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# Essential self-adjointness for combinatorial Schrödinger operators I- Metrically complete graphs

Nabila Torki-Hamza \*

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## Abstract

We introduce the weighted graph Laplacian  $\Delta_{\omega,c}$  and the notion of Schrödinger operator of the form  $\Delta_{1,a} + W$  on a locally finite graph  $G$ . Concerning essential self-adjointness, we extend Wojciechowski's and Dodziuk's results for graphs with vertex constant weight. The main result in this work states that on any metrically complete weighted graph with bounded degree, the Laplacian  $\Delta_{\omega,c}$  is essentially self-adjoint and the same holds for Schrödinger operators provided the associated quadratic form is bounded from below. We construct for the proof a strictly positive and harmonic function which allows us to write any Schrödinger operator  $\Delta_{1,a} + W$  as a Laplacian  $\Delta_{\omega,c}$  modulo a unitary transform.

## 1 Introduction

This work is the first of a series of three articles (the others are [5] et [6]) dealing with spectral theory of Laplacians and Schrödinger operators on infinite graphs. We extend for infinite graphs some classical results of Laplacians and Schrödinger operators on non compact Riemannian manifolds.

One of the main results, Theorem 6.2, states that the Laplacian of a metrically complete weighted graph with bounded degree is essentially self-adjoint. Theorem 1.3.1 in [25] and Theorem 3.1 in [12] are Corollaries of this result. The notion of completeness used here for the weighted graphs is related to a distance built

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\*Université de Carthage; Faculté des Sciences de Bizerte; Mathématiques et Applications (05/UR/15-02); 7021-Bizerte (Tunisie); [nabila.torki-hamza@fsb.rnu.tn](mailto:nabila.torki-hamza@fsb.rnu.tn); [torki@fourier.ujf-grenoble.fr](mailto:torki@fourier.ujf-grenoble.fr)

according to the vertex weight and the edge conductance. The second article discusses the non complete case for which we will give conditions of potential increasing to insure essential self-adjointness of a Schrödinger operator. And the third article deals with the case of combinatorial Schrödinger operators with magnetic fields.

One of the classical famous questions in mathematical physics is to find conditions of essential self-adjointness for Schrödinger operators. Many works study this problem in the case of  $\mathbb{R}^n$ . It is mentioned in [1], that the first article in this topic is that of Weyl [23], and the classical results can be found in the famous four-books [16] of Reed-Simon.

Later Gaffney proved, in [9] and [10] (see also [3] and [21]), that the Laplacian of a complete Riemannian manifold is essentially self-adjoint. And it is proved (see [16], [18] and [19]) that on a complete Riemannian manifold, a Schrödinger operator is essentially self-adjoint if the potential satisfies a bounded condition. The Beltrami-Laplacian on a Riemannian manifold has many analogues on graphs: Laplacians on quantum graphs (see [8], [14], [2]); combinatorial Laplacians (see [4], [25], [11],[12]), or physical Laplacians (see [24]).

In this article, we introduce a different Laplacian, denoted by  $\Delta_{\omega,c}$  "the *weighted graph Laplacian*", for a locally finite weighted graph with a weight  $\omega$  on the vertices and a conductance  $c$  on the edges. It generalizes the "combinatorial Laplacian" of [25] (it is nothing but  $\Delta_{1,1}$ ); as well as the "graph Laplacian" of [12] (which is  $\Delta_{1,c}$ ). This notion had been introduced in the case of finite graphs, see [4] and [22].

In Section 2, we give immediate properties of the weighted graph Laplacian  $\Delta_{\omega,c}$  and we prove that it is unitary equivalent to a Schrödinger operator:  $\Delta_{1,a} + W$ , modulo a diagonal transform.

In Section 3, we prove that if the weight  $\omega$  is constant, the operator  $\Delta_{\omega,c}$  is essentially self-adjoint. The idea is inspired from Wojciechowski's method [25]. The same procedure can be used to prove that if we add a potential  $W$  which is bounded from below, it stills essentially self-adjoint.

Section 4 consists on building a strictly positive function  $\Phi$  which is harmonic for a positive Schrödinger operator. We need for this construction a discrete version of local Harnack inequality, a solved Dirichlet problem and a discrete minimum principle.

We use such function  $\Phi$ , in Section 5, to prove the important result that *every positive Schrödinger operator is unitary equivalent to a Laplacian*.

In Section 6, we consider graphs with bounded degree. For a given Schrödinger operator  $\Delta_{1,a} + W$ , we introduce a distance  $\delta_a$  on the graph, and we prove that *for a metrically complete weighted graph, the Schrödinger operator  $\Delta_{1,a} + W$  is essentially self-adjoint if its quadratic form is bounded from below*. Then we give a counter-example to show that this Theorem is not a particular case of Theorem 3.2. In the same section, we deduce a similar Theorem for the Laplacian  $\Delta_{\omega,c}$ . It

is the main result of this article which is a generalization for metrically complete graphs of Gaffney's theorem.

This paper is in fact a translation of [21]. We correct the end of the proof of Lemma 4.1 and we add Remark 6.4. Furthermore we update some recent references.

## 2 Preliminaries

Let  $G$  an infinite locally finite connected graph. We denote by  $V$  the set of vertices and by  $E$  the set of edges. If  $x$  and  $y$  are two vertices of  $V$ , we denote by  $x \sim y$  if they are connected by an edge which would be indicated by  $\{x, y\} \in E$ . Sometimes when  $G$  is assumed to be oriented, we denote by  $[x, y]$  the edge from the origin  $x$  to the extremity  $y$ , and by  $\overline{E}$  the set of all oriented edges. It is to mention that no result depends on the orientation.

The simplest natural infinite locally finite connected graph is the *graph*  $\mathbb{N}$  which is the graph with  $V \equiv \mathbb{N}$  and  $E = \{\{n, n + 1\}; n \in \mathbb{N}\}$ .

