Li-Yau inequality on virtually Abelian groups

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We show that Cayley graphs of virtually Abelian groups satisfy a Li-Yau type gradient estimate despite the fact that they do not satisfy any known variant of the curvature-dimension inequality with non-negative curvature.

1. Introduction

Li and Yau [6] proved an upper bound on the gradient of positive solutions of the heat equation on manifolds with Ricci curvature bounded from below. The simplest variant of their result is

(1.1)
$$|\nabla \log u|^2 - \partial_t (\log u) = \frac{|\nabla u|^2}{u^2} - \frac{\partial_t u}{u} \le \frac{n}{2t},$$

where u is a positive solution of the heat equation $(\Delta - \partial_t)u = 0$ on an *n*dimensional compact manifold with non-negative Ricci curvature. The proof is based on a specific property of such manifolds, the *curvature-dimension inequality* (CD-inequality)

(1.2)
$$\frac{1}{2}\Delta |\nabla f|^2 \ge \langle \nabla f, \nabla \Delta f \rangle + \frac{1}{n} (\Delta f)^2.$$

It was an important insight by Bakry and Emery [1] that one can use it as a substitute for the lower Ricci curvature bound on spaces where a direct generalization of Ricci curvature is not available. The direct discrete version of the CD-inequality was introduced in [7]. It is a local notion in the sense that it only depends on 2-step neighborhoods of the nodes of the graph. Its properties were subsequently studied in [3], where the authors showed that the discrete CD-inequality implies a weak Harnack-type inequality, but fell short of proving the Li-Yau gradient estimate.

In the break-through paper [2] a variant of the CD-inequality was introduced: the so called the exponential curvature-dimension (CDE) inequality. This is still a local notion, its validity depends only on 2-step neighborhoods in the graph. However, for the first time, it was shown that this inequality implies a version of the Li-Yau gradient estimate.

Theorem 1.3 ([2]). Let G be a finite graph satisfying CDE(n, 0), and let u be a positive solution to the heat equation on G. Then for all t > 0

(1.4)
$$\frac{|\nabla(\sqrt{u})|^2}{u} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} \le \frac{n}{2t}$$

1.1. Main result

It was shown in [2] that the curvature notion based on CDE-inequality behaves "as expected": complete graphs have positive curvature, lattices have 0 curvature, trees have negative curvature. However, the fact that the CDEinequality only depends on 2-step neighborhoods leads to an unexpected and undesirable side-effect. The hexagonal lattice, and in more general Cayley graphs of virtually-Abelian groups (these include periodic planar tilings, among others), will not satisfy a CDE type inequality with non-negative curvature. In fact, their 2-step neighborhoods are the same as that of trees, whose curvature is known to be negative. This is completely counter-intuitive to the observation that these graphs are essentially flat and hence should ideally have 0 curvature. Our intuition is hence that they should satisfy a Li-Yau type gradient estimate. That is exactly what we show in this paper.

Theorem 1.5. Let Φ be a virtually Abelian group and $\tilde{\Phi} \leq \Phi$ a normal Abelian subgroup of index $k < \infty$. Let $S \subset \Phi$ be a finite, symmetric generating set and denote $G = \text{Cay}(\Phi, S)$ the associated Cayley graph. Similarly, let $\tilde{S} \subset \tilde{\Phi}$ be a finite, symmetric, conjugation-invariant generating set of $\tilde{\Phi}$. There exist constants K, C > 0 such that for any solution $w : G \times [0, \infty) \rightarrow [0, 1]$ of the heat equation on G, the shifted solution $u = w + \sqrt{k}$ satisfies

$$\frac{\overline{\Gamma}(\sqrt{u})}{Ku} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} \le \frac{C}{t} \ .$$

Here $\tilde{\Gamma}$ stands for the usual "gradient squared" operator Γ of $\tilde{G} = \operatorname{Cay}(\Phi, \tilde{S})$, the graph on the full group obtained by generators of the Abelian subgroup. For the exact definitions and notation see Section 1.2.

Remark 1. A big drawback of this theorem is the need to shift the solutions of the heat equation by \sqrt{k} . Even though the size of the shift is

independent of the solution, it is still bigger than the infinity norm of it. This means that the theorem cannot be used to prove Harnack-type inequalities (a typical application of the gradient estimate), since the shifted solutions automatically satisfy such an inequality.

On the other hand, we believe that shifting is only a technical artifact of the proof, and that the theorem ought to be true without it. The main issue is that the family of weight functions $f_{\chi,j}$ constructed in Section 3 aren't non-negative. One possibility of avoiding the shift could be to construct a better family of such functions.

