroup $A_* \subset A$ containing Id_A and generated by a finite set S_{A_*}. Let us introduce in A_* the distance to the identity element as follows

$$d_{A_*}(a, \mathrm{Id}_A) = \min\{m : a = c_1 c_2 \ldots, c_m, \ c_1, c_2, \ldots, c_m \in S_{A_*}\}$$

(in general, $d_{A_*}(a, b)$ is not defined for arbitrary $a, b \in A_*$). Consider also balls in A_*

$$B_{A_*}(r) = \{a \in A_* : d_{A_*}(a, \mathrm{Id}_A) < r\}$$

and truncated balls

$$B_{A_*}(r, \rho) = B_{A_*}(r) \cap \{a \in A_* : d_A(a, \complement A_*) > \rho\}.$$

We say that A_* has polynomial volume growth of degree D if, for some $\varepsilon > 0$ and all r large enough,

$$\#B_{A_*}(r) \simeq \#B_{A_*}(r, \varepsilon r) \simeq r^D$$

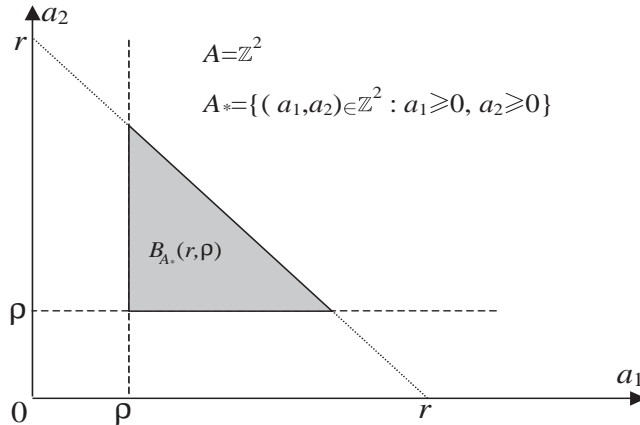(see Fig. 11). Here d_A denotes the graph distance on (A, S_A).

Figure 11 The semigroup A_* has polynomial volume growth of degree 2.

The following statement provides some way of constructing norms satisfying the hypotheses (A), (T), (D), (V).

Corollary 7.6 *Let $G = U \rtimes A$ be a finitely generated group, and S be a finite symmetric set of generators of G not containing the identity. Assume that the following conditions hold:*

(i) There is a finitely generated semigroup $A_* \subset A$ containing Id_A and such that

$$d_{A_*}(a, \mathrm{Id}_A) = d_A(a, \mathrm{Id}_A), \ \forall a \in A_* \tag{7.17}$$

where d_{A_*} is related to a finite set S_{A_*} of generators of A_*.

(ii) There is a finitely generated subgroup $U_* \subset U$ such that

$$S_U \subset U_*$$

and U_* is stable under the action of A_*, that is

$$a(U_*) \subset U_* \quad \forall a \in A_*. \tag{7.18}$$

(iii) The group U_* and the semigroup A_* both have polynomial volume growth.

Then the heat kernel on $\Gamma = (G, S)$ satisfies the estimate

$$\varphi_\Gamma(k) \geq \exp(-Ck^{1/3}),$$

for all even k.

Proof. Let S_{U_*} be a finite symmetric set of generators of U_* not containing Id_U. Since $U_* \supset S_U$, we may assume without loss of generality $S_{U_*} \supset S_U$. Define a norm $|a|$ on A by

$$|a| = d_A(a, \mathrm{Id}_A)$$

and a norm $\|\cdot\|$ on U by

$$\|u\| = \begin{cases} d_{U_*}(u, \mathrm{Id}_U), & u \in U_* \\ +\infty, & u \notin U_* \end{cases}$$

where d_{U_*} is the graph distance on (U_*, S_{U_*}). Obviously, hypotheses (A), (T) and (V) of Theorem 7.5 are satisfied.