The space of real functions on the graph  $G$  is considered as the space of real functions on  $V$  and is denoted by

$$C(V) = \{f : V \longrightarrow \mathbb{R}\}$$

and  $C_0(V)$  is its subset of finite supported functions. We consider, for any weight  $\omega : V \longrightarrow \mathbb{R}_+^*$  on vertices, the space

$$l_\omega^2(V) = \left\{ f : V \longrightarrow \mathbb{R} ; \sum_{x \in V} \omega_x^2 |f(x)|^2 < \infty \right\} .$$

It is a Hilbert space when equipped by the scalar product given by

$$\langle f, g \rangle_{l_\omega^2} = \sum_{x \in V} \omega_x^2 f(x) . g(x)$$

This space is isomorphic to

$$l^2(V) = \left\{ f : V \longrightarrow \mathbb{R} ; \sum_{x \in V} |f(x)|^2 < \infty \right\}$$

with respect to the unitary transform

$$U_\omega : l_\omega^2(V) \longrightarrow l^2(V)$$

defined by

$$U_\omega(f) = \omega f$$

which preserves the set  $C_0(V)$  of finite supported real functions on  $V$ .

**Remark 2.1** *If the weight  $\omega$  is constant equal to  $\omega_0 > 0$  (ie. for any vertex  $x \in V$ , we have  $\omega_x = \omega_0$ ), then*

$$l_{\omega_0}^2(V) = l^2(V) .$$

**Definition 2.1** *The weighted graph Laplacian on  $G$  with the vertex weight  $\omega : V \rightarrow \mathbb{R}_+^*$  and the edge conductance  $c : E \rightarrow \mathbb{R}_+^*$ , is the operator on  $l_{\omega}^2(V)$ , which is denoted by  $\Delta_{\omega,c}$  and is given by:*

$$(\Delta_{\omega,c}f)(x) = \frac{1}{\omega_x^2} \sum_{y \sim x} c_{x,y} (f(x) - f(y)) \quad (1)$$

for any function  $f$  in  $l_{\omega}^2(V)$  and any vertex  $x$  in  $V$ .

**Remark 2.2** *These Laplacians satisfy elementary properties, some of them are taken from [4] and [7]:*

1. *The operator  $\Delta_{\omega,c}$  is symmetric on  $l_{\omega}^2(V)$  with domain  $C_0(V)$  and its associated quadratic form given by*

$$Q_c(f) = \sum_{\{x,y\} \in E} c_{x,y} (f(x) - f(y))^2$$

*is positive.*

2. *If the weight  $\omega$  is in  $l^2(V)$ , the constant functions are  $\Delta_{\omega,c}$ -harmonic.*
3. *The sums in the expression of  $\Delta_{\omega,c}$  are finite as the graph  $G$  is locally finite, so this operator is well defined on  $C_0(V)$ .*
4. *It is a local operator, in the sense that  $(\Delta_{\omega,c}f)(x)$  depends only on the values of  $f$  on the neighbors of  $x$ . The Laplacian  $\Delta_{\omega,c}$  can be considered as a differential operator on the graph  $G$ .*
5. *It is an elliptic operator, as for any edge  $\{x,y\}$  of the graph  $G$ , the coefficient  $c_{\{x,y\}}$  does not vanish.*
6. *The weight  $c$  does not depend on the orientation, and we have:  $c_{x,y} = c_{y,x}$ , for each neighbors  $x$  and  $y$ .*

To work on the same function space  $l^2(V)$ , we use the unitary transform  $U_{\omega}$ . More precisely, the Proposition 2.1, asserts that  $\Delta_{\omega,c}$  is unitary equivalent to a Schrödinger operator of the graph  $G$ . Let us first give the definition of a combinatorial Schrödinger operator.

**Definition 2.2** *A Schrödinger operator of the graph  $G$  is an operator of the form  $\Delta_{1,a} + W$  acting on functions of  $l^2(V)$ , where the potential  $W$  is a real function on  $V$  and the conductance  $a$  is a strictly positive function on  $E$ .*

**Proposition 2.1** *If*

$$\widehat{\Delta} = U_\omega \Delta_{\omega,c} U_\omega^{-1}$$

*then  $\widehat{\Delta}$  is a Schrödinger operator of  $G$  and we have*

$$\widehat{\Delta} = \Delta_{1,a} + W$$

*where  $a$  is a strictly positive function on  $E$  given by:*

$$a_{x,y} = \frac{c_{x,y}}{\omega_x \omega_y}$$

*and the potential  $W : V \rightarrow \mathbb{R}$  is given by :*

$$W = -\frac{1}{\omega} \Delta_{1,a} \omega .$$

*Proof.*

For any  $g$  in  $C_0(V)$  and  $x$  in  $V$ , we have:

$$\begin{aligned} (\widehat{\Delta}g)(x) &= \omega_x (\Delta_{\omega,c} U_\omega^{-1}g)(x) \\ &= \frac{1}{\omega_x} \sum_{y \sim x} c_{x,y} \left( \frac{g(x)}{\omega_x} - \frac{g(y)}{\omega_y} \right) \\ &= \sum_{y \sim x} \frac{c_{x,y}}{\omega_x \omega_y} (g(x) - g(y)) + g(x) \frac{1}{\omega_x} \sum_{y \sim x} c_{x,y} \left( \frac{1}{\omega_x} - \frac{1}{\omega_y} \right) \\ &= (\Delta_{1,a}g)(x) + W(x)g(x) , \end{aligned}$$

where  $\Delta_{1,a}$  denotes the Laplacian on  $G$  weighted by the vertex constant weight  $\omega \equiv 1$  and by the strictly positive function  $a$  on  $E$  given by:

$$a_{x,y} = \frac{c_{x,y}}{\omega_x \omega_y}$$

and where the potential  $W : V \rightarrow \mathbb{R}$  is given by:

$$W(x) = \frac{1}{\omega_x} \sum_{y \sim x} c_{x,y} \left( \frac{1}{\omega_x} - \frac{1}{\omega_y} \right) = -\frac{1}{\omega_x} (\Delta_{1,a}\omega)(x) .$$

