# Some properties of (elliptic (non)) selfadjoint differential operators on locally finite weighted graphs

We survey some properties of selfadjoint and non selfadjoint operators in the discrete case. The author first motivation was to understand and try to reformulate Lieb-Thirring type inequalities and ideas from [Bög21] in a different setting. It is the perfect opportunity for the author to face and cope with a variety of new objects that are easier to handle on locally finite weighted graphs. **FINISH**

A peculiar attention is devoted to justify arguments more or less ignored by some authors...

This undergraduate research project considered arXiv, sciencedirect... as a giant puzzle. It was a fun game to play whose objective was to build from (really) dispersed informations. This document is a sort of compilation of results the author tried to learn.

At the end of the document, one can find notes of a mini-course by G. Berkolaiko given at the *Institut de Mathématiques de Toulouse* (3rd and 4th July, 2024). Moreover, I've added two notes taken during the summer.

*Per loca pastorum deserta atque otia dia.*

Contents

This research project started to emerge after discussions at the end of the *Fourier series* course. I deeply thank Julien Royer (*merci Julien!!*) for guiding me, giving me the opportunity to assist to the 2024 MAQM Conference *Spectral and Scattering theory* and to the mini-course of Gregory Berkolaiko *Counting zeros of graphs eigenfunctions*. It was really tough to follow (*je crois que j'ai survécu!*) but of the biggest interest. I am glad to have met Laurens Lavielle and truly hope you'll find a way to tackle your $\lambda$, $\alpha$, $\xi$ and way more!

**Attention.** On demande au lecteur de ne pas être trop exigeant. Ce texte a été écrit pour l'essentiel dans un court laps de temps (un peu plus d'une semaine) et n'est rien de plus qu'une compilation de résultats trouvés ici et là. Tout au plus, on comble certains trous en introduisant ce qui semblait naturellement manquer. Honnêtement, comme aucune contrainte n'était imposée (merci!!!), ce texte n'est pas plus qu'un petit jeu d'exploration un peu enfantine. On ne s'aventure pas trop dans les détails. Cela sous-entend qu'il faudra reprendre (beaucoup plus) sérieusement le travail plus tard. Ce texte ne prétend à aucune originalité mais cherche à rassembler, certes un peu maladroitement, diverses idées. Toute erreur est fait de l'auteur.

L'auteur espère poursuivre sa voie sur un versant plus algébrique du sujet sans pour autant négliger l'aspect analytique qui lui tient tant à cœur. Ce fut une grande joie de découvrir ce sentiment d'obsession pour une idée.

Beaucoup de remarques resteront en suspens et l'on ne trouvera en fin de compte, malheureusement, pas tant de non autoadjoint que cela... D'une manière générale, s'il fallait retenir une chose de ce projet, qui ne transparaît malheureusement que bien peu dans ce rapport, ce serait la suivante: les graphes constituent un modèle jouet qui en dit souvent bien plus qu'on ne le penserait!

– *This organisation, do you know what it's called?*
– *No.*
– *Spectre. It's name is Spectre.*

007 Spectre

## 1. Introduction

The selfadjoint world is nearly idyllic whereas the non selfadjoint world seems repelling, exhausting and demanding. Roughly speaking, there is no fundamental theorem of non selfadjoint operators (even if some authors argue the contrary, see for instance [Rob14, theorem 1.2]). Moreover, one cannot easily get an orthonormal decomposition in terms of the eigenvectors of a given operator or localise its eigenvalues. On a more practical viewpoint, it is tough to find monographs, textbooks or even surveys and articles discussing the non selfadjoint framework.

We first present what was the author first contact and starting point with the non selfadjoint world. The author had got the opportunity to attend the 2024 MAQM Conference at Toulouse where Sabine Bögli presented her work.

### 1.1. Bögli article.

In $\mathrm{L}^2(\mathbf{R}^d)$, the classical Lieb-Thirring inequality [LT05] for the (classical) Schrödinger operator $-\Delta + V$ is formulated as:

$$\sum_{\lambda \in \sigma_d(-\Delta+V)} |\lambda|^{p-d/2} \leq C_{d,p} \|V\|_{\mathbf{L}^p}^p \tag{1}$$

up to certain constraints on $p$ and $d$. It is, physically speaking, a trace inequality allowing to control the sum of observable energies in terms of a real potential (as soon as one knows what the trace of an operator means in an infinite dimensional vector space). When the potential is complex, the Schrödinger operator is no more necessarily selfadjoint. Demuth, Hansmann and Katriel [DHK09] treated the complex potential case. Then, Bögli [Bög21] improved it.

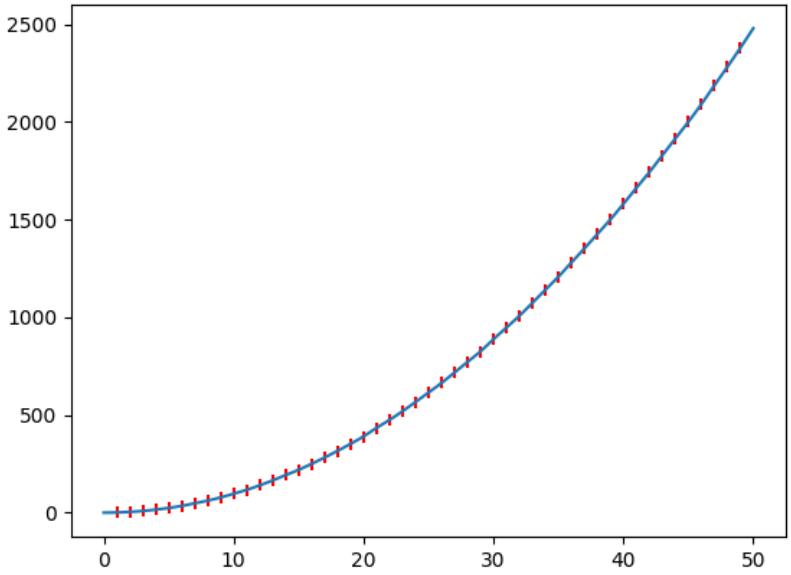
**Theorem 1.** *Let $d \in \mathbf{N}$ and $p \geq d/2+1$. Let $f : [0,+\infty[ \to ]0,+\infty[$ be a continuous non-increasing function. If $\int_0^{+\infty} f(s)d(s) < +\infty$, then there exists $C_{d,p,f}$ such that, for any $V \in \mathrm{L}^p(\mathbf{R}^d)$, the following inequality holds:*

$$\sum_{\lambda \in \sigma_d(-\Delta+V)} \frac{\operatorname{dist}(\lambda, [0,+\infty[)^p}{\lambda^{d/2}} f\left( -\log\left( \frac{\operatorname{dist}(\lambda, [0,+\infty[)}{|\lambda|} \right) \right) \leq C_{d,p,f} \|V\|_{\mathrm{L}^p}^p. \tag{2}$$

As a natural generalisation, one can ask for a version involving elliptic differential operator instead of the usual Laplacian operator perturbed by a multiplication operator.