To prove hypothesis (D), it suffices to show that, for all $v \in S_{U_*}$ and $a \in A_*$

$$\|v^a\| \leq \beta^{|a|}, \tag{7.19}$$

with some number β. First observe that $\|v^a\| < +\infty$ because $v \in U_*$ and hence $v^a \in U_*$. If $a \in S_{A_*}$ then (7.19) holds for

$$\beta = \max_{a \in S_{A_*}, v \in S_{U_*}} \|v^a\|.$$

Before we prove (7.19) for all $a \in A_*$, let us first verify that, for any $c \in S_{A_*}$ and any $u \in U_*$,

$$\|u^c\| \leq \beta\|u\|. \tag{7.20}$$

If $u \in S_{U_*}$ then this follows from the definition of β. If $\|u\| > 1$, write $u = vw$ where $w \in S_{U_*}$ and $\|v\| = \|u\| - 1$. Hence, by the triangle inequality and the inductive hypothesis,

$$\|u^c\| = \|v^c w^c\| \leq \|v^c\| + \|w^c\| \leq \beta\|v\| + \beta = \beta\|u\|.$$

Now we prove (7.19) for arbitrary $a \in A_*$ by induction on $|a|$. If $|a| = 1$ then, again, this follows from the definition of β. Assume $|a| > 1$. By the hypothesis (7.17), $|a| = d_{A_*}(a, \mathrm{Id}_A)$. Hence, a can be represented as $a = cb$ where $b \in A_*$, $c \in S_{A_*}$, and $|b| = |a| - 1$. By (7.20) and by the inductive hypothesis, we obtain

$$\|v^a\| = \|(v^b)^c\| \leq \beta\|v^b\| \leq \beta\beta^{|b|}\|v\| = \beta^{|a|}\|v\|.$$

∎

7.4 Some semi-direct products related to homotheties

The main result of this section is Theorem 7.8 that can be regarded as an application of Corollary 7.6. Let D be a positive integer and $\lambda = (\lambda_1, ..., \lambda_D) \in \mathbb{R}^D$ so that all components $\lambda_i \neq 0$. Then $\mathbb{Z}^D$ acts on $\mathbb{R}$ by homotheties

$$a(u) := \lambda^a u \tag{7.21}$$

where $a = (a_1, ..., a_D) \in \mathbb{Z}^D$, $u \in \mathbb{R}$ and

$$\lambda^a := \lambda_1^{a_1} \lambda_2^{a_2} ... \lambda_D^{a_D}.$$

This action defines a semi-direct product $\mathbb{R} \rtimes \mathbb{Z}^D$.

Consider the additive group $\mathbb{Z}_\lambda \subset \mathbb{R}$ generated by all numbers λ^a with $a \in \mathbb{Z}^D$, that is

$$\mathbb{Z}_\lambda = \left\{ m_1 \lambda^{a(1)} + m_2 \lambda^{a(2)} + ... + m_l \lambda^{a(l)} : l \in \mathbb{N}^*, \ m_i \in \mathbb{Z}, \ a(i) \in \mathbb{Z}^D, \ i = 1, ..., l \right\}.$$

Obviously, $\mathbb{Z}_\lambda$ is stable under the action (7.21) so that the following group is defined:

$$G_\lambda := \mathbb{Z}_\lambda \rtimes \mathbb{Z}^D.$$

We claim that G_λ is finitely generated; moreover, the following set S generates G_λ

$$S = \{(\pm 1, 0), (0, \pm e_1), ..., (0, \pm e_D)\}, \tag{7.22}$$

where $e_1, e_2, ..., e_D$ is the canonical basis of $\mathbb{Z}^D$. Indeed, this can be seen from the identities

$$(u, a)(\pm 1, 0) = (u \pm \lambda^a, a) \quad \text{and} \quad (u, a)(0, \pm e_i) = (u, a \pm e_i)$$

where $u \in \mathbb{Z}_\lambda$ and $a \in \mathbb{Z}^D$.

The group G_λ admits a representation in the affine transformation group of the real line. Indeed, the generator $(1, 0)$ corresponds to the translation $x \to x + 1$ of $\mathbb{R}$ and the generator $(0, e_i)$ corresponds to the homothety $x \to \lambda_i x$. The representation is faithful if and only if $\log |\lambda_1|, ..., \log |\lambda_D|$ are linearly independent over the rationals.

Recall that a real number α is called *algebraic* if it is a root of a polynomial with integer coefficients. The minimal degree of such a polynomial is called the degree of α. If in addition the highest coefficient of the polynomial is equal to 1 then α is called an *integral algebraic number*. Hence, if n is the degree of an integral algebraic number α then

$$\alpha^n = c_0 + c_1 \alpha + c_2 \alpha^2 + ... + c_{n-1} \alpha^{n-1} \tag{7.23}$$

for some integers $c_0, c_1, ..., c_{n-1}$.