□

**Remark 2.3** *In Proposition 2.1, the function  $W$  might be obtained strictly negative, while the Laplacian is positive : we can take for example, the graph  $G$  with  $V = \mathbb{N}^*$  and  $n \sim n+1$  for any  $n \in \mathbb{N}^*$ , and we suppose that  $G$  is weighted by the vertex weights  $\omega_n = \frac{1}{n}$  and the edge conductance  $c_{n,n+1} = (n+1)^2$ ; then we find  $W(n) = -n(2n+1) < 0$  .*

### 3 Extension of Wojciechowski and Dodziuk's results

Our first two theorems are extensions of results due to J. Dodziuk [7] and R.K. Wojciechowski [25] concerning essential self-adjointness. Let us remind the following definitions.

**Definition 3.1** *An unbounded symmetric linear operator on a Hilbert space is called essentially self-adjoint if it has a unique self-adjoint extension.*

To prove essential self-adjointness, we use the following useful and practical criterion, deduced from Theorem X.26 in [17] .

**Criterion 3.1** *The definite positive symmetric operator  $\Delta : C_0(V) \longrightarrow l^2(V)$  is essentially self-adjoint if and only if  $\text{Ker}(\Delta^* + 1) = \{0\}$  .*

From the definition the adjoint operator  $\Delta^*$  of  $\Delta : C_0(V) \longrightarrow l^2(V)$  , we can deduce:

$$\text{Dom}(\Delta^*) = \{f \in l^2(V) ; \Delta f \in l^2(V)\} .$$

Using an idea in the proof of Theorem 1.3.1 of [25] , we prove the following result:

**Theorem 3.1** *If the weight  $\omega$  is constant on  $V$  then for any conductance  $c$  on  $E$ , the Laplacian  $\Delta_{\omega,c}$  , with domain  $C_0(V)$  , is essentially self-adjoint.*

*Proof.*

Let  $\omega_0$  a strictly positive real number, and  $\omega \equiv \omega_0$  on  $V$  . We consider a function  $g$  on  $V$  satisfying:

$$\Delta_{\omega_0,c} g + g = 0 .$$

Let us assume that there is a vertex  $x_0$  in  $V$  such that  $g(x_0) > 0$  .

The equality

$$\Delta_{\omega_0,c} g(x_0) + g(x_0) = 0$$

implies

$$\frac{1}{\omega_0^2} \sum_{y \sim x_0} c_{x_0,y} (g(x_0) - g(y)) + g(x_0) = 0 .$$

Then there exists at least a vertex  $x_1$  for which  $g(x_0) < g(x_1)$  , since  $\omega_0 > 0$  and  $c_{x,y} > 0$  for any edge  $\{x,y\}$  in  $E$  . We repeat the procedure with  $x_1$  ... Hence we build a strictly increasing sequence of strictly positive real numbers  $(g(x_n))_n$  . We deduce that the function  $g$  is not in  $l^2(V)$  .

A similar way is used to have the same conclusion when we take the assumption  $g(x_0) < 0$  .

□

**Remark 3.1** *Theorem 1.3.1 of Wojciechowski in [25] deals with the Laplacian  $\Delta_{1,1}$ , so it is a particular case of Theorem 3.1.*

We can prove similarly the following Theorem.

**Theorem 3.2** *If  $W : V \rightarrow \mathbb{R}$  is a bounded from below potential and if  $\omega_0$  is a constant weight on  $V$ , then for any conductance  $c : E \rightarrow \mathbb{R}_+$ , the Schrödinger operator  $\Delta_{\omega_0,c} + W$ , with domain  $C_0(V)$ , is essentially self-adjoint.*

*Proof.*

Let  $\kappa$  a real number bounding from below the potential  $W$ . We proceed as in the proof of Theorem 3.1, considering a function  $g$  on  $V$  satisfying:

$$\Delta_{\omega_0,c}g + Wg + \kappa_1g = 0,$$

avec  $\kappa + \kappa_1 \geq 1$ .

□

**Remark 3.2** *J. Dodziuk states in Theorem 1.2 (see [7]) that the operator  $A+W$  is essentially self-adjoint when  $A$  is a bounded positive symmetric operator on  $l^2(V)$  and when the potential  $W$  is bounded from below.*

*The operator  $A$  is  $\Delta_{1,c}$  in Theorem 3.2, and we can conclude that this Theorem is more general than Dodziuk's, since the Schrödinger operator  $\Delta_{1,c} + W$  is essentially self-adjoint when  $W$  is bounded from below, even if the operator  $A = \Delta_{1,c}$  is unbounded on  $l^2(V)$ , taking for example the locally finite graph  $G$  with unbounded degree and affected of a constant conductance  $c \equiv 1$ .*

## 4 Harmonic function on vertices

We are going to build a function  $\Phi$  strictly positive and harmonic on  $V$  which is useful on Section 5.

**Theorem 4.1** *Let  $P$  a Schrödinger operator on the graph  $G$  such that*

$$\langle Pf, f \rangle_{l^2} > 0,$$

*for any  $f$  in  $C_0(V) \setminus \{0\}$ .*

*Then there exists a  $P$ -harmonic strictly positive function  $\Phi$  on  $V$ .*

The proof of Theorem 4.1 uses Lemma 4.1 which gives a local Harnack's inequality for graphs. At first we present the following definitions:



**Definition 4.1** A subgraph  $G'$  of  $G$  is a graph having the set of its vertices included in  $V$  and the set of its edges a subset of  $E$  .