The idea of the proof is the following. From [2] we know that any positive solution of the heat equation on \tilde{G} satisfies (1.4) for $n = 2|\tilde{S}|$. We will express solutions of the heat equation on G as a linear combination of solutions of the heat equation on \tilde{G} . Then we show that positive linear combinations preserve the validity of (1.4). Finally we show that shifting the original solution by a positive constant allows us to turn the original linear combination into a positive linear combination.

In general, (1.1) is a stronger conclusion than (1.4), and it is an easy computation to show that the direct discrete analogue of (1.1) does not hold on graphs. However, on a manifold, the inequality (1.1) is equivalent to

(1.6)
$$-\Delta \log u(x,t) \le n/2t$$

and Münch [8] found a new variant of the CD-inequality that implies (1.6) for finite graphs. In particular, he shows that for finite, locally Abelian graphs there exists a constant n depending only on the degree such that (1.6) holds. We shall use this result to prove the following analogue of Theorem 1.5.

Theorem 1.7. Under the conditions of Theorem 1.5, we have

$$-\tilde{\Delta}\log u \leq \frac{C}{t},$$

where $\tilde{\Delta}$ denotes the Laplace operator on \tilde{G} .

1.2. Notation

For a given locally finite graph G we define the Laplace operator $\Delta = \Delta_G$ acting on a function $f: G \to \mathbb{R}$ as

$$\Delta f(x) = \sum_{y \sim x} (f(y) - f(x)).$$

We will often consider a graph \tilde{G} on the same vertex set at the same time. For convenience we will often abbreviate $\Delta_{\tilde{G}}$ as $\tilde{\Delta}$.

For a given function $g: G \to [0, \infty)$ the heat equation for $u: G \times [0, \infty) \to [0, \infty)$ with initial condition g is the system

$$\Delta u(x,t) = \partial_t u(x,t), \quad u(x,0) = g(x),$$

where Δ acts on the first variable of u.

The gradient operator $\Gamma = \Gamma_G$ is defined as

$$\Gamma(f)(x) = \sum_{y \sim x} (f(y) - f(x))^2.$$

We will also use the notation $\widetilde{\Gamma} = \Gamma_{\tilde{G}}$.

Throughout the paper we consider a fixed virtually Abelian group Φ with a finite, symmetric generating set S. The unit element will always be denoted by 1. The Cayley graph associated to this generating set will be denoted by G. (Edges are given by multiplication by generators on the right.) Since Φ is virtually Abelian, it has a finite index free Abelian normal subgroup $\tilde{\Phi} \leq \Phi$. We fix a generating set \tilde{S} for $\tilde{\Phi}$, and denote by \tilde{G} the graph whose vertex set is the same as that of G, but the edges are given by multiplication by elements of \tilde{S} . Thus, \tilde{G} is a disjoint union of finitely many copies of $\operatorname{Cay}(\tilde{\Phi}, \tilde{S})$.

Every element $x \in \Phi$ defines an automorphism $\phi_x : \tilde{\Phi} \to \tilde{\Phi}$ by the map $y \mapsto x^{-1} * y * x$. The map $x \mapsto \phi_x$ defines a representation $\Phi \to \operatorname{Aut}(\tilde{\Phi})$ that factors through the quotient $\Phi/\tilde{\Phi}$, hence there are at most k different automorphisms obtainable this way and they form a group.

We will assume that the set \tilde{S} is invariant under the automorphisms ϕ_x . By the previous remarks such a finite generating set always exists. For example, if $\tilde{\Phi}$ is in the center of Φ , any finite generating set can be chosen.

Remark 2. A simple consequence of the invariance of \tilde{S} is that for any $z \in \Phi$ the following two sets are the same:

(1.8)
$$\{z * s : s \in \tilde{S}\} = \{s * z : s \in \tilde{S}\}.$$

Let $f: G \to \mathbb{C}$ be any function, and let $f_z(x) = f(x * z)$. Then (1.8) immediately implies the following identities:

$$\tilde{\Delta}f_z(x) = (\tilde{\Delta}f)(x*z),$$

and

$$\widetilde{\Gamma}(f_z)(x) = \widetilde{\Gamma}(f)(x * z).$$

2. Relating the heat equation on G and \tilde{G}

In this section we explain how to obtain a solution to the heat equation on G as a (possibly infinite) linear combination of solutions to the heat equation on \tilde{G} .