Proposition 7.7 *Let $\lambda_1, \lambda_2, ..., \lambda_D$ be non-zero real integral algebraic numbers. Then the heat kernel on $\Gamma_\lambda = (G_\lambda, S)$ satisfies the estimate*

$$\varphi_\Gamma(k) \geq \exp(-Ck^{1/3}),$$

for even k.

Proof. Denote $U = \mathbb{Z}_\lambda$, $A = \mathbb{Z}^D$ and set

$$A_* = \mathbb{Z}_+^D := \left\{ a \in \mathbb{Z}^D : a_1 \geq 0, a_2 \geq 0, ..., a_D \geq 0 \right\}.$$

Let U_* be the subgroup of U generated by all numbers λ^a with $a \in \mathbb{Z}_+^D$. Obviously, U_* is stable under multiplication by λ^b with $b \in A_*$ so that $A_*(U_*) \subset U_*$. It is also obvious that the semigroup

distance d_{A_*} associated with the canonical generating set $e_1, ..., e_D$ is equal to the restriction of d_A to A_*. Notice that $U_* \supset \{\pm 1\} = S_U$ and that the volume growth of A_* is polynomial.

Let us verify that U_* is finitely generated. Indeed, if λ_i has degree n_i then $\lambda_i^{a_i}$ with any $a_i \geq n_i$ can be expressed in the form $m_0 + m_1 \lambda_i + m_2 \lambda_i^2 + ... + m_{n_i-1} \lambda_i^{n_i-1}$ with integer m_j. Therefore, λ^a with $a \in A_*$ can be expressed as a sum of terms like $\pm \lambda_1^{b_1} \lambda_2^{b_2} ... \lambda_D^{b_D}$ where $0 \leq b_i < n_i$, which means that U_* is finitely generated. Since U_* is abelian, U_* also has polynomial volume growth, whence the lower bound for φ_Γ follows by Corollary 7.6. ∎

Theorem 7.8 Let $\lambda_1, \lambda_2, ..., \lambda_D$ be non-zero real algebraic numbers at least one of them being not equal to ± 1. Then the heat kernel on $\Gamma_\lambda = (\mathbb{Z}_\lambda \rtimes \mathbb{Z}^D, S)$ satisfies the estimate

$$\varphi_\Gamma(k) \asymp \exp(-k^{1/3}),$$

for even k.

Proof. Each λ_i satisfies an equation

$$m_i \lambda_i^{n_i} = c_{0,i} + c_{1,i} \lambda_i + c_{2,i} \lambda_i^2 + ... + c_{n-1,i} \lambda_i^{n_i-1}, \tag{7.24}$$

with some positive integers n_i, m_i and integers $c_{k,i}$. Introduce the vector

$$\nu = (m_1 \lambda_1, m_1, m_2 \lambda_2, m_2, ..., m_D \lambda_D, m_D) \in \mathbb{R}^{2D},$$

and observe that all components ν_j of ν are integral algebraic numbers, which follows from (7.24) by multiplication by $m_i^{n_i-1}$. Therefore, by Proposition 7.7, the heat kernel on the group

$$G_\nu = \mathbb{Z}_\nu \rtimes \mathbb{Z}^{2D}$$

admits lower bound $\exp(-Ck^{1/3})$. By a result of [34], the same lower bound is true for any finitely generated subgroup of G_ν.

Thus, we are left to show that G_λ is isomorphic to a subgroup of G_ν. Indeed, $\mathbb{Z}_\lambda$ is naturally identified with a subgroup of $\mathbb{Z}_\nu$ because $\lambda_i = \nu_{2i-1}/\nu_{2i}$. For any $a \in \mathbb{Z}^D$, consider

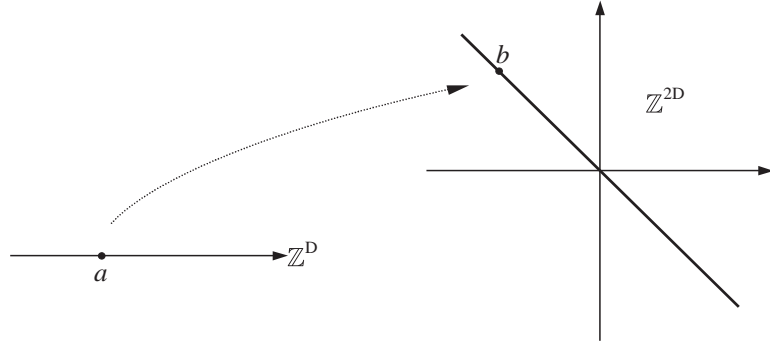$$b_a := (a_1, -a_1, a_2, -a_2, ..., a_D, -a_D) \in \mathbb{Z}^{2D}.$$

Figure 12 The map $a \mapsto b_a$.