**Definition 4.2** For a subgraph  $G'$  of  $G$  with the set of vertices  $K$  , we mix up  $G'$  with  $K$ , and we define:

- the interior of  $K$  denoted by  $\overset{\circ}{K}$

$$\overset{\circ}{K} = \{x \in K; y \sim x \Rightarrow y \in K\}$$

- the boundary of  $K$  denoted by  $\partial K$

$$\partial K = K \setminus \overset{\circ}{K} = \{x \in K ; \exists y \in V \setminus K, y \sim x\}$$

- $K$  is connected if and only if for any vertices  $x, y$  in  $K$ , there exist vertices  $x_1, x_2, \dots, x_n$  , such that

$$x_i \in K, x_1 = x, x_n = y, \{x_i, x_{i+1}\} \in E(G')$$

for any  $1 \leq i \leq n - 1$  .

**Lemma 4.1** (Harnack) Let  $P$  a Schrödinger operator on the graph  $G$  . Let  $G'$  a sub-graph of  $G$ , and let us denote its set of vertices by  $K$ . We assume that the interior of  $K$  is finite connected. Then there exists a constant  $k > 0$  such that, for any function  $\varphi : V \rightarrow \mathbb{R}$  strictly positive on  $K$  and satisfying

$$(P\varphi) \upharpoonright \overset{\circ}{K} \equiv 0 ,$$

we have:

$$\frac{1}{k} \leq \frac{\varphi(x)}{\varphi(y)} \leq k$$

for any  $x, y$  in  $\overset{\circ}{K}$  .

The resolution of the Dirichlet problem given by Lemma 4.2 is useful to prove Theorem 4.1 .

**Lemma 4.2** (Dirichlet) Let  $P$  a Schrödinger operator on the graph  $G$  such that for any  $f \in C_0(V) \setminus \{0\}$  we have

$$\langle Pf, f \rangle_{l^2} > 0 .$$

Then for any subgraph  $G'$  of  $G$  such that the interior of the set  $K$  of its vertices is finite connected and for any function  $u : \partial K \rightarrow \mathbb{R}$  , there exists a unique function  $f$  on  $K$  satisfying the following two conditions:

$$(i) \quad (Pf) \upharpoonright \overset{\circ}{K} \equiv 0 .$$

$$(ii) \quad f \upharpoonright \partial K \equiv u .$$

Furthermore, if  $u$  is positive and not identically null, then  $f$  is strictly positive on  $\overset{\circ}{K}$  .

To prove the strict positivity in Lemma 4.2 , we will use a discrete version of the "minimum principle" , given by Lemma 4.3 in [7] .

**Lemma 4.3** (Minimum principle) *Let  $P = \Delta_{1,a} + W$  Schrödinger operator on the graph  $G$  , where  $W > 0$  , and let  $G'$  a subgraph of  $G$  such that the set  $K$  of its vertices has a finite connected interior. We assume that there exist a function  $f$  satisfying*

$$\langle Pf, f \rangle_{l^2} \geq 0$$

*in the interior of  $K$  and an interior vertex  $x_0$  so that  $f(x_0)$  is minimum and negative. Then  $f$  is constant on  $K$  .*

### Proof of lemma 4.2

We proceed by steps.

- For the uniqueness, we suppose the existence of two functions  $f$  and  $g$  with finite support in  $K$  satisfying the two conditions of the theorem. Then it follows that  $P(f - g) \upharpoonright \overset{\circ}{K} \equiv 0$  , and  $(f - g) \upharpoonright \partial K \equiv 0$  . This implies

$$\langle P(f - g), f - g \rangle_{l^2} = 0 .$$

By the hypothesis on  $P$ , we deduce the nullity of  $(f - g)$  .

- The uniqueness give the existence since the function space on  $K$  is finite dimensional.
- We take a positive not identically null function  $u$  and we argue by contradiction, to show that  $f$  is strictly positive in the interior of  $K$  . Assume the existence of a vertex in  $\overset{\circ}{K}$  which has a negative image by  $f$ . Let  $x_0$  the vertex realizing the minimum of  $f$  on  $\overset{\circ}{K}$  which is finite and connected. Thus we have  $f(x_0) \leq 0$  and  $Pf$  vanishes on  $\overset{\circ}{K}$  . And from Lemma 4.3 , the function  $f$  is constant and negative on  $K$  . This contradicts  $f \upharpoonright \partial K \equiv u$  since the function  $u$  is supposed a non identically null function. Hence  $f$  est strictly positive on  $K$  .

□

The proof of Harnack's inequality is inspired from proofs of Lemma 1.6 and Corollary 2.3 in [7], noticing that the constant  $k$  does not depend on the function  $\varphi$ .

**Proof of lemma 4.1**

Let us consider a finite subgraph  $K$  with a connected interior, and a function  $\varphi : V \rightarrow \mathbb{R}$  strictly positive on the set of vertices of  $K$  and  $P$ -harmonic on the set of the vertices of  $\overset{\circ}{K}$ . Let  $x$  and  $y$  two vertices of  $\overset{\circ}{K}$ .