A first problem occurs when one tries to derive a similar inequality on a locally finite weighted graph: the dimension $d$ makes no sense but one would be eager to have available discrete Lieb-Thirring inequalities. More generally, combinatorial graphs are convenient but a bit too flexible frameworks to work in. Furthermore, contrary to appearances, it is not that easy to perform actual calculations or analysis on graphs. But, at least for finite graphs, one can hope to obtain a Lieb-Thirring type inequality and maybe a sharp bound relying on the structure of the graph. For infinite graphs, a more detailed study of the graph spectrum is needed.

Some numerical evidences let one to think that there should be a parameter playing the role of the dimension $d$. Here is an illustration, in the self adjoint case (real potential) of the growth of $\max \sum_{\lambda \in \sigma_d(-\Delta+V)} |\lambda|$ with respect to the size of the Laplacian matrix of a family of random graphs:




The red marks are the maxima and the blue curve is the quadratic interpolation (approximately, $0.998 - 0.421x + 0.954x^2$). (*The non selfadjoint case seems manageable, at least numerically!*) See [Pac91] to maybe find a path to a discrete generalisation. There also exists some works on this subject using Jacobi gap matrices.

## 1.2. **Motivations from examples.**

1.2.1. *Spectrum of some finite graphs.* A graph, per sé, do not have spectrum. We define the spectrum of the graph as the spectrum of an operator acting on the graph, usually the Laplacian. There are many possibilities to define the discrete Laplace operator. We opt for the followings.

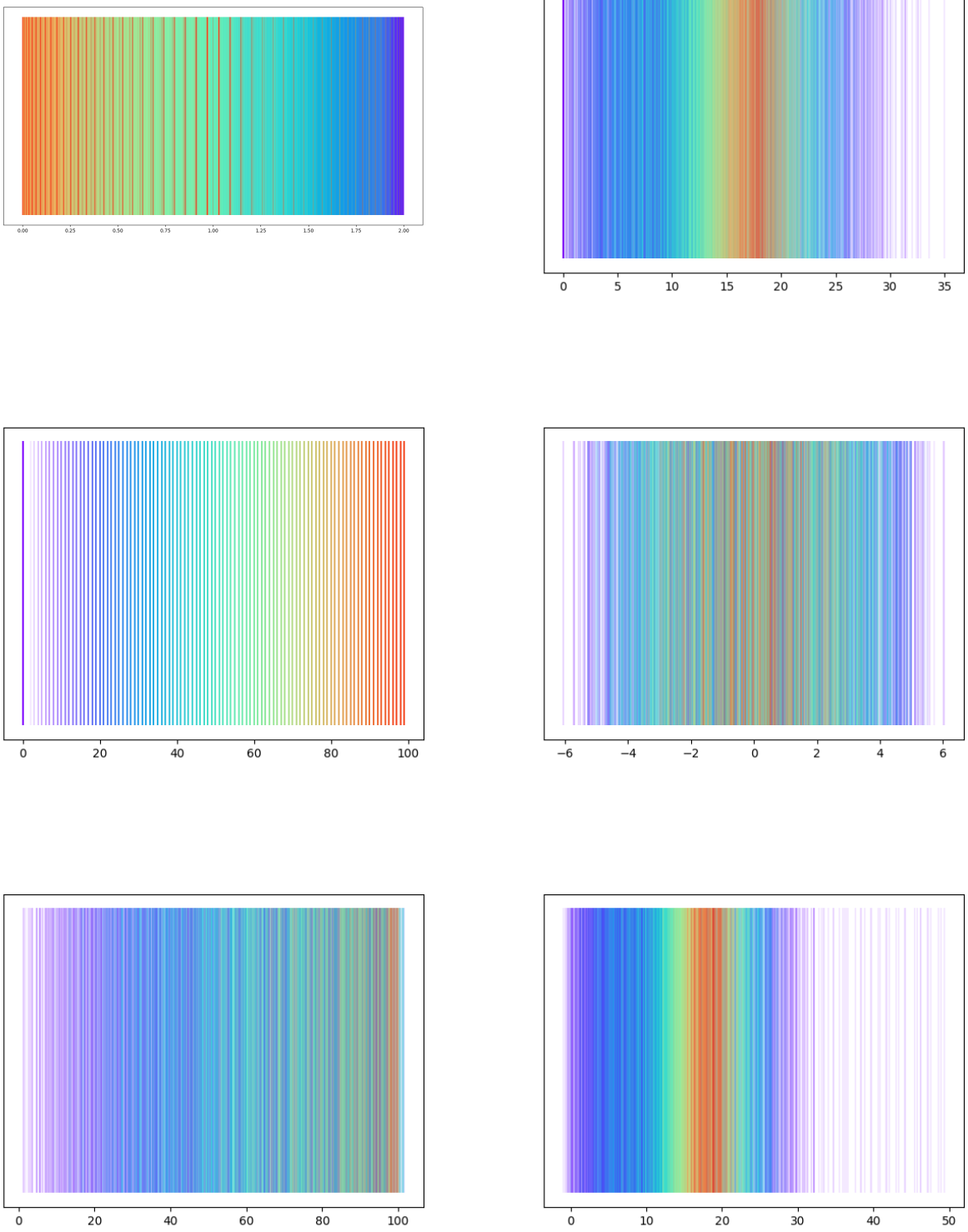
**Definition 2.** *Let $G = (V, E, \mu)$ a locally finite weighted graph. For any function $f : V \to \mathbf{C}$, we define the discrete (normalised) Laplace operator as:*

$$\Delta_\mu f(x) = \frac{1}{\mu(x)} \sum_{y \sim x} f(y)\mu_{xy} - f(x). \tag{3}$$

*The (matrix) Laplacian operator is defined as $D - A$, where $D$ is the degree matrix and $A$ the adjacency matrix.*

Most of the time, the weighted Laplacian will be simple (i.e. $\mu_{xy} = 1$). In this case, we can omit the $\mu$ subscript and write $\Delta f(x)$. Note that we must be careful when considering the Laplacian or the negative of the Laplacian (as physicists do), the context will make it clearer.