Since the action of $a \in \mathbb{Z}^D$ on $\mathbb{Z}_\lambda$ is given by

$$a(u) = \lambda^a u = (m_1 \lambda_1)^{a_1} m_1^{-a_1} ... (m_D \lambda_D)^{a_D} m_D^{-a_D} u = \nu^{b_a} u,$$

and the action of $b \in \mathbb{Z}^{2D}$ on $\mathbb{Z}_\nu$ is given by $b(u) = \nu^b u$, we see that $b_a(u) = a(u)$ on $\mathbb{Z}_\lambda$. This implies that the map from G_λ to G_ν defined by

$$(u, a) \longmapsto (u, b_a)$$

is a morphism of G_λ into G_ν.

The condition $\lambda_i \neq \pm 1$ for some i implies that G_λ has exponential volume growth (to see this, one can imitate the argument in [40], Lemma 3), so that the upper bound for the heat kernel on G_λ follows from Corollary 7.4. ∎

Assume that all λ_i's are integers, and set $q = \lambda_1 \lambda_2 ... \lambda_D$. Then $\mathbb{Z}_\lambda$ coincides with $\mathbb{Z}[\frac{1}{q}]$ (cf. Section 5.1 for the case $D = 1$). Theorem 7.8 (or Proposition 7.7) implies immediately the following result which generalizes Theorem 5.1.

Corollary 7.9 *Let all λ_i be integers not equal to $0, \pm 1$, and let $q = \lambda_1 \lambda_2 ... \lambda_D$. Then the heat kernel on the Cayley graph $\Gamma = (\mathbb{Z}[\frac{1}{q}] \rtimes \mathbb{Z}^D, S)$ admits the estimate*

$$\varphi_\Gamma(k) \asymp \exp(-k^{1/3}),$$

for even k.

Remark 7.2 If $D = 1$ and λ_1 is transcendental, then G_λ can be shown to be isomorphic to $\mathbb{Z} \wr \mathbb{Z}$. In this case one has

$$\varphi_{\Gamma_\lambda}(k) \asymp \exp(-k^{1/3}(\log k)^{2/3})$$

(see [35] and [33]). If $\lambda_1 = \pm 1$ then G_λ is commensurable with $\mathbb{Z}$, i.e. they contain isomorphic subgroups of finite index. Namely, if $\lambda_1 = 1$ then $G_\lambda = \mathbb{Z}$ and if $\lambda_1 = -1$ then G_λ is the non-trivial split extension of $\mathbb{Z}$ by $\mathbb{Z}_2$. In both cases, by the result of [34],

$$\varphi_{\Gamma_\lambda}(k) \simeq k^{-1/2}.$$

7.5 Appendix: Polycyclic groups

The aim of this appendix is to give a self-contained proof of a result first proved by Alexopoulos ([2]). His original proof relies on certain non-trivial estimates for random walks on $\mathbb{Z}^D$ which we do not use here. For general information on polycyclic groups, we refer to [36], Chap. 4, or [38].

The scheme with contraction of graphs may also apply for a finitely generated group G with abelian quotient A even if the short exact sequence

$$1 \to U \to G \to A \to 1$$

does not split.

By a theorem of Mal'cev, any polycyclic group G (up to finite index) contains a normal subgroup $U \lhd G$ which is a nilpotent group, and such that G/U is abelian (see, for example, [38, p.35], [37]). Therefore, the scheme which will be described below is well suited for polycyclic groups.