- (i) First we suppose that  $\{x, y\}$  is an edge.  
As  $(P\varphi)(x) = 0$ , ie

$$\sum_{z \sim x} a_{x,z} [\varphi(x) - \varphi(z)] + W(x) \varphi(x) = 0,$$

then

$$\left( \sum_{z \sim x} a_{x,z} \right) \varphi(x) + W(x) \varphi(x) = \sum_{z \sim x} a_{x,z} \varphi(z).$$

By the positivity of the functions  $\varphi$  and  $a$ , We obtain the following inequality:

$$\left[ W(x) + \sum_{z \sim x} a_{x,z} \right] \varphi(x) \geq a_{x,y} \varphi(y).$$

Let us denote by  $\alpha = \min \{a_{r,s}; r, s \in K, r \sim s\}$  and

$$A = \sum_{r,s \in K, r \sim s} a_{r,s}.$$

The finiteness of  $K$  induce  $\alpha > 0$  et  $A < \infty$ . Hence denoting:

$$k_0 = \frac{\max(0, \max_K W) + A}{\alpha},$$

we have:  $k_0 > 0$ , and we find

$$\frac{1}{k_0} \leq \frac{\varphi(x)}{\varphi(y)} \leq k_0.$$

- (ii) If the vertices  $x$  and  $y$  are not neighbors, by the connectedness of  $\overset{\circ}{K}$ , there exists a path connecting  $x$  to  $y$  in  $\overset{\circ}{K}$ . Let us denote

the consecutive vertices of the path by:  $x_1 = x, x_2, x_3, \dots, x_d = y$ .  
So we have:

$$\frac{1}{k_0} \leq \frac{\varphi(x_i)}{\varphi(x_{i+1})} \leq k_0, \quad \text{pour } 1 \leq i \leq d-1,$$

hence we deduce:

$$\frac{1}{k_0^d} \leq \frac{\varphi(x)}{\varphi(y)} \leq k_0^d.$$

Then, noticing that  $k_0 \geq 1$  and taking  $k = k_0^D$ , with  $D$  the number of edges of the subgraph  $K$ , we obtain

$$\frac{1}{k} \leq \frac{\varphi(x)}{\varphi(y)} \leq k.$$

□

### Proof of Theorem 4.1

Assume that  $\langle Pf, f \rangle > 0$  for any function  $f \in C_0(V) \setminus \{0\}$ . Let  $x_0$  a fixed vertex in  $V$ , which we take as an “origin”. Consider for  $n \geq 1$ , the subgraph  $G_n$  of  $G$ , such that the set of its vertices is the ball centered in  $x_0$  with a radius  $n$  denoted by  $\mathcal{B}_n$ ,

$$\mathcal{B}_n = \{x \in V; d(x_0, x) \leq n\}$$

where  $d(x, y)$  is the combinatorial distance between the vertices  $x$  and  $y$  in  $V$ , which is the number of the edges of the shortest path connecting  $x$  to  $y$ . The ball  $\mathcal{B}_n$  is connected and we apply Lemma 4.2, taking it as  $K$ , and choosing as function  $u$  the constant function 1 on  $\partial\mathcal{B}_n$ .

We proceed on three steps:

- First step: There exists a function  $\psi_n \in C_0(V)$  satisfying  $P\psi_n \equiv 0$ , and such that  $\psi_n > 0$  in the interior of  $\mathcal{B}_n$  and constant 1 on  $\partial\mathcal{B}_n$ . Then we consider the function  $\Phi_n \in C_0(V)$  given by:

$$\Phi_n(x) = \frac{\psi_n(x)}{\psi_n(x_0)}.$$

It satisfies the four following conditions:

- $\Phi_n(x_0) = 1$ .
- $P\Phi_n \equiv 0$  in the interior of  $\mathcal{B}_n$ .
- $\Phi_n \upharpoonright \partial\mathcal{B}_n \equiv \frac{1}{\psi_n(x_0)}$  strictly positive constant.
- $\Phi_n > 0$  on  $\mathcal{B}_n$ .

- Second step: Let  $x$  a vertex in  $V$  , and  $n_0$  a fixed integer such that  $x$  is in the interior of  $\mathcal{B}_{n_0}$  .

Then for any  $n \geq n_0$  , we have:  $\mathcal{B}_{n_0} \subseteq \mathcal{B}_n$  . Furthermore  $\Phi_n$  is strictly positive  $\mathcal{B}_{n_0}$  and  $P$ -harmonic in the interior of  $\mathcal{B}_{n_0}$  . Then from Lemma 4.1 , there exists a constant  $k_{n_0} > 0$  such that

$$\frac{1}{k_{n_0}} \leq \frac{\Phi_n(x)}{\Phi_n(x_0)} \leq k_{n_0} .$$

As  $\Phi_n(x_0) = 1$  , we obtain:

$$\frac{1}{k_{n_0}} \leq \Phi_n(x) \leq k_{n_0} .$$

It follows that the set  $\{\Phi_n(x)\}_{n \geq n_0}$  is included in the segment  $\left[ \frac{1}{k_{n_0}}, k_{n_0} \right]$  .

- Third step: Let us consider the subset  $C$  of  $\mathbb{R}^V$  defined by:

$$C = \prod_{x \in V} \left[ \frac{1}{k_{n_0}}, k_{n_0} \right] .$$

The sequence  $(\Phi_n)_{n \geq n_0}$  is in the compact  $C$  , so it has a convergent subsequence  $(\Phi_{h(n)})_{n \geq n_0}$  for the topology of  $\mathbb{R}^V$  to a function  $\Phi$  satisfying in particular the two following conditions:

- $\Phi$  is strictly positive on  $V$  , since  $\Phi(x) \in \left[ \frac{1}{k_{n_0}}, k_{n_0} \right]$  , for any vertex  $x$  in  $V$  .
- $P\Phi \equiv 0$  on  $V$  , since  $\lim_{n \rightarrow \infty} P\Phi_{h(n)}(x) = P\Phi(x)$  , for any vertex  $x$  in  $V$  .

□

The function  $\Phi$  given by Theorem 4.1 is used to build a unitary transform in Theorem 5.1 .

## 5 Any positive Schrödinger operator is unitary equivalent to a Laplacian

We prove that under a positivity condition, a Schrödinger operator is unitary equivalent to a Laplacian  $\Delta_{\omega,c}$  .