Let $w(x,t): \hat{G} \times [0,\infty)$ be the solution of $\Delta w = \partial_t w$ with the initial condition $w(x,0) = \delta_{x=1}$. As a first attempt, let us fix a $\beta > 0$ and try to construct a solution to $\Delta u = \partial_t u$ in the form

(2.1)
$$u(x,t) = \sum_{z \in \Phi} f(z)w(x * z^{-1}, \beta t).$$

Uniform convergence of this sum will be ensured by choosing a nonnegative bounded weight function $f : \Phi \to \mathbb{R}_{\geq 0}$. That is sufficient, since w decays super-exponentially in space according to the continuous time version of the Carne-Varopoulos bound [5].

Now we can compare Δu and $\partial_t u$, and find a sufficient condition on f that ensures u is a solution of the heat equation.

$$\begin{array}{ll} (2.2) & \Delta u(x,t) = \sum_{s \in S} (u(x*s) - u(x)) \\ & = \sum_{z \in \Phi} \sum_{s \in S} f(z)(w(x*s*z^{-1},\beta t) - w(x*z^{-1},\beta t)) \\ & = \sum_{z \in \Phi} f(z) \sum_{s \in S} (w(x*(z*s^{-1})^{-1},\beta t) - w(x*z^{-1},\beta t)) \\ & = \sum_{z \in \Phi} w(x*z^{-1},\beta t) \sum_{s \in S} (f(z*s) - f(z)) \\ & = \sum_{z \in \Phi} (\Delta f)(z) \cdot w(x*z^{-1},\beta t). \end{array}$$

In order to compute the time derivative, we will exploit that w satisfies $\tilde{\Delta}w = \partial_t w$, as well as Remark 2. Let us temporarily denote $w_z(x,t) = w(x * t)$

 z^{-1}, t).

(2.3)

$$\partial_t u(x,t) = \sum_{z \in \Phi} f(z)\beta \cdot (\partial_t w)(x * z^{-1}, \beta t)$$

$$= \sum_{z \in \Phi} f(z)\beta \cdot (\tilde{\Delta}w)(x * z^{-1}, \beta t)$$

$$= \beta \sum_{z \in \Phi} f(z)\tilde{\Delta}w_z(x, \beta t)$$

$$= \beta \sum_{z \in \Phi} (\tilde{\Delta}f)(z)w_z(x, \beta t)$$

$$= \beta \sum_{z \in \Phi} (\tilde{\Delta}f)(z)w(x * z^{-1}, \beta t).$$

Thus combining (2.2) and (2.3) leads to the following observation.

Lemma 2.4. If $\beta \tilde{\Delta} f = \Delta f$ then the function u defined in (2.1) satisfies $\Delta u = \partial_t u$.

The next step is to find a family of functions f that satisfy the conditions of Lemma 2.4. This will be facilitated by the observation that Δ and $\tilde{\Delta}$ commute. Thus we will be able to find functions f that satisfy the condition of Lemma 2.4 by constructing joint eigenfunctions of Δ and $\tilde{\Delta}$.

Claim 2.5. $\Delta \widetilde{\Delta} f = \widetilde{\Delta} \Delta f$ for any function f.

Proof. Writing out the definitions, what we need to check is that

$$\sum_{s \in S} \sum_{\tilde{s} \in \tilde{S}} f(x \ast \tilde{s} \ast s) = \sum_{s \in S} \sum_{\tilde{s} \in \tilde{S}} f(x \ast s \ast \tilde{s}),$$

but this follows immediately from Remark 2.

3. Constructing periodic solutions

In this section we will build solutions to the heat equation on G that have almost arbitrary "periodic" initial conditions. Fix n > 1. Denote by Φ_n the finite quotient $\Phi_n = \Phi/\langle s^n : s \in \tilde{S} \rangle$ and by $\tilde{\Phi}_n$ the finite Abelian quotient $\tilde{\Phi}_n = \tilde{\Phi}/\langle s^n : s \in \tilde{S} \rangle$). The associated graphs will be denoted by G_n and \tilde{G}_n respectively. Let us introduce the quotient map by $\pi_n : \Phi \to \Phi_n$.

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Definition 3.1. We say that a function $g : \Phi \to \mathbb{C}$ is (n-) periodic if $g(x) = g(x * s^n)$ for any $s \in \tilde{S}$. Since $\tilde{\Phi}$ is normal in Φ , this is equivalent to saying that $g(s^n * x) = g(x)$ for all $s \in \tilde{S}$. It is also equivalent to the existence of a function $h : \Phi_n \to \mathbb{C}$ such that $g = h \circ \pi_n$.