Let G be a finitely generated group and let U be a normal subgroup of G. Assume that U is also finitely generated, and that $A := G/U = \mathbb{Z}^D$. Let $\pi : G \to A$ be the natural homomorphism with kernel U. Denote by $\{e_1, e_2, ..., e_D\}$ the canonical basis in $\mathbb{Z}^D$. For each e_i choose some $g_i \in \pi^{-1}(e_i)$ (see Fig. 13) and denote

$$\tilde{S}_A := \bigcup_{i=1}^{D} \{g_i, g_i^{-1}\} \subset G.$$

Let $\tilde{S}_U = \{v_j\}$ be a finite symmetric set of generators in U. Then the set $S := \tilde{S}_U \cup \tilde{S}_A$ is a finite symmetric set of generators of G. Denote by Γ the Cayley graph (G, S).
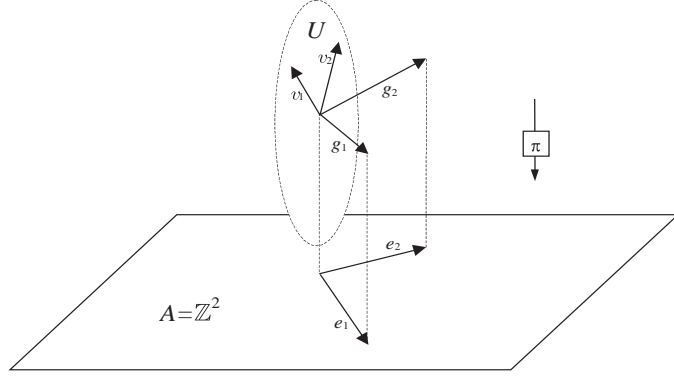
Figure 13 The generating set S of G is the union of $\{v_i\}$, $\{g_i\}$ and $\{g_i^{-1}\}$.

Theorem 7.10 *Let G be a finitely generated group and U be a normal subgroup of G. If U is a finitely generated group with polynomial volume growth and $A := G/U = \mathbb{Z}^D$, then the heat kernel on the Cayley graph $\Gamma = (G, S)$ admits the lower bound*

$$\varphi_\Gamma(k) \geq \exp(-Ck^{1/3}) \tag{7.25}$$

for all even k.

In particular, this theorem covers polycyclic groups. Indeed, as was mentioned above, any polycyclic group up to finite index is of this kind. However, a theorem of [34] implies that passing to a finite index subgroup does not change the asymptotic behavior of $\varphi_\Gamma(k)$.

Proof. It suffices to verify that all hypotheses (LT), (W) and (DT) of Theorem 6.1 are satisfied for $\Gamma = (G, S)$ and $\mathcal{A} = (A, S_A)$ (where S_A consists of e_i's and their inverses). Note that the homomorphism $\pi : G \to A$ can be considered as a projection $\pi : \Gamma \to \mathcal{A}$ so that $\mathcal{A}$ is a contraction of Γ. Let $|\cdot|$ be the distance norm on A, that is the graph distance to the identity element on $\mathcal{A}$. Then the hypothesis (LT) is trivially true.

Similarly, let $\|\cdot\|$ be a distance norm on U with respect to the Cayley graph $(U, \tilde{S}_U)$. Next, we would like to extend $\|\cdot\|$ to a norm $\||\cdot\||$ on G. We cannot use equality (7.16) as it was possible in the case of semi-direct products. However, the fact that A is abelian (hence admits nice normal forms) allows to define a (set-theoretic) section with good enough properties. For each $a = a_1 e_1 + ... + a_D e_D \in \mathbb{Z}^D$, denote

$$\sigma^a := g_1^{a_1} g_2^{a_2} ... g_D^{a_D} \in G$$

and observe that

$$\pi(\sigma^a) = a_1 e_1 + ... + a_D e_D = a.$$

If $x \in \pi^{-1}(a)$, let

$$u := x(\sigma^a)^{-1} \in U.$$

We see that any $x \in G$ can be uniquely represented in the form:

$$x = u\sigma^a, \quad u \in U, \, a \in \mathbb{Z}^D. \tag{7.26}$$

Hence, if we fix the choice of the g_i's then we can define a norm on G by

$$\||u\sigma^a\||_G = \|u\|. \tag{7.27}$$

Let us verify condition (W). Let $B_A(r)$ and $B_a(r)$ be the balls defined by (6.4) and (6.3), that is

$$B_A(r) = \{a \in A : |a| < r\}$$

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and, for any $a \in A$,

$$B_a(r) = \{x \in \Gamma_a : |||x||| < r\} = \{u\sigma^a \in G : \|u\| < r\} .$$

Note that $B_a(r)$ is in one-to-one correspondence with the ball $B_U(r)$ in the Cayley graph $(U, \tilde{S}_U)$, which is defined by

$$B_U(r) = \{u \in U : \|u\| < r\} .$$

Let $V_A(r)$ and $V_U(r)$ be the cardinalities of the balls $B_A(r)$ and $B_U(r)$, respectively. By hypothesis, both functions $V_A(r)$ and $V_U(r)$ are polynomial, whence condition (W) follows.