**Theorem 5.1** *Let  $P$  a Schrödinger operator on a graph  $G$  . We assume that*

$$\langle Pf, f \rangle_{l^2} > 0$$

*for any function  $f \in C_0(V) \setminus \{0\}$  .*

*Then there exist a weight function  $\omega : V \longrightarrow \mathbb{R}_+^*$  on  $V$  and a conductance  $c : E \longrightarrow \mathbb{R}_+^*$  on  $E$  such that the operator  $P$  is unitary equivalent to the weighted graph Laplacian  $\Delta_{\omega,c}$  on  $G$  .*

*Proof.*

We will use a function  $\Phi$  which is  $P$ -harmonique and strictly positive, given by Theorem 4.1. Let  $P = \Delta_{1,a} + W$  a Schrödinger operator satisfying the hypothesis of the Theorem. By Theorem 4.1 , there exists a strictly positive  $P$ -harmonique function  $\Phi$  on  $V$ . Then we obtain:

$$W = -\frac{\Delta\Phi}{\Phi} .$$

Let us set  $\omega = \Phi$  and for any  $g \in l^2(V)$  ,  $f = \frac{g}{\Phi}$  .

We will prove that  $\langle Pg, g \rangle_{l^2} = \langle \Delta_{\omega,c}f, f \rangle_{l^2_\omega}$  .

Let us compute

$$\begin{aligned} \langle Pg, g \rangle_{l^2} &= \langle \Delta(f\Phi) + Wf\Phi, f\Phi \rangle_{l^2} \\ &= \langle \Delta(f\Phi) - f\Delta\Phi, f\Phi \rangle_{l^2} \\ &= \sum_{x \in V} \left[ \sum_{y \sim x} a_{x,y} (f(x)\Phi(x) - f(y)\Phi(y)) \right. \\ &\quad \left. - f(x) \left( \sum_{y \sim x} a_{x,y} [\Phi(x) - \Phi(y)] \right) f(x)\Phi(x) \right] \\ &= \sum_{x \in V} f(x)\Phi(x) \sum_{y \sim x} a_{x,y} \Phi(y) [f(x) - f(y)] \\ &= \sum_{x \in V} \Phi^2(x) f(x) \frac{1}{\Phi^2(x)} \sum_{y \sim x} a_{x,y} \Phi(x)\Phi(y) [f(x) - f(y)] . \end{aligned}$$

Setting

$$c_{x,y} = a_{x,y} \Phi(x)\Phi(y) ,$$

we deduce:

$$\langle Pg, g \rangle_{l^2} = \langle \Delta_{\omega,c}f, f \rangle_{l^2_\omega} .$$

So

$$P = U^{-1} \Delta_{\omega,c} U ,$$

where  $U : l^2(V) \longrightarrow l^2_\omega(V)$  is given by

$$U(g) = \frac{g}{\Phi} .$$

Thus  $P$  is unitary equivalent to the Laplacian  $\Delta_{\omega,c}$ , with the weight  $\omega \equiv \Phi$  and the conductance  $c$  given by

$$c_{x,y} = a_{x,y} \Phi(x) \Phi(y) .$$

□

## 6 Metrically complete graphs

We adapt to graphs the G. and I. Nenciu's method (see [15]) in the proof of Theorem 6.1 , using Agmon's estimates which are given by the following technical lemma.

**Lemma 6.1** *Let  $H = \Delta_{1,a} + W$  a Schrödinger operator on  $G$ ,  $\lambda$  a real number and  $v \in C(V)$  . We assume that  $v$  is a solution of the equation:*

$$(H - \lambda)(v) = 0 . \tag{2}$$

Then for any  $f \in C_0(V)$  , we have:

$$\begin{aligned} \langle fv, (H - \lambda)(fv) \rangle_{l^2} &= \sum_{\{x,y\} \in E} a_{x,y} v(x) v(y) [f(x) - f(y)]^2 \\ &= \frac{1}{2} \sum_{x \in V} v(x) \sum_{y \sim x} a_{x,y} v(y) [f(x) - f(y)]^2 . \end{aligned}$$

*Proof.*

Let us assume that:  $(H - \lambda)(v) = 0$  , ie. for any vertex  $x \in V$  ,

$$\sum_{y \sim x} a_{x,y} (v(x) - v(y)) + W(x) v(x) = \lambda v(x)$$

Let us compute  $S = \langle fv, (H - \lambda)(fv) \rangle_{l^2}$

$$\begin{aligned} S &= \sum_{x \in V} f(x) v(x) [(H - \lambda)(fv)](x) \\ &= \sum_{x \in V} f(x) v(x) W(x) f(x) v(x) - \lambda f(x) v(x) \\ &\quad + \sum_{x \in V} \sum_{y \sim x} a_{x,y} [f(x) v(x) - f(y) v(y)] . \end{aligned}$$

And by the assumption on  $v$  , we have:

$$\lambda f(x) v(x) - W(x) f(x) v(x) = \sum_{y \sim x} a_{x,y} f(x) [v(x) - v(y)] .$$

Then, replacing in the precedent expression, we find:

$$\begin{aligned} S &= \sum_{x \in V} f(x) v(x) \sum_{y \sim x} a_{x,y} v(y) [f(x) - f(y)] \\ &= \sum_{x \in V} \sum_{y \sim x} a_{x,y} v(x) v(y) [f^2(x) - f(x) f(y)] \end{aligned}$$

As  $a_{x,y} = a_{y,x}$  , the expression becomes:

$$S = \sum_{\{x,y\} \in E} a_{x,y} v(x) v(y) [f^2(x) - f(x) f(y) + f^2(y) - f(x) f(y)]$$

Finally:

$$\begin{aligned} \langle f v, (H - \lambda)(f v) \rangle_{l^2} &= \sum_{\{x,y\} \in E} a_{x,y} v(x) v(y) [f(x) - f(y)]^2 \\ &= \frac{1}{2} \sum_{x \in V} v(x) \sum_{y \sim x} a_{x,y} v(y) [f(x) - f(y)]^2 . \end{aligned}$$

□

**Definition 6.1** A graph  $G$  is called with bounded degree if there exists an integer  $N$  such that for any  $x \in V$  we have:  $\#\{y \in V; y \sim x\} \leq N$  .