It is then a fun game to generate spectrum of graphs as chemists would do. We plot the eigenvalues of sequences of matrices indexed by their dimension. Note that each ray represents an eigenvalue and the lighter the colour is (violet) the smaller is the dimension of the matrix. The colours range from violet to red (following the rainbow colours). Here are some examples.




Some observations can be made, sometimes the spectrum tends to accumulate, sometimes to be evenly spaced. There mostly always seems to exist a pattern. Not an easy game (inverse problem): try to find the sequence of matrices associated to each spectrum.

Note that, sometimes, explicit formulas can be derived to characterise the elements of the spectrum of classes of graphs. For instance, see [BH11, p. 17] and [BB21, § 4.1].

1.2.2. *A generalised eigenvalue equation.* From an historical but also from a personal interest, quantum chemistry contributed to the study of certain differential operators on likely discrete structures [Ver98, § 3.7.]. One of the main protagonist was Erich Hückel, see [Hüc31].

We will have in mind the following principle (or approximation): the chemical framework is characterised by complete graphs of $n + N$ vertices where $n + N \ll 10'000$ (approximately),

$n$ represents the number of electrons and $N$ the number of nuclei. But, from a mathematical standpoint, one is absolutely not forced to study only complete graphs! Nevertheless, we restrict here ourselves to such case. See [Gar24] to get few (and small) ideas.

1.2.3. *Elliptic operators and PDEs.* Agmon [Agm10] defines a linear differential operator $A$ of order $\ell$ as:

$$A(x,D) := \sum_{|\alpha|\leq \ell} a_\alpha(x) D^\alpha \tag{4}$$

where the multi-index notation was used: $\alpha = (\alpha_1, \dots, \alpha_n)$, with $n$ the dimension of the vector space. Thus: $|\alpha| = \alpha_1 + \cdots + \alpha_n$, and $D^\alpha = D_1^{\alpha_1} D_2^{\alpha_2} \dots D_n^{\alpha_n} = \frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \dots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_n}}$. The coefficients $a_\alpha(x)$ are complex valued functions defined in an open set of the considered vector space.

As a natural generalisation, it may be fruitful to consider $A(x,d)$ for $d$ an abstract derivation (in the differential algebra setting).

A linear differential operator is said elliptic if a condition holds on its principal part

$$A'(x,\xi) := \sum_{|\alpha|=\ell} a_\alpha(x) \xi^\alpha. \tag{5}$$

**Definition 3.** *The linear differential operator $A$ is elliptic at $x_0$ if for any real non zero $\xi$, $A'(x_0,\xi) \neq 0$. Furthermore, if for every $x$ in a domain $\Omega$ and for all real non zero $\xi$, there exists a constant $C$ such that:*

$$\frac{1}{C}|\xi|^\ell \leq |A'(x,\xi)| \leq C|\xi|^\ell \tag{6}$$

*then $A$ is said uniformly elliptic. The operator $A$ is strongly elliptic if there exists a function $C(x)$ such that for any real non null $\xi$:*

$$\Re(C(x)A'(x,\xi)) > 0. \tag{7}$$

This definition will motivate the one given in the discrete setting, see definition 7.

For the sake of clarity and concreteness, consider $\ell = 1$ and $n = 1$. The principal part simply is a polynomial in $\xi$ (up to the dependence in $x$):

$$A'(x,\xi) = a_1(x)\xi. \tag{8}$$

The ellipticity condition reduces to $a_1(x) \neq 0$. Elliptic operators form a class of interesting operators because it contains $-\Delta$. Recall its definition in $\mathbf{R}^d$:

$$-\Delta := -\sum_{i=1}^{d} \partial_i^2. \tag{9}$$

**Proposition 4.** *The negative of the Laplacian in $\mathbf{R}^d$ is uniformly elliptic.*

This is not the only reason why one shall care about elliptic operators. The elliptic equation $Au = f$ always has a (weak) solution from local and global perspectives (up to some assumptions on $f$ and the coefficients of $A$).

We will (try to) derive some results from Agmon book for locally finite weighted graphs (especially from chapter 8) in the following sections.

For a general bibliography, see [Bre10, p. 312]. For some spectral properties and inverse problems, see [Bre10, chapter 9, § 13]

1.2.4. *The wave equation.* In [LX21], an initial boundary problem for the inhomogeneous wave equation is introduced. After introducing it, we solve it in a slightly more general setting than the one introduced in the article. The situation seems, at least at the beginning, quite similar to the one in subdomains of $\mathbf{R}^d$.

This subsection will be very classical but is quite new for the author and he needs to treat it carefully at least one time. Here is our problem: let $G = (V,E)$ a locally finite weighted graph

and $\Omega$ a bounded domain. We want to solve the inhomogeneous wave equation on the graph, i.e.

$$\begin{cases} \partial_t^2 u(t,x) - \Delta u(t,x) = f(t,x), & (t,x) \in [0,+\infty[\times\Omega^o \\ u(0,x) = g(x), \partial_t u(0,x) = h(x), & x \in \Omega^o \\ u(t,x) = 0, & (t,x) \in [0,+\infty[\times\partial\Omega \end{cases} \tag{10}$$

where the domain of the Laplacian is restricted to $\Omega^o$, the function $f : [0,+\infty[\times\Omega^o \to \mathbf{R}$ is given and continuous in t, and $g$ and $h$ are unknown function from $\Omega^o$ to $\mathbf{R}$.