We are left to verify the hypothesis (DT). Let us first prove two lemmas.

Lemma 7.11 *For all $v \in U$ and $a \in \mathbb{Z}^D$,*

$$\left\|\sigma^a v (\sigma^a)^{-1}\right\| \leq \eta^{|a|} \|v\| , \tag{7.28}$$

for some large enough number η.

    Proof. First observe that $\sigma^a v (\sigma^a)^{-1} \in U$ so that the left-hand side of (7.28) makes sense. By induction on $|a|$, (7.28) amounts to

$$\left\|gvg^{-1}\right\| \leq \eta \|v\| , \tag{7.29}$$

for any $g \in \tilde{S}_A$.

Let us prove (7.29) by induction on $\|v\|$. The inductive basis for $\|v\| = 0$ is obvious. If $\|v\| > 0$ then v can be represented as $v = ws$ where $w \in U$, $s \in \tilde{S}_U$ and $\|w\| = \|v\| - 1$. Hence,

$$gvg^{-1} = \left(gwg^{-1}\right)\left(gsg^{-1}\right)$$

and, by the triangle inequality,

$$\left\|gvg^{-1}\right\| \leq \left\|gwg^{-1}\right\| + \left\|gsg^{-1}\right\| . \tag{7.30}$$

By the inductive hypothesis,

$$\left\|gwg^{-1}\right\| \leq \eta \|w\| = \eta(\|v\| - 1). \tag{7.31}$$

Define η by

$$\eta := \max_{s \in \tilde{S}_U} \max_{g \in \tilde{S}_A} \left\|gsg^{-1}\right\| . \tag{7.32}$$

Then (7.29) follows from (7.30), (7.31) and (7.32). $\blacksquare$

Define a commutator in the group G by

$$c(x, y) = xyx^{-1}y^{-1}. \tag{7.33}$$

Since $G/U = A$ is abelian, $\pi(c(x, y)) = 0_A$ whence $c(x, y) \in U$. The next lemma provides an estimate for a norm in U of certain commutators.

Lemma 7.12 *For all $a \in \mathbb{Z}^D$ and $h \in \tilde{S}_A$,*

$$\|c(\sigma^a, h)\| \leq \beta^{|a|}, \tag{7.34}$$

for some large enough β.

Proof. If $|a| = 0$ then $c(\sigma^a, h) = \text{Id}_U$ and the claim is trivial. If $|a| = 1$ then $\sigma^a = g$ for some $g \in \tilde{S}_A$. Therefore, inequality (7.34) holds provided β is big enough so that

$$\beta \geq \max_{g, h \in \tilde{S}_A} \|c(g, h)\|. \tag{7.35}$$

For $|a| \geq 2$, let us prove (7.34) inductively on $|a|$. Let i be the smallest index for which $a_i \neq 0$ so that

$$a = a_i e_i + a_{i+1} e_{i+1} + \dots + a_D e_D.$$

Depending on the sign of a_i, let us set $b = a - e_i$ or $b = a + e_i$ so that $|b| = |a| - 1$. By the inductive hypothesis, $w := c(\sigma^b, h)$ satisfies the inequality

$$\|w\| \leq \beta^{|b|} = \beta^{|a|-1}. \tag{7.36}$$

Clearly, we have

$$\sigma^a = g_i^{a_i} g_{i+1}^{a_{i+1}} \dots g_D^{a_D} = g\sigma^b$$

where $g = g_i$ or g_i^{-1}. Applying the general identity

$$c(gg', h) = g\, c(g', h) g^{-1} c(g, h), \tag{7.37}$$

for $g' = \sigma^b$, we obtain

$$c(\sigma^a, h) = (gwg^{-1}) c(g, h). \tag{7.38}$$

By (7.29), (7.35) and (7.36), we obtain

$$\|c(\sigma^a, h)\| \leq \|gwg^{-1}\| + \|c(g, h)\| \leq \eta \|w\| + \beta \leq \eta\beta^{|a|-1} + \beta. \tag{7.39}$$