It is easy to check that the operators Δ and $\hat{\Delta}$ descend to G_n and that, for either of these operators, a periodic function $g: \Phi \to \mathbb{C}$ is an eigenfunction if and only if it is a lift of an eigenfunction $h: \Phi_n \to \mathbb{C}$.

Let

$$Ch(\tilde{\Phi}_n) = \{\chi : \tilde{\Phi}_n \to \mathbb{C} : \chi(x * y) = \chi(x)\chi(y)\}$$

denote the set of multiplicative characters on $\tilde{\Phi}_n$. Fix a multiplicative character $\chi :\in Ch(\tilde{\Phi}_n)$. Next we consider the possible extensions χ to each coset of $\tilde{\Phi}$ as follows. Define the complex vector space

(3.2)
$$V_{\chi} = \{g : \Phi_n \to \mathbb{C} : \forall x \in \Phi_n, \forall s \in \tilde{S}, g(s * x) = \chi(s)g(x)\}.$$

Clearly for any $g \in V_{\chi}$ we have, by (1.8),

$$\tilde{\Delta}g(x) = \sum_{s \in \tilde{S}} (g(x * s) - g(x)) = \sum_{s \in \tilde{S}} (g(s * x) - g(x)) = \lambda_{\chi}g,$$

where $\lambda_{\chi} = \sum_{s \in \tilde{S}} (\chi(s) - 1)$. It is also clear from the symmetry of \tilde{S} that $\lambda_{\chi} \in \mathbb{R}_{\leq 0}$, and $\lambda_{\chi} = 1$ if and only if $\chi \equiv 1$. Let $\mathbb{1}$ denote the constant 1 character.

We have dim $V_{\chi} = |\Phi_n : \tilde{\Phi}_n| = k$, and the formula

(3.3)
$$\langle g,h\rangle = \sum_{x\in\Phi_n} g(x)\overline{h(x)}$$

defines a scalar product on V_{χ} .

Claim 3.4. V_{χ} is an invariant subspace for Δ .

Proof. For any $s \in \tilde{S}$ we have

$$\begin{aligned} \Delta g(s*x) &= \sum_{t \in S} (g(s*x*t) - g(s*x)) \\ &= \sum_{t \in S} (\chi(s)g(x*t) - \chi(s)g(x)) = \chi(s)\Delta g(x). \end{aligned}$$

Thus Δ is a negative definite, self-adjoint operator on V_{χ} so there are k eigenfunctions $f_{\chi,1}, \ldots, f_{\chi,k} \in V_{\chi}$ of Δ with respective eigenvalues $\lambda_{\chi,1}, \ldots, \lambda_{\chi,k}$ that form an orthonormal basis with respect to the scalar product (3.3).

Since different characters are orthogonal on $\tilde{\Phi}_n$, and there are exactly $|\tilde{\Phi}_n|$ of them, we get that the system

$$\{f_{\chi,j}: \chi \in \operatorname{Ch}(\tilde{\Phi}_n), 1 \le j \le k\}$$

forms an orthonormal basis of Δ -eigenfunctions on G_n . One virtue of this particular eigenbasis is that we can bound the supremum norm of its elements.

Lemma 3.5. $\|f_{\chi,j}\|_{\infty} \leq \sqrt{k/|\Phi_n|}$

Proof. Write $f = f_{\chi,j}$ for short. We know by construction that |f| is constant along each coset of Φ_n . Let these constants be $c_1, \ldots, c_k \ge 0$. Then we can write

$$1 = \sum_{x \in \Phi_n} |f(x)|^2 = \sum_{i=1}^k c_i^2 |\tilde{\Phi}_n| \ge \max_i (c_i^2) |\tilde{\Phi}_n|.$$

Thus

$$||f||_{\infty} = \max_{i}(c_i) \le \sqrt{\frac{1}{|\tilde{\Phi}_n|}} = \sqrt{\frac{k}{|\Phi_n|}}.$$

For each $f_{\chi,j}$ we define

$$0 < \beta_{\chi,j} = \lambda_{\chi,j} / \lambda_{\chi}.$$

This can be done unless $\chi = \mathbb{1}$. The positivity follows from the fact that both λ_{χ} and $\lambda_{\chi,j}$ are negative. The subspace $V_{\mathbb{I}}$ is special, it contains all the functions that are constant along the cosets of $\tilde{\Phi}_n$. We may assume that $f_{1,1}$ is the constant function and define $\beta_{\mathbb{I},1} = 1$. Thus the following statement holds.