We first treat the homogeneous setting (i.e. $f = 0$). We make the assumption that $u$ can be decomposed in a basis of eigenvectors $\phi$ so that

$$u(t,x) = \sum_n c_n(t)\phi_n(x). \tag{11}$$

The homogeneous equation can be rewritten:

$$0 = \partial_t^2\Big(\sum_n c_n(t)\phi_n(x)\Big) - \sum_n c_n(t)\Delta\phi_n(x) = \sum_n c_n''(t)\phi_n(x) - \sum_n c_n(t)\lambda_n\phi_n(x). \tag{12}$$

Since $\{\phi_n\}_n$ is a basis of $\ell^2(V,\mu)$ (we are not perfectly rigorous on this point), we must have the following implication:

$$\sum_n \big(c_n''(t) - c_n(t)\lambda_n\big)\phi_n(x) = 0 \Longrightarrow c_n''(t) - c_n(t)\lambda_n = 0. \tag{13}$$

Hence:

$$c_n(t) = C_{1,n}e^{\sqrt{\lambda_n}t} + C_{2,n}e^{-\sqrt{\lambda_n}t}. \tag{14}$$

To determine the constant (for $t$) $C_{1,n}$ and $C_{2,n}$ we use the initial value conditions. Expand the initial value in the orthogonal basis $\{\phi_n\}_n$:

$$u(0,x) = g(x) = \sum_n g_n\phi_n(x),$$
$$\partial_t u(0,x) = h(x) = \sum_n h_n\phi_n(x).$$

By uniqueness of the decomposition, we have : $C_{1,n} + C_{2,n} = g_n$. The same way, we find that $h_n = \sqrt{\lambda_n}\big(C_{1,n} - C_{2,n}\big)$ because:

$$\partial_t u(t,x) = \sum_n \Big(C_{1,n}\sqrt{\lambda_n}e^{\sqrt{\lambda_n}t} - C_{2,n}\sqrt{\lambda_n}e^{-\sqrt{\lambda_n}t}\Big)\phi_n(x) \tag{15}$$

and evaluating at $t = 0$ yields the result.

Solving the system hereinbelow, we find an expression for $C_{1,n}$ and $C_{2,n}$:

$$\begin{cases} C_{1,n} + C_{2,n} = g_n \\ C_{1,n} - C_{2,n} = \dfrac{h_n}{\sqrt{\lambda_n}} \end{cases} \tag{16}$$

for $\lambda_n \neq 0$.

Injecting this altogether, we find the following homogeneous solution:

$$\begin{aligned}
u(t,x) &= \sum_n \Big(C_{1,n}\mathrm{e}^{\sqrt{\lambda_n}t} - C_{2,n}\mathrm{e}^{-\sqrt{\lambda_n}t}\Big)\phi_n(x) \\
&= \sum_n \left(\Big(\frac{g_n}{2} + \frac{h_n}{2\sqrt{\lambda_n}}\Big)\mathrm{e}^{\sqrt{\lambda_n}t} + \Big(\frac{g_n}{2} - \frac{h_n}{2\sqrt{\lambda_n}}\Big)\mathrm{e}^{-\sqrt{\lambda_n}t}\right)\phi_n(x) \\
&= \sum_n \frac{g_n}{2}\mathrm{e}^{\sqrt{\lambda_n}t}\phi_n(x) + \sum_n \frac{h_n}{2\sqrt{\lambda_n}}\mathrm{e}^{\sqrt{\lambda_n}t}\phi_n(x) + \sum_n \frac{g_n}{2}\mathrm{e}^{-\sqrt{\lambda_n}t}\phi_n(x) - \sum_n \frac{h_n}{2\sqrt{\lambda_n}}\mathrm{e}^{-\sqrt{\lambda_n}t}\phi_n(x) \\
&= \sum_n g_n \frac{\mathrm{e}^{\sqrt{\lambda_n}t} + \mathrm{e}^{-\sqrt{\lambda_n}t}}{2}\phi_n(x) + \sum_n \frac{h_n}{\sqrt{\lambda_n}}\frac{\mathrm{e}^{\sqrt{\lambda_n}t} - \mathrm{e}^{-\sqrt{\lambda_n}t}}{2}\phi_n(x) \\
&= \sum_n g_n \cosh\big(\sqrt{\lambda_n}t\big)\phi_n(x) + \sum_n \frac{h_n}{\sqrt{\lambda_n}}\sinh\big(\sqrt{\lambda_n}t\big)\phi_n(x) \\
&= \sum_n \left(g_n \cosh\big(\sqrt{\lambda_n}t\big) + \frac{h_n}{\sqrt{\lambda_n}}\sinh\big(\sqrt{\lambda_n}t\big)\right)\phi_n(x)
\end{aligned}$$

We could be surprised to not find the same result as [LX21, theorem 1.4]. It is just a matter of convention (physics or not, that is the question): in equation 12, we assumed that $\Delta\phi_n(x) = \lambda_n\phi_n(x)$. But we could have considered the eigenvalues and eigenvectors of $-\Delta$. That way, we would have found:

$$u(t,x) = \sum_n \left(g_n \cos\big(\sqrt{\lambda_n}t\big) + \frac{h_n}{\sqrt{\lambda_n}}\sin\big(\sqrt{\lambda_n}t\big)\right)\phi_n(x) \tag{17}$$

Some facts were not completely clear, not sufficiently precise... For instance, what is the range of the index $n$ in every sum? What precisely are the spaces considered? This are important questions that must be treated.

One can remark that nothing was really particular to the graph setting (despite the eluded question above). Most of the question lies in determining the eigenvectors $\phi_n$ ! That's precisely the problem in general!

**FINISH**

1.2.5. *The heat equation.* For a careful treatment of the heat equation on a finite graph, see [Cot19], for some investigations, see [Dod05] and [DM05]. We consider the following problem: let $G = (V, E)$ a graph, solve

$$\begin{aligned}
Au(t,x) + \partial_t u(t,x) &= 0, \\
u(x,0) &= u_0(x)
\end{aligned}$$

where $t \in [0, +\infty[$, $x \in V$, for $u_0(x)$ a given initial value condition and $A$ a given operator acting on the graph vertices. The classical situation occurs when $A$ is the usual (discrete) Laplace operator. We would like to find a basis expansion of the solution, as it is done in the introduction of [Roy24a]. Stated otherwise, we want to "diagonalize" the operator $A$, if possible.