**Definition 6.2** Let  $a$  a strictly positive function on the edges of the graph  $G$  . We define the  $a$ -weighted distance on  $G$  , which we denote by  $\delta_a$  :

$$\delta_a(x, y) = \min_{\gamma \in \Gamma_{x,y}} L(\gamma)$$

where  $\Gamma_{x,y}$  is the set of all edge paths  $\gamma : x_1 = x, x_2, \dots, x_n = y$  , linking the vertex  $x$  to the vertex  $y$  ; and

$$L(\gamma) = \sum_{1 \leq i \leq n} \frac{1}{\sqrt{a_{x_i x_{i+1}}}}$$

the length of the edge path  $\gamma$  .

**Theorem 6.1** Let  $H = \Delta_{1,a} + W$  a Schrödinger operator on an infinite graph  $G$  with bounded degree and such that metric associated to the distance  $\delta_a$  is complete. We assume that there exists a real number  $k$  so that

$$\langle Hg, g \rangle_{l^2} \geq k \|g\|_{l^2}^2$$

for any  $g \in C_0(V)$ . Then the operator  $H$  , with domain  $C_0(V)$ , is essentially self-adjoint.



*Proof.*

Let  $\lambda < k - 1$ , we would prove that if  $v \in l^2(V)$  and satisfies the equation

$$Hv = \lambda v ,$$

then  $v$  vanishes.

We set  $R > 0$  and a vertex  $x_0$  as the origin. Let us denote:

$$B_R = \{x \in V; \delta_a(x_0, x) \leq R\}$$

the ball centered in  $x_0$  and with radius  $R$  for the distance  $\delta_a$ .

Let us consider the function  $f$  defined on  $V$  by

$$f(x) = \min(1, \delta_a(x, V \setminus B_{R+1})) .$$

Hence we have:

$$f \upharpoonright B_R \equiv 1, \quad f \upharpoonright V \setminus B_{R+1} \equiv 0, \quad f(B_{R+1} \setminus B_R) \subseteq [0, 1]$$

The support of  $f$  is in the bounded ball  $B_{R+1}$  which is finite by the completeness of the metric associated to the distance  $\delta_a$ .

By the assumption on  $H$  and the finiteness of the support of  $fv$  in  $B_{R+1}$ , we find the following inequalities:

$$\langle fv, (H - \lambda)(fv) \rangle_{l^2} \geq (k - \lambda) \sum_{x \in B_{R+1}} (fv)^2(x) \geq \sum_{x \in B_R} v^2(x)$$

On the other hand, using Lemma 6.1, we find:

$$\begin{aligned} \langle fv, (H - \lambda)(fv) \rangle_{l^2} &= \frac{1}{2} \sum_{x \in V} \sum_{y \sim x} a_{x,y} v(x) v(y) [f(x) - f(y)]^2 \\ &\leq \frac{1}{2} \sum_{x \in V} \sum_{y \sim x} a_{x,y} v^2(x) [f(x) - f(y)]^2 \end{aligned}$$

using the fact that  $a_{x,y} = a_{y,x}$  and that:

$$v(x) v(y) \leq \frac{1}{2} (v^2(x) + v^2(y)) .$$

As every restriction of  $f$  to  $B_R$  and to  $V \setminus B_{R+1}$  are constant functions, then the preceding inequality becomes:

$$\begin{aligned} \langle fv, (H - \lambda)(fv) \rangle_{l^2} &\leq \frac{1}{2} \sum_{x \in B_{R+1} \setminus B_R} \sum_{y \sim x} a_{x,y} v^2(x) [f(x) - f(y)]^2 \\ &\leq \frac{1}{2} \sum_{x \in B_{R+1} \setminus B_R} \sum_{y \sim x} a_{x,y} v^2(x) (\delta_a(x, y))^2 \end{aligned}$$

The last inequality is obtained by the fact that  $f$  is a 1-Lipschitz continuous function since it is the minimum of two 1-Lipschitz continuous functions.

Since the distance  $\delta_a$  satisfies the condition:

$$\delta_a(x, y) \leq \frac{1}{\sqrt{a_{x,y}}}$$

if  $\{x, y\}$  is an edge, and the degree of  $G$  is bounded by  $N$ , we have:

$$\langle fv, (H - \lambda)(fv) \rangle_{l^2} \leq \frac{1}{2}N \sum_{x \in B_{R+1} \setminus B_R} v^2(x)$$

Hence, for any  $R > 0$ , we find:

$$\sum_{x \in B_R} v^2(x) \leq \langle fv, (H - \lambda)(fv) \rangle_{l^2} \leq \frac{1}{2}N \sum_{x \in B_{R+1} \setminus B_R} v^2(x)$$

And since  $v \in l^2(V)$ , making  $R$  tend to  $\infty$ , it results that:

$$\lim_{R \rightarrow \infty} \sum_{x \in B_{R+1} \setminus B_R} v^2(x) = 0.$$

It follows  $\|v\|_{l^2}^2 = 0$ .