We may choose $\beta \geq 2\eta$ which implies, for any $n \geq 2$,

$$\eta\beta^{n-1} + \beta \leq \frac{1}{2}\beta^n + \beta \leq \beta^n.$$

Then (7.39) yields (7.34) which finishes the proof. ∎

Now we can prove the condition (DT) which can be stated as follows: there exists a positive number β such that, for all $x \in G$ and $s \in S$,

$$|||xs||| \leq |||x||| + \beta^{|\pi(x)|}. \tag{7.40}$$

Recall that any $x \in G$ can be uniquely represented as $x = u\sigma^a$ where $u \in U$ and $a = \pi(x) \in \mathbb{Z}^D$. By definition (7.27) of the norm in G, we have $|||x||| = \|u\|$. Hence, it suffices to prove the inequality

$$|||xs||| \leq \|u\| + \beta^{|a|}. \tag{7.41}$$

Choose β to be large enough so that it satisfies the conclusion of Lemma 7.12 and is larger than η from Lemma 7.11. Since $S = \tilde{S}_U \cup \tilde{S}_A$, we consider two cases.

Case 1. Assume $s \in \tilde{S}_U$. Then

$$xs = u\sigma^a s = u(\sigma^a s(\sigma^a)^{-1})\sigma^a = uv\sigma^a$$

where

$$v := \sigma^a s(\sigma^a)^{-1} \in U.$$

By Lemma 7.11 and $\|s\| = 1$, we have

$$\|v\| = \|\sigma^a s(\sigma^a)^{-1}\| \leq \beta^{|a|} \|s\| = \beta^{|a|}.$$

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Since $xs = (uv)\sigma^a$, we have, by (7.27) and (T),

$$|||xs||| = \|uv\| \leq \|u\| + \|v\| \leq \|u\| + \beta^{|a|},$$

which was to be proved.

Case 2. Assume $s \in \tilde{S}_A$. Then $s = g_i$ or $s = g_i^{-1}$ for some $i = 1, 2, ..., D$. Split a as $a = a' + a''$ where

$$a' = a_1 e_1 + ... + a_i e_i \quad \text{and} \quad a'' = a_{i+1} e_{i+1} + ... + a_D e_D,$$

and write

$$xs = u\sigma^a s = u\sigma^{a'} \sigma^{a''} s = u\sigma^{a'} c(\sigma^{a''}, s) s \sigma^{a''}. \tag{7.42}$$

Denote $w := c(\sigma^{a''}, s) \in U$, then (7.42) yields

$$xs = u \left[\sigma^{a'} w (\sigma^{a'})^{-1} \right] (\sigma^{a'} s \sigma^{a''}). \tag{7.43}$$

Since

$$\sigma^{a'} w (\sigma^{a'})^{-1} \in U$$

and

$$\sigma^{a'} s \sigma^{a''} = g_1^{a_1} ... g_i^{a_i \pm 1} ... g_D^{a_D} = \sigma^b,$$

where $b = a \pm e_i$, the relation (7.43) provides a representation of xs as a product of an element of U by σ^b. By definition (7.27) of the norm in G and by Lemmas 7.11, 7.12, we obtain

$$\begin{aligned} |||xs||| &= \|u\sigma^{a'} w(\sigma^{a'})^{-1}\| \leq \|u\| + \|\sigma^{a'} w(\sigma^{a'})^{-1}\| \\ &\leq \|u\| + \beta^{|a'|} \|w\| \leq \|u\| + \beta^{|a'| + |a''|} = \|u\| + \beta^{|a|}, \end{aligned}$$

which was to be proved. ∎

There is an alternative way of proving heat kernel estimates on a polycyclic group. Indeed, any polycyclic group G has a finite index subgroup which is a discrete cocompact subgroup in a simply-connected solvable Lie group. The heat kernel estimate on the Lie group is given by Theorem 3.3. Then one can use [34] as it was mentioned in the Introduction.

8   Appendix: δ-regularity

Lemma 8.1 *Let $\rho \in C^1(0, +\infty)$ be a positive non-decreasing function such that $v\frac{\rho'(v)}{\rho(v)}$ is non-increasing for large enough v. Define $\gamma(t)$ by the identity*

$$t = \int_{\gamma_0}^{\gamma(t)} \rho^2(v) \frac{dv}{v} \tag{8.1}$$

for some $\gamma_0 > 0$. Then the function γ is δ-regular for some $\delta > 0$.