On a finite graph, the problem reduces to a system of linear equations. Assume $A$ is represented by the matrix $(a_{ij})_{(i,j)\in[\![1,d]\!]^2}$, with $d = |V|$. We can restrict our study to a basis of $\mathbf{C}^d$, namely $(e_1, \dots, e_d)$. Let $x$ be an element of the (Hilbert) space of (finitely supported) functions from $V$ to $\mathbf{C}$, write $x$ as $x_1e_1 + \cdots + x_de_d$. We simply develop expand componentwise and formally get:

$$Au(t,x) + \partial_t u(t,x) = \sum_{i=1}^{d} x_i\big(A + \partial_t\big)u(t,e_i) = 0. \tag{18}$$

Thus, for each $i \in [\![1,d]\!]$ and $t \in [0, +\infty[$:

$$\big(A + \partial_t\big)u(t,e_i) = 0. \tag{19}$$

To fix ideas, we will consider the case $A = \Delta$, the simple discrete Laplace operator (i.e. weights fixed to 1). For a more general case (not restricted to graphs), see [Roy24b] for instance. It

seems that a "control" over the operator allows to get the existence of a solution (via semi-group theory, not studied). To have such a result, one needs to state that the Laplace operator is dissipative., i.e. $\Re\langle -\Delta u, u\rangle \leq 0$, for $u \in \mathbf{C}^d$.

**Proposition 5.** *The simple discrete Laplace operator is dissipative.*

*Proof.* We first need to compute the following quantity (in the case of a real-valued dot product, feel free to adapt for a complex-valued dot product):

$$0 \leq \langle \Delta f, \Delta f\rangle := \sum_{x\in V} \Delta f(x)\Delta f(x)\deg(x) \tag{20}$$

$$= \sum_{x\in V} \Big(\frac{1}{\deg(x)} \sum_{y\sim x} \big(\nabla_{xy} f\big)\Big)^2 \deg(x) \tag{21}$$

$$= \sum_{x\in V} \frac{1}{\deg(x)} \Big(\sum_{y\sim x} \big(\nabla_{xy} f\big)\Big)^2. \tag{22}$$

Observe that the equality is true by definition:

$$\sum_{y\sim x} \nabla_{xy} f = \sum_{y\sim x} \big(f(y) - f(x)\big) = \sum_{y\sim x} f(y) - \deg(x) f(x). \tag{23}$$

We bound from above the former quantity using Cauchy-Schwarz:

$$0 \leq \langle \Delta f, \Delta f\rangle \leq \sum_{x\in V} \frac{1}{\deg(x)} \left[\sum_{y\sim x} \big(\nabla_{xy} f\big)^2 \sum_{y\sim x} 1^2\right] = \sum_{x\in V} \sum_{y\sim x} \big(\nabla_{xy} f\big)^2. \tag{24}$$

We then apply Green equality (cf. [Gri18, theorem 2.1, case $\Omega = V$]) and find:

$$0 \leq \sum_{x\in V, y\sim x} \big(\nabla_{xy} f^2\big) = -2 \sum_{x\in V} \big(\Delta f(x)\big) f(x)\deg(x) = -2\langle \Delta f, f\rangle. \tag{25}$$

This concludes. □

In this then possible to check that the solution is $u(t,x) = e^{-t\Delta} u_0(x) = \sum_{i=1}^{d} e^{-t\lambda_i} \langle f, \mu_i\rangle \mu_i$, where the eigenvalues and eigenvectors of the Laplacian appear.

1.3. **Some resources.** To get an overview of some of the main objects introduced in this mini report, see:

- analysis on graphs: [Ver98], [Gri18], [FT04], [Sal12] [KR16], [JP09],
- standard functional analysis: [Bre10],
- non selfadjoint operators: [Agm10, chapter 15], [CFS24], [Vog15], [Pra06], [Pra19], [Hen13], [Bal18], [Roy22], [BST20], [Sjo08],
- miscellaneous: [Bre10, p. 312], [Gri24], [Han21], [SCV14].

## 2. Elliptic differential operators

Fix a locally finite weighted graph $G = (V, E, \mu)$. Functions on the graph are assumed to be complex-valued (we won't discuss the case of functions defined over an arbitrary field).

2.1. **Ellipticity.** Following Colin de Verdière [Ver98] and Dodziuk [Dod05], we first introduce elliptic operators and see how the discrete setting preserve ideas from the continuous one.

**Definition 6.** *An endomorphism $A$ of $\mathbf{C}^V$ is local on $G$ if its value on a vertex only depends of its neighbours, i.e. its matrix representation $(a_{xy})_{x,y\in V}$ is such that $a_{xy} = 0$ whenever $x \not\sim y$ and $x \neq y$. A local endomorphism is called a differential operator.*

Due to locality, a differential operator $A \in \mathcal{L}(\mathbf{C}^V)$ is represented as follow. Let $f : V \to \mathbf{C}$ and $x \in V$ a vertex, then:

$$Af(x) := a_{xx} f(x) + \sum_{y\sim x} a_{xy} f(y). \tag{26}$$

Introduce $V(x) = a_{xx} + \sum_{y\sim x} a_{xy}$. Thus, $A$ can be decomposed as the sum of two operators:

$$\begin{aligned} Af(x) &:= a_{xx}f(x) + \sum_{y\sim x} a_{xy}f(y) \\ &= \Big(a_{xx} + \sum_{y\sim x} a_{xy}\Big)f(x) - \sum_{y\sim x} a_{xy}\big(f(x) - f(y)\big) \\ &= Vf(x) + Bf(x) \end{aligned}$$

where $V$ is a multiplication operator and $B$ is the local operator above. Physically, a local operator can be decomposed as a sum of a potential and an other operator. For an example of a nonlocal operator, see [ZLY24b].

**Definition 7.** *A local operator $A$ is elliptic if the coefficients $(a_{xy})$ of equation 26 are all non-null. A local operator $A$ is uniformly elliptic if it is elliptic and there exists positive constants $\gamma$ and $\Gamma$ such that $\gamma \le a_{xy} \le \Gamma$ for all edges $\{x, y\}$.*

Examples will come in a next subsection. For now, we'll derive some properties of elliptic operators on locally finite weighted graphs.

2.1.1. *Basic properties.* Since the zero operator is not elliptic, the elliptic operators cannot form a vector space. Note that they form a cone because of the stability by non-zero scaling but they are not necessarily stable by addition.

2.1.2. *Survey.* The two main references about elliptic operators appear to be [Ver98] and [Dod05]. Many other developments have been made. More generally, the study of differential equations on graphs seems to be increasingly a subject of research (maybe not that much in France or even Europe ?). We present, without a (clear) critical examination, some results obtained on the theme of the discretisation of PDEs on graphs and spectral analysis on graphs. This should motivate some paths to follow in the following subsections.