□

**Theorem 6.2** *Let  $G$  an infinite graph with bounded degree and which is weighted by  $\omega$  on  $V$  and a conductance  $c$  on  $E$ . We assume that the metric associated to the distance  $\delta_a$  is complete, where  $a$  is the function given by*

$$a_{x,y} = \frac{c_{x,y}}{\omega_x \omega_y}.$$

*Then the Laplacian  $\Delta_{\omega,c}$ , with domain  $C_0(V)$ , is essentially self-adjoint.*

*Proof.*

By Lemma 2.1, the operator  $\Delta_{\omega,c}$  is unitary equivalent to the Schrödinger operator  $H = \Delta_{1,a} + W$ , where

$$a_{x,y} = \frac{c_{x,y}}{\omega_x \omega_y}$$

and

$$W(x) = \frac{1}{\omega_x^2} \sum_{y \sim x} c_{x,y} \left( 1 - \frac{\omega_x}{\omega_y} \right).$$

And we apply Theorem 6.1 for the operator  $H$  which satisfies the assumptions, since  $\Delta_{\omega,c}$  is positive and

$$\langle Hg, g \rangle_{l^2} = \left\langle \Delta_{\omega,c} \frac{g}{\omega}, \frac{g}{\omega} \right\rangle_{l^2_\omega}$$

in the proof of Theorem 5.1 .

□

**Remark 6.1** *Theorem 6.1 is not particular case of Theorem 3.2. In fact in Theorem 6.1, the potential  $W$  is not necessarily bounded from below. For example let  $G$  the graph such that  $V = \mathbb{N} \setminus \{0, 1\}$  and  $n \sim n + 1$  for any  $n$  . We assume that  $G$  is weighted by the vertex weight  $\omega_n = \frac{1}{n \log n}$  and by the constant edge conductance  $c_n = 1$  . The distance  $\delta_a$  is given by:*

$$\delta_a(n_0, n) = \sum_{n_0 \leq k \leq n} \frac{1}{\sqrt{a_{k,k+1}}}$$

but

$$\frac{1}{\sqrt{a_{k,k+1}}} = \frac{1}{\sqrt{k(k+1) \log k \log(k+1)}} \sim \frac{1}{k \log k} ,$$

then

$$\delta_a(n_0, n) \xrightarrow{n \rightarrow \infty} \infty ,$$

and the associated metric is complete.

Furthermore, setting

$$H = \Delta_{1,a} + W ,$$

we have:

$$\langle Hg, g \rangle_{l^2} = \left\langle \Delta_{\omega,c} \frac{g}{\omega}, \frac{g}{\omega} \right\rangle_{l^2_\omega} \geq 0 ,$$

for any  $g \in C_0(V)$  .

While the potential  $W$  is not bounded from below, since we obtain, after calculation:

$$W(n) = 2n^2 \log^2 n - n \log n [(n+1) \log(n+1) + (n-1) \log(n-1)] \underset{\infty}{\sim} -\log n$$

which goes to  $-\infty$  .

**Remark 6.2** *In the Example of Remark 6.1 , the choice of the weight according to log is crucial. In fact, setting power functions, we can not have at the same time the metric  $\delta_a$  complete and the potential  $W$  not bounded from below. For example let  $G$  the graph such that  $V = \mathbb{N} \setminus \{0, 1\}$  and  $n \sim n + 1$  for any  $n$  ,*

and assume  $G$  weighted by the vertex weight  $\omega_n = \frac{1}{n^\alpha}$  and the edge conductance  $c_n = \frac{1}{n^\beta}$ . The distance  $\delta_a$  is given by:

$$\delta_a(n_0, n) = \sum_{n_0 \leq k \leq n} \left( \frac{k^\beta}{(k^\alpha(k+1)^\alpha)} \right)^{\frac{1}{2}} .$$

And an easy calculation show that

$$\delta_a \text{ is complete if and only if } \alpha - \frac{1}{2} \beta \leq 1 .$$

We obtain easily for the potential:

$$W_n \sim -\alpha(\alpha - \beta - 1)n^{2\alpha - \beta - 2} .$$

Hence for  $\alpha - \frac{1}{2} \beta \leq 1$ , the potential  $W$  is bounded from below.

**Remark 6.3** The completeness of the metric  $\delta_a$  is not a necessary condition to essential self-adjointness of the Laplacian  $\Delta_{\omega,c}$  (or the Schrödinger operator  $\Delta_{1,a} + W$  .)

In fact, let  $G$  the graph  $\mathbb{N}$ . For any edge conductance  $a$ , the Laplacian  $\Delta_{1,a}$  is essentially self-adjoint by Theorem 3.1 . While the metric given by the distance  $\delta_a$  is not necessarily complete: for example when  $a_n = (n+1)^{-2-\varepsilon}$ , for an  $\varepsilon > 0$  .

We give in the paper [5] some increasing conditions of the potential insuring the essential self-adjointness of a Schrödinger operator on metrically non complete graphs.

**Remark 6.4** Theorem 6.2 and Keller-Lenz's Theorem are not deduced one from another. For example, let  $G$  the graph  $\mathbb{N}$  . We consider the two following cases:

1. Let us choose the vertex weight  $\omega_n = \frac{1}{n+1}$  and the constant edge conductance  $c_n = 1$ . For a fixed vertex  $n_0$ , we have

$$\delta_a(n_0, n) = \sum_{n_0 \leq k \leq n} \frac{1}{\sqrt{k(k+1)}} \xrightarrow{n \rightarrow \infty} \infty ,$$

So the associated metric is complete. Hence by Theorem 6.2, we conclude that the Laplacian  $\Delta_{\omega,1}$  is essentially self-adjoint.

But the sum  $\sum_n \omega_n^2$  is finite, so the assumption (A) is not satisfied. Hence we can not conclude by Keller-Lenz's Theorem.

2. Let us choose now the vertex weight  $\omega_n = \frac{1}{\sqrt{n+1}}$  and the edge conductance  $c_n = n^2$ . Then

$$\delta_a(n_0, n) = \sum_{n_0 \leq k \leq n} \frac{1}{k((k+1)(k+2))^{\frac{1}{4}}},$$

which is convergent. Then the associated metric is non complete, and we can not apply Theorem 6.2 here. While Keller-Lenz's Theorem can be applied as  $\sum_n \omega_n^2$  is not finite.

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