Claim 3.6.

$$\beta_{\chi,j}\tilde{\Delta}f_{\chi,j} = \Delta f_{\chi,j},$$

unless $\chi = 1$ and $j \geq 2$. Hence the same also holds for $c + f_{\chi,j} \circ \pi_n : G \to \mathbb{C}$ where c is an arbitrary constant, so these functions satisfy the condition Lemma 2.4. Now let $g: G_n \to \mathbb{C}$ be a function that is orthogonal to $f_{1,j}: j \geq 2$. Then we can express it as a linear combination of all the other eigenfunctions:

$$g = \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n), j = 1, \dots, k} c_{\chi, j} f_{\chi, j},$$

where $c_{1,j} = 0$ if $j \ge 2$.

Let us further choose constants $a_{\chi,j}\in\mathbb{C}$ whose value will be determined later. Let us set

(3.7)
$$B = \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k c_{\chi,j} a_{\chi,j}.$$

Finally, define $u: G \to \mathbb{C}$ with the formula

$$u(x,t) = \sum_{\chi \in Ch(\tilde{\Phi}_n)} \sum_{j=1}^k \sum_{z \in \Phi} c_{\chi,j} \cdot \left(f_{\chi,j} \circ \pi_n(z) + a_{\chi_j} \right) \cdot w(x * z^{-1}, \beta_{\chi,j}t) - B.$$

Theorem 3.9. The function u defined in (3.8) satisfies the heat equation on G with initial condition $u(x, 0) = g \circ \pi_n(x)$.

Proof. That $\Delta u = \partial_t u$ holds follows from Lemma 2.4 combined with Claim 3.6. The only thing we have to show is that u satisfies the initial condition. This is a simple calculation based on the choice of $w(x,0) = \delta_{x=1}$.

$$u(x,0) = \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k \sum_{z \in \Phi} c_{\chi,j} \cdot \left(f_{\chi,j} \circ \pi_n(z) + a_{\chi_j} \right) \cdot w(x * z^{-1}, 0) - B$$
$$= \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k \sum_{z \in \Phi} c_{\chi,j} \cdot \left(f_{\chi,j} \circ \pi_n(z) + a_{\chi_j} \right) \cdot \delta_{x * z^{-1} = 1} - B$$
$$= \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k c_{\chi,j} \cdot \left(f_{\chi,j} \circ \pi_n(x) + a_{\chi_j} \right) - B$$
$$= \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k c_{\chi,j} \cdot f_{\chi,j} \circ \pi_n(x) = g(x)$$

We are interested in non-negative real initial conditions g(x) for which the solution u(x,t) will also be real and non-negative. Then we can take the real part of both sides of (3.8) to obtain

$$(3.10)$$

$$u(x,t) = \sum_{\chi \in \operatorname{Ch}(\tilde{\Phi}_n)} \sum_{j=1}^k \sum_{z \in \Phi} \Re \left(c_{\chi,j} \cdot \left(f_{\chi,j} \circ \pi_n(z) + a_{\chi_j} \right) \right) \cdot w(x * z^{-1}, \beta_{\chi,j} t)$$

$$- \Re(B).$$

The main idea of the proof of Theorem 1.5 is to express the solution u(x,t) as a non-negative linear combination of solutions on \tilde{G} for which the gradient estimate is already known.

Our goal with introducing the constants $a_{\chi,j}$ is to force all coefficients appearing in (3.10) to be non-negative. This can be done by setting

(3.11)
$$a_{\chi,j} = \begin{cases} \frac{|c_{\chi,j}|}{c_{\chi,j}} \|f_{\chi,j}\|_{\infty} & : \quad c_{\chi,j} \neq 0\\ 0 & : \quad c_{\chi,j} = 0 \end{cases}$$

Unfortunately the use of the constants $a_{\chi,j}$ come at the cost of having to deal with the constant *B*. Next we show that *B* can be bounded in terms of *g* but independently of *n*.

Lemma 3.12. If the $a_{\chi,j}$'s are chosen according to (3.11) then $B = \sum a_{\chi,j} c_{\chi,j} \leq \sqrt{k} ||g||_2$.