Here are two very classical results (they admit a nearly trivial proof).

**Proposition 8** (Maximum principle, [Dod05])**.** *Let $L = B + V$ where $B$ is positive, symmetric and $V$ is nonnegative. Suppose $V_1 \subset V$ is such that $\overset{\circ}{V}_1$ is connected. Let $f$ be a function on $V_1$ respecting:*

$$Lf(x) = Bf(x) + V(x)f(x) \ge 0 \text{ for } x \in \overset{\circ}{V}_1.$$

*If $f$ has a minimum at $x_0 \in \overset{\circ}{V}_1$ and $f(x_0) \le 0$, then $f$ is constant on $V_1$.*

**Proposition 9** (Harnack inequality, [Dod05])**.** *Suppose $B$ and $V$ satisfy the same assumptions as in proposition 8. Let $V_1 \subset V$, $x$ and $y$ in $\overset{\circ}{V}_1$ are such that $x \sim y$. If:*

$$Lf(x) = Bf(x) + V(x)f(x) \ge 0 \text{ and } f > 0 \text{ for } x \in V_1,$$

*then:*

$$\frac{a_{xy}}{V(x) + \sum_{z\sim x} a_{xz}} \le \frac{f(x)}{f(y)} \le \frac{V(y) + \sum_{z\sim y} a_{yz}}{a_{xy}}.$$

This inequality and this principle can be used to prove, under natural but restrictive hypotheses on a graph, that there might exist a unique bounded solution to the discrete heat equation.

Many continuous objects can have a discrete analogue. For instance, see [DM05] for a Kato inequality, [JZ23] for Cheeger inequalities, [PG20] for isoperimetric inequalities, [Gol11] for Hadry inequality.

Some solutions to equations on (locally finite) graphs : [YXZ24], [BCK22], [KX21], [Sun24], [GLY15], [LX21], see [ZLY24a] for equations with fractional Laplacian operator.

Some general considerations on Sobolev spaces on locally finite graphs [SYZ23], on the Ricci flow [MY24].

2.2. **Examples.** We encountered elliptic operators in preceding subsections, among which the famous and prototypical Laplacian operator.

2.3. **Spectral properties.**

2.4. **Analysis.**

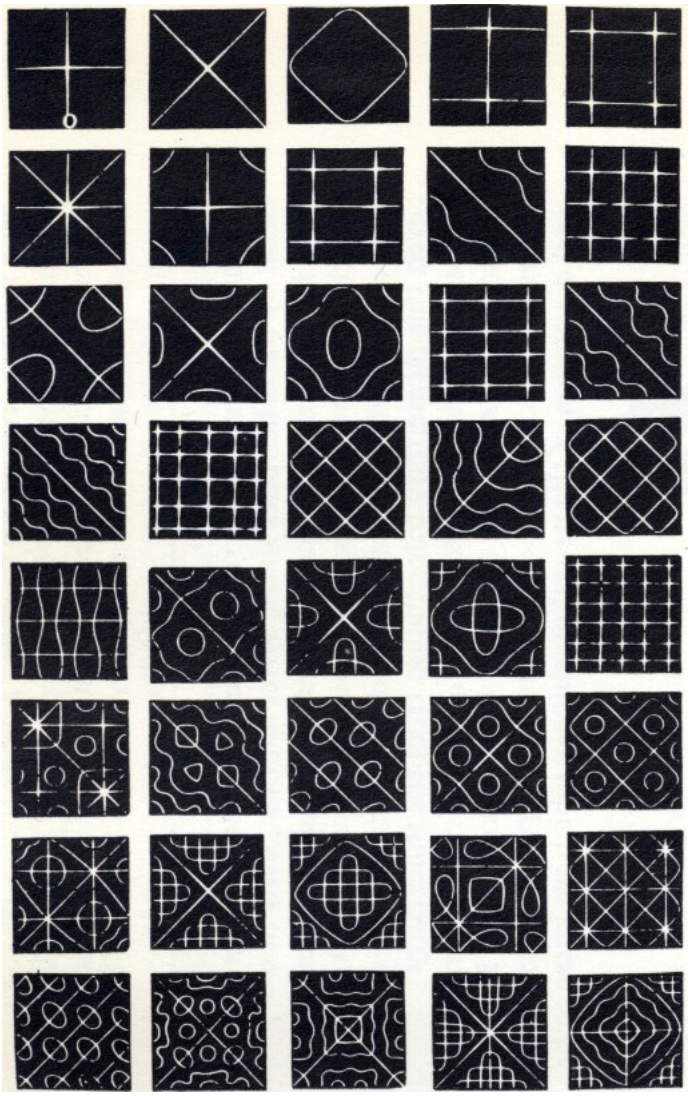
## Appendix: Counting zeros of graph eigenfunctions, a mini-course by Gregory Berkolaiko

### Lecture 1. Eigenvalue interlacing from Cauchy to Weyl to Dirichlet-Neumann bracketing.

**Overview.** In this lecture we will introduce the concept of eigenvalue interlacing, starting with symmetric matrices (Cauchy and Weyl interlacing) and proceeding to the Laplacian of a metric graph. The proofs proceed using the well-known tools: quadratic forms and the minimax characterisation of the eigenvalues.

The focus will be put on the discrete Laplacian but the methods involved also extend to differential operator on metric graph (but won't have enough time to treat them).