Proof. Set $\eta(v) = \rho^2(v)$; $v\frac{\eta'(v)}{\eta(v)} = 2v\frac{\rho'(v)}{\rho(v)}$ is non-increasing for large enough v. By definition of δ-regularity (see Section 2) we need to show that, for some $\delta > 0$ and all $0 < t \leq s \leq 2t$,

$$\frac{\gamma'(s)}{\gamma(s)} \geq \delta \frac{\gamma'(t)}{\gamma(t)}. \tag{8.2}$$

Let us first show that (8.2) is implied by the following condition: for some $t_0 \geq 0$,

$$(t - t_0) \frac{\gamma'(t)}{\gamma(t)} \quad \text{increases for } t \text{ large enough.} \tag{8.3}$$

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Indeed, if t is large enough then by (8.3)

$$(t - t_0) \frac{\gamma'(t)}{\gamma(t)} \le (s - t_0) \frac{\gamma'(s)}{\gamma(s)} \le (2t - t_0) \frac{\gamma'(s)}{\gamma(s)}$$

whence

$$\frac{\gamma'(s)}{\gamma(s)} \ge \frac{t - t_0}{2t - t_0} \frac{\gamma'(t)}{\gamma(t)},$$

and (8.2) follows with some $0 < \delta < 1/2$. For a bounded range of t (and s), we have, by differentiating (8.1) and by continuity of η and γ,

$$\frac{\gamma'(t)}{\gamma(t)} = \frac{1}{\eta(\gamma(t))} \simeq \frac{1}{\eta(\gamma_0)}$$

so that (8.2) holds again with some $\delta > 0$.

Now let us prove (8.3). We have already noticed that

$$\frac{\gamma'(t)}{\gamma(t)} = \frac{1}{\eta(\gamma(t))}.$$

Applying (8.1) again, we obtain

$$t - t_0 = \int_{\gamma(t_0)}^{\gamma(t)} \eta(v) \frac{dv}{v}$$

whence

$$(t - t_0) \frac{\gamma'(t)}{\gamma(t)} = \frac{1}{\eta(\gamma(t))} \int_{\gamma(t_0)}^{\gamma(t)} \eta(v) \frac{dv}{v}.$$

Therefore, the increasing of $(t - t_0) \frac{\gamma'(t)}{\gamma(t)}$ will follow from the increasing of the function

$$\theta \longmapsto \frac{1}{\eta(\theta)} \int_{\theta_0}^{\theta} \eta(v) \frac{dv}{v}, \tag{8.4}$$

where $\theta_0 = \gamma(t_0)$. By differentiating the function (8.4) in θ, we are left to verify the inequality

$$-\frac{\eta'(\theta)}{\eta^2(\theta)} \int_{\theta_0}^{\theta} \eta(v) \frac{dv}{v} + \frac{1}{\theta} \ge 0. \tag{8.5}$$

Since η is increasing, we have $\eta' \ge 0$. If $\eta'(\theta) = 0$, then (8.5) trivially holds. If $\eta'(\theta) > 0$ then rewrite (8.5) as

$$\frac{1}{\eta(\theta)} \int_{\theta_0}^{\theta} \eta(v) \frac{dv}{v} \le \frac{\eta(\theta)}{\theta \eta'(\theta)}.$$

Using the generalized mean value theorem and the fact that $v \frac{\eta'(v)}{\eta(v)}$ decreases, we obtain, for some $\xi \in (\theta_0, \theta)$,

$$\frac{1}{\eta(\theta)} \int_{\theta_0}^{\theta} \eta(v) \frac{dv}{v} \le \frac{\int_{\theta_0}^{\theta} \eta(v) \frac{dv}{v}}{\eta(\theta) - \eta(\theta_0)} = \frac{\eta(\xi)}{\xi \eta'(\xi)} \le \frac{\eta(\theta)}{\theta \eta'(\theta)},$$

which finishes the proof. ∎

Note added in proof: Applying the method developed in this paper, Ch.Pittet and L.Saloff-Coste have recently established the on-diagonal lower bound $\exp\left(-Ck^{1/3}\right)$ for the heat kernel decay in finitely generated solvable groups of finite rank.

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