Proof. First, it is clear that $B \leq \sum |c_{\chi,j}| \cdot ||f_{\chi,j}||_{\infty}$. Let us recall that $c_{\chi,j} = \langle g, f_{\chi,j} \rangle$ Then, by Cauchy-Schwarz and Lemma 3.5 we get

$$B \le \sqrt{\sum |\langle g, f_{\chi,j} \rangle|^2} \sqrt{\sum \|f_{\chi,j}\|_{\infty}^2} \le \|g\|_2 \sqrt{|\Phi_n| \frac{k}{\Phi_n}} = \sqrt{k} \|g\|_2.$$

We can summarize the results of this section as follows.

Corollary 3.13. Let $g: G_n \to [0, \infty)$ be orthogonal to the span of $\{f_{1,j}: 2 \leq j \leq k\}$. Let u(x,t) denote solution of the heat equation on G with initial conditions $u(x,0) = g \circ \pi_n(x)$. Then there exist a non-negative bounded weight function $q(\chi, j, z)$ such that

(3.14)
$$u(x,t) + \sqrt{k} \|g\|_2 = \sum_{\chi,j,z} q(\chi,j,z) w(x * z^{-1}, \beta_{\chi,j} t).$$

Remark 3. The condition that g be orthogonal to the eigenfunctions $f_{1,j}$: $2 \leq j \leq k$ is equivalent to requiring that the sum of g along any coset of $\tilde{\Phi}_n$ is the same. This is clear, since the orthogonal projection of g onto V_1 is obtained by averaging g along each coset, and thus g is orthogonal to $f_{1,j}: 2 \leq j \leq k$ if and only if this projection coincides with $f_{1,1}$ – the constant function.

4. Gradient estimate

Let us recall from [2] that since w(x,t) is a solution of the heat equation on the Abelian Cayley graph \tilde{G} , it satisfies the Li-Yau estimate

$$\frac{\tilde{\Gamma}(\sqrt{w})}{w} - \frac{\partial_t w}{2w} \le \frac{C}{t}$$

with a constant C depending only on $|\tilde{S}|$. Then, by Remark 2, the function $w_{\beta,z}(x,t) = w(x * z^{-1}, \beta t)$ satisfies

$$\frac{\Gamma(\sqrt{w_{\beta,z}})}{w_{\beta,z}} - \frac{\partial_t w_{\beta,z}}{2\beta w_{\beta,z}} \le \frac{C}{\beta t},$$

or equivalently

(4.1)
$$\beta \tilde{\Gamma}(\sqrt{w_{\beta,z}}) - \partial_t w_{\beta,z}/2 \le \frac{C}{t} w_{\beta,z}.$$

The β values appearing are the $\beta_{\chi,j}$ introduced in the previous section; to make (4.1) effective we now derive a global lower bound on these β s.

Lemma 4.2. There is a constant K depending only on Φ, S, \tilde{S} such that for any fixed n we have $\beta_{\chi,j} \geq 1/K$ for all $1 \neq \chi \in Ch(\tilde{\Phi}_n)$ and $1 \leq j \leq k$.

Proof. Let's fix χ and j, and let's write $\beta = \beta_{\chi,j}$ and $f = f_{\chi,j}$ for short. By Claim 3.6 we have $\beta \tilde{\Delta} f = \Delta f$. Since $f_{\chi,j}$ is defined on the finite graph G_n , we can take scalar product of both sides with $f_{\chi,j}$ and use "integration by parts" to get

(4.3)
$$\beta_{\chi,j} \sum_{x \in G_n} \sum_{t \in \tilde{S}} (f(x * t) - f(x))^2 = \sum_{x \in G_n} \sum_{s \in S} (f(x * s) - f(x))^2.$$

Each $t \in \tilde{S}$ can be written as a word in S. Suppose $t = s_{t,1}s_{t,2}\ldots s_{t,r}$ where $s_{t,1}, s_{t,2}, \ldots, s_{t,r} \in S$. (Of course r = r(t) may depend on t.) Then we can use Cauchy-Schwarz to obtain

$$(f(x * t) - f(x))^{2} = \left(\sum_{i=1}^{r} (f(x * s_{t,1} * s_{t,2} * \dots * s_{t,i}) - f(x * s_{t,1} * s_{t,2} * \dots * s_{t,i-1}))\right)^{2} \le r \sum_{i=1}^{r} (f(x * s_{t,1} * s_{t,2} * \dots * s_{t,i}) - f(x * s_{t,1} * s_{t,2} * \dots * s_{t,i-1}))^{2}.$$

Summing this for all $x \in G_n$, for any *i* the expression $x * s_{t,1} * \cdots * s_{t,i-1}$ also runs exactly over each element of G_n . Thus we get

$$\sum_{x \in G_n} (f(x * t) - f(x))^2 \le r \sum_{i=1}^{r(t)} (f(x * s_{t,i}) - f(x))^2.$$