Before the modern foundation of the theory by Sturm in the 1840s (*oscillation theory of Sturm-Liouville operators*), the subject goes back to observations of high vibrational modes which oscillate on a finer scale thus they have many zeros (need to properly explain what is intended). The first observations were made by da Vinci, Galileo and Hooke and it was Chladni who really experienced the visualisation of zeros of eigenfunctions. See for instance the following pictures from [Bog13]:

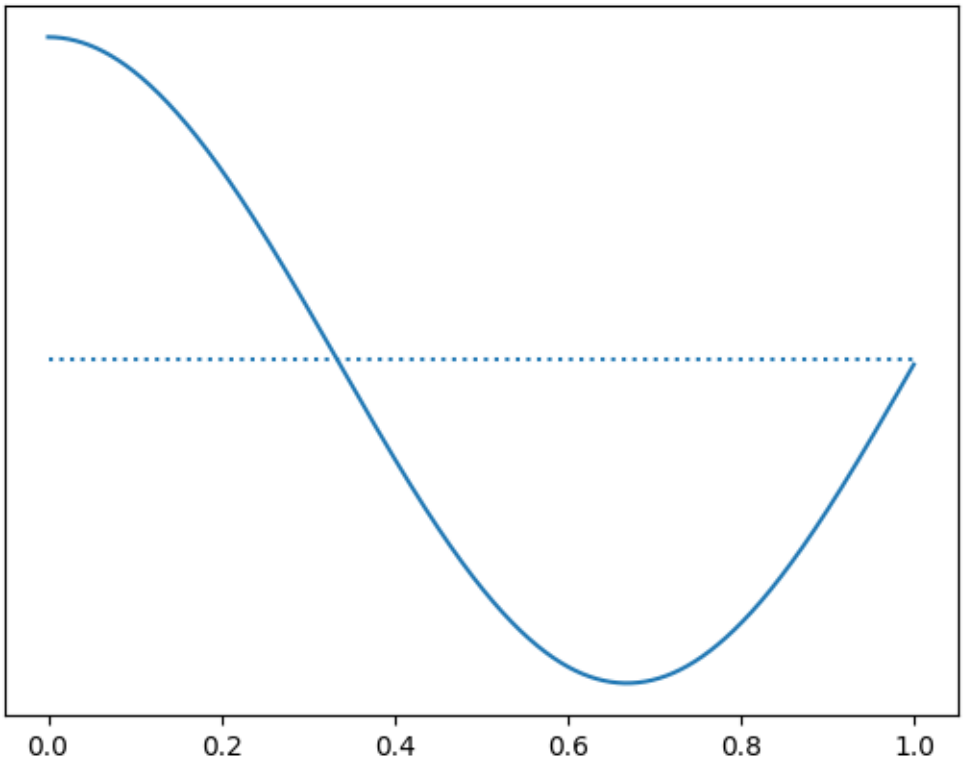


***Motivations.*** One of the main idea inherited from the modern theory is, broadly speaking, that on an interval, the $k$-th eigenfunction has $k-1$ zeros.

For instance, in the one dimensional case, consider the interval $[0,1]$ with boundary conditions $f'(0) = 0$ and $f(1) = 0$. On the interval, acts the following differential operator : $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$, i.e. the one dimensional Laplace operator. One would like to solve to generalised eigenvalue equation:

$$-\frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2} = \lambda f(x) \tag{27}$$

with the imposed boundary conditions. Here is the plot of the shape of the second eigenvector ($\lambda = 2$):




One effectively sees only one zero (the boundary condition do not count).

In the two dimensional case, a similar problem is posed still for the Dirichlet condition. The main result can be traced back to Courant in 1923 : the number of nodal domains (seen as connected components) of the $k$-th eigenfunction is bounded above by $k$. For Neumann boundary condition, a similar result exists and it is quite recent. Many questions arise from this setting.

***Some questions.*** Denote by $\nu(f_k)$ the number of nodal domains of the $k$-th eigenfunction. Can one estimate the following quantity:

$$\limsup_{k\to+\infty} \frac{\nu(f_k)}{k} = \ ? \tag{28}$$

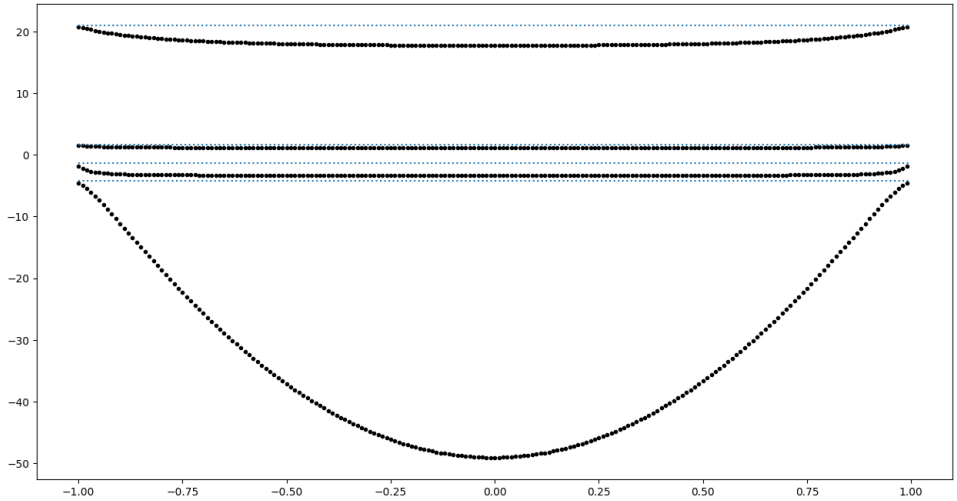
A bound was given by Pleijel in the fifties in terms of zero of the Bessel function. We thus have $\limsup_{k\to+\infty} \frac{\nu(f_k)}{k} \lessapprox 0.7$. (This seems to be related to Faber-Krahn inequality and Weyl asymptotic.) More directly, one can ask for the superior limit of $\nu(f_k)$. It was investigated by Hoffmann-Ostenhof and solved by Jung-Zelditch. An other problem relies on giving a distribution of $\frac{\nu(f_k)}{k}$. Numerics shows that the distribution looks different in function of the shape of the studied domain. There are works of Smilansky and a famous conjecture by Bogonolny with progress by Nazarov-Sodin. At last, one can expect *universality* of nodal surplus distribution on graphs (see Alon, Band, Berkolaiko and Goresky).

Some problems treat the measure of the nodal set. See Yau, Donnely-Feffermann and recent progresses by Logunov-Malinnikova. Things can get really wild (for instance in three dimensions).

Jerison and his collaborators studied the morphology of the second nodal curve.

A domain where Helffer contributed a lot with his collaborators relates to spectral minimal partitions.

***Eigenvalue interlacing.*** Given a matrix $M$, form the symmetric matrix $H = \frac{M + {}^tM}{2}$. Consider a perturbation of $H$ (for instance, we replace $H_{2,2}$ by $H_{2,2}+s$, where $s$ is the perturbation parameter) denoted by $H(s)$. We want to see how eigenvalues evolve in terms of $s$ and compare it with the non perturbed matrix $H$. Here is an example of a plot for a random matrix $M$.