Now we sum this last expression for all $t \in \tilde{S}$ to get

$$\sum_{x \in G_n} \sum_{t \in \tilde{S}} (f(x * t) - f(x))^2 \le r \sum_{x \in G_n} \sum_{t \in \tilde{S}} \sum_{i=1}^{r(t)} (f(x * s_{t,i}) - f(x))^2 \le r M \sum_{x \in G_n} \sum_{s \in S} (f(x * s) - f(x))^2,$$

where M is the largest of the multiplicities of the elements of the multiset $\{s_{t,i} : t \in \tilde{S}, 1 \leq i \leq r(t)\}$. Combining the last estimate with (4.3) we get $\beta \geq 1/(rM)$, so K = rM is a valid choice.

Lemma 4.4. $\tilde{\Gamma}(\sqrt{\cdot})$ is a convex operator, that is for non-negative weights c_i and non-negative functions f_i we have

$$\tilde{\Gamma}\left(\sqrt{\sum_{i} c_{i} f_{i}}\right) \leq \sum_{i} c_{i} \tilde{\Gamma}\left(\sqrt{f_{i}}\right).$$

Proof. By the definition of $\tilde{\Gamma}$ all we have to check is that, assuming all sums are convergent and all numbers are non-negative,

$$\left(\sqrt{\sum_{i} c_{i} a_{i}} - \sqrt{\sum_{i} c_{i} b_{i}}\right)^{2} \leq \sum_{i} c_{i} \left(\sqrt{a_{i}} - \sqrt{b_{i}}\right)^{2}.$$

This is a simple Cauchy-Schwarz inequality after opening the brackets and canceling as much as possible. $\hfill \Box$

Corollary 4.5. For any nonnegative bounded weight function $q(\chi, j, z)$, we have

$$\tilde{\Gamma}\left(\sqrt{\sum_{\chi,j,z} q(\chi,j,z)w_{\beta_{\chi,j},z}}\right) \leq \sum_{\chi,j,z} q(\chi,j,z)\tilde{\Gamma}(\sqrt{w_{\beta_{\chi,j},z}}).$$

We are ready to prove Theorem 1.5. We will actually show the following slightly stronger statement.

Theorem 4.6. Let $g \in L_2(G)$ a non-negative function. Let u(x,t) denote the solution of the heat equation on G with initial condition $u(x,0) = g(x) + k ||g||_2$. Then

$$\frac{\widetilde{\Gamma}(\sqrt{u})}{Ku} - \frac{\partial_t(\sqrt{u})}{\sqrt{u}} \leq \frac{C}{t} \ .$$

Proof. For each n > 1, choose a subset $H_n \subset G$ that contains exactly one element from each set $\pi_n^{-1}(x) : x \in \Phi_n$ in such a way that $1 \in H_n$ but that this element 1 is as far from the boundary of H_n as possible with respect to the graph distance. (The set H_n will look like a (skew) ball around the element 1 in G.) In particular we have $H_1 \subset H_2 \subset H_3 \ldots$, and the distance between 1 and the boundary of H_n clearly goes to infinity as n goes to infinity.

Now we describe a simple way to modify g and turn it into a function that satisfies the conditions of Corollary 3.13. Let h_n denote the "restriction" of g to Φ_n through H_n . That is, let $h_n : \Phi_n \to \mathbb{R}$ be the function defined by $h_n(x) = g(\pi_n^{-1}(x) \cap H_n)$. Note that $h_n \circ \pi_n$ coincides with g on H_n and is periodic.

However h_n still might not be orthogonal to the subspace spanned by $f_{1,j}: 2 \leq j \leq k$. We can ensure this orthogonality, according to Remark 3, by modifying g on $H_n \setminus H_{n/2}$ in such a way that for any coset D of $\tilde{\Phi}_n$ in Φ_n , the expression $\sum_{x \in D} g(\pi_n^{-1}(x) \cap H_n)$ is independent of D. This increases $\|g_{|H_n|}\|_2$ at most \sqrt{k} -fold. (The worst case is when g was 0 on all but one of the cosets.) Let g'_n denote the modified function, and let h'_n denote its restriction to Φ_n as explained in the previous paragraph.

We get that $||h'_n||_2 \leq \sqrt{k}||g||_2$, and that h'_n is orthogonal to the eigenfunctions $f_{1,j}: 2 \leq j \leq k$. Finally $h'_n \circ \pi_n$ is a periodic function that coincides with g on $H_{n/2}$. Let us denote by $u_n(x,t)$ the solution of the heat equation

with initial conditions $u(x, 0) = h'_n \circ \pi_n(x)$. Then by Corollary 3.13 there is a bounded non-negative weight function $q(\chi, j, z)$ such that

$$u_n + \sqrt{k} \|h'_n\|_2 = \sum_{\chi,j,z} q(\chi,j,z) w_{\beta_{\chi,j},z}.$$

By Lemma 4.2 there is a constant K independent of n such that each $\beta_{\chi,j} \ge 1/K$, hence by (4.1), for every χ, j pair

$$\frac{1}{K}\widetilde{\Gamma}(\sqrt{w_{\beta_{\chi,j},z}}) - \partial_t w_{\beta_{\chi,j},z}/2 \leq \frac{C}{t} w_{\beta_{\chi,j},z}$$

Thus by Corollary 4.5 the same holds for $u_n + \sqrt{k} ||h'_n||_2$, and thus also for $v_n = u_n + k ||g||_2$. So we get that for any point $x \in G$ and any $t \ge 0$

(4.7)
$$\frac{\overline{\Gamma}(\sqrt{v_n})(x,t)}{Kv_n(x,t)} - \frac{\partial_t v_n(x,t)}{2v_n(x,t)} \le \frac{C}{t}.$$

Finally, we let $n \to \infty$. The theorem then follows from Claim 4.8 below.

Claim 4.8. For any $x \in G$ and $t \ge 0$ we have $\lim_{n\to\infty} u_n(x,t) = u(x,t)$ and $\lim_{n\to\infty} \partial_t u_n(x,t) = \partial_t u(x,t)$.

Proof. Let $p_n(x) = g(x) - h'_n \circ \pi_n(x)$, and denote $U_n(x,t)$ the solution of the heat equation with initial conditions $U_n(x,0) = p_n(x)$. Then clearly $u(x,t) = U_n(x,t) + u_n(x,t)$. Note that $\partial_t u_n$, and $\partial_t U_n$ are also solutions of the heat equation with initial conditions $\Delta g, \Delta g - p_n, \Delta p_n$ respectively.

Let us denote the heat kernel on G by k. That is, $k(\cdot, y, t)$ is the probability density, at time t, of a continuous time random walk started at y. Then

$$U_n(x,t) = \sum_y p_n(y)k(x,y,t).$$

The continuous time version of the Carne-Varopoulos bound [5] implies that if d(x, y)/t is large enough, then

(4.9)
$$k(x,y,t) \le \exp\left(-cd(x,y)\ln\frac{d(x,y)}{ct}\right)$$

For a fixed x, if n is large enough, the initial condition function p_n vanishes on a ball of radius R_n around x. Since p_n is bounded on the whole G, and t

is fixed, by (4.9) we get

$$U_n(x,t) \le c \|p_n\|_{\infty} \sum_{y:d(x,y)>R_n} e^{-cd(x,y)\ln\frac{d(x,y)}{ct}}.$$

Since the volume of the balls of radius R_n grow polynomially, this sum clearly decays exponentially to 0 as $R_n \to \infty$. The same holds for $\partial_t U_n$, since Δp_n also vanishes on a ball of radius growing to infinity around any particular point x as $n \to \infty$.

Finally let briefly indicate what modifications are necessary to obtain Theorem 1.7.

Proof of Theorem 1.7. From [8] we get that there is a constant C > 0 such that for any solution $w : \tilde{G} \to [0, \infty)$ of the equation $\tilde{\Delta}w = \partial_t w$ that is periodic with respect to $\langle s^n : s \in \tilde{S} \rangle$ satisfies

(4.10)
$$-\tilde{\Delta}\log w \le \frac{C}{t}.$$

The reason w is a priori required to be periodic is because [8] only proves (4.10) for finite graphs. However, by the same method as used in the proof of Theorem 1.5, and in particular by Claim 4.8 this implies that (4.10) holds for arbitrary w. Then, just as in (4.1), we find that $-\beta \log w_{\beta,z} \leq \frac{C}{t}$. Thus the statement follows, as long as we provide the analog of Lemma 4.4 for $-\tilde{\Delta} \log$. However $\tilde{\Delta}$ is linear, and log is concave, so $-\tilde{\Delta} \log$ is convex, so $-\log \sum c_i f_i \leq -\sum c_i \log f_i$ for real numbers $c_i \geq 0$ and functions $f_i \geq 0$. \Box

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