One can guess that $\lambda_k(s)$, the $k$-th eigenvalue of $H(s)$, is increasing if $s \geq 0$ and $\lambda_k(0) \leq \lambda_k(s) \leq \lambda_{k+1}(0)$ for $s \geq 0$. But there is nothing special with zero, we must have more generally $\lambda_k(s') \leq \lambda_k(s) \leq \lambda_{k+1}(s')$ for $s \geq s'$.

Since the sequence $(\lambda_k(s))_k$ is bounded and increasing, it must have a limit. Is it $\lambda_{k+1}(0)$ ? No. May it be $\lim_{s' \to -\infty} \lambda_{k+1}(s)$ ? To investigate the behaviour at $\pm\infty$, we can make the change of variable $s = \tan(t)$.

From numeric we can guess the following Weyl interlacing theorem.

**Theorem 10.** *Let $H$ be a real symmetric matrix, $P$ a rank one perturbation (equal to $(\vec{z}, \cdot)\vec{z}$, where the dot product is linear in the second variable). We thus have:*

$$\lambda_k H \leq \lambda_k(H + P) \leq \lambda_{k+1}(H). \tag{29}$$

Here is the proof idea: use minimax characterisation of the eigenvalues:

$$\lambda_k(A) = \min_{\substack{V \subset \mathcal{C}^n \\ \dim(V)=k}} \max_{\substack{\|u\|=1 \\ u \in V}} Q_A(\vec{u}) = \min_{\substack{V \subset \mathcal{C}^n \\ \dim(V)=k}} \max_{\substack{\|u\|=1 \\ u \in V}} (\vec{u}, A\vec{u}). \tag{30}$$

Apply to $H + P$, then find a one codimensional subspace ignoring $P$.

Here is an other interlacing inequality: Cauchy interlacing.

**Theorem 11.** *Suppose $H'$ is a principal minor of $H$. Then:*

$$\lambda_k(H) \leq \lambda_k(H') \leq \lambda_{k+1}(H). \tag{31}$$

The proof idea is the same: use minimax and observe that $Q_{H'} = Q_H$ restricted to subspace of codimension 1.

We introduce some notations. We say $V \subset_1 W$ if $W/V$ is one dimensional. Let $\mathcal{H}$ be a not necessarily finite dimensional Hilbert space, $Q : \mathrm{dom}(Q) \times \mathrm{dom}(Q) \to \mathbf{C}$ a sesquilinear form bounded from below, closed and hermitian (i.e. $Q(u, v) = \overline{Q(v, u)}$) with discrete spectrum. We define $f$ as an eigenvector with eigenvalue $\lambda$ if $Q(u, f) = \lambda(u, f)_{\mathcal{H}}$, for all $u \in \mathrm{dom}(Q)$.

Note that there are other characterisations of the minimax principle (maximin!):

$$\lambda_k(A) = \min_{\substack{V\subset \mathrm{dom}(Q)\\ \dim(V)=k}} \max_{\substack{\|u\|=1\\ u\in V}} Q_A(\vec{u},\vec{u})$$
$$= \max_{\substack{W\subset \mathrm{dom}(Q)\\ \dim(W)=k-1}} \min_{\substack{u\in W^\perp\\ \|u\|=1}} Q_A(\vec{u},\vec{u}).$$

**Definition 12** (see Birman-Solomyak book)**.** *The operator $\tilde{Q}$ is a rank one non negative perturbation of $Q$ if:*

- *$\exists Z \subset dom(Q)$ such that $Q\big|_Z = \tilde{Q}\big|_Z$ and*
- *either $dom(\tilde{Q}) \subset_1 dom(Q)$ (and $Z = dom(\tilde{Q})$) or $dom(\tilde{Q}) = dom(Q)$ and $\tilde{Q} \geq Q$ (for every vector).*

Here is a general interlacing inequality.

**Theorem 13.** *Let $\tilde{Q}$ be a non negative rank one perturbation of $Q$. Then:*

$$\lambda_k(Q) \leq \lambda_k(\tilde{Q})\lambda_{k+1}(Q). \tag{32}$$

*Furthermore, if $\Lambda$ has multiplicity $m$ and $\tilde{m}$ is in the spectrum (resp.) of $Q$, $\tilde{Q}$, then:*

$$|m-\tilde{m}| \leq 1 \text{ and } \dim(E(Q,\lambda)\cap E(\tilde{Q},\lambda)) = \min(m,\tilde{m}) \tag{33}$$

*where $E(Q,\lambda)$ is the eigenspace of $Q$ for the eigenvalue $\lambda$.*

For more informations, see *Surgery principles for the spectral analysis of quantum graphs* by Berkolaiko-Kennedy-Kurasov-Mugnolo, TAMS 2019. (Due to the title of the article, Berkolaiko got surprisingly invited to many medical conferences!)

**Lecture 2. Interlacing inequalities and nodal estimates.**

> **Overview.** In this lecture we will use interlacing inequalities to derive the estimates on the number of zeros of the n-th eigenfunction on a graph (both discrete and metric). That the number of zeros of an eigenfunction is related to the label of the corresponding eigenvalue is an old idea of Sturm, developed in higher dimensions by Courant, Pleijel and others. We will see that metric graphs behave as if they have a little more than one dimension to them, quantified by the first Betti number of the graph.

Our objective is to get non trivial estimates of zeros of eigenfunctions on grpahs $\Gamma = (V,E)$ where $V = \{1,\dots,n\}$ is the set of vertices and $E$ the set of edges. (The graph is considered by no loops and even connected).

The graph Laplacian is the following operator (there exists many alternatives definitions in terms of what we expect about it): $L : \mathbf{C}^V \to \mathbf{C}^V$ such that

$$(L\psi)_u = \sum_{v\sim u}(\psi_u - \psi_v). \tag{34}$$

A (generalised discrete) Schrödinger operator $H : \mathbf{C}^V \to \mathbf{C}^V$ is real symmetric and respect for all $u \neq v$, $H_{u,v} \neq 0 \iff u \sim v$. Pay attention, $H_{u,u}$ can be zero.

Let $\psi \in \mathbf{C}^V$, $H$ be as above. We define the edge count function:

$$\phi_H(\psi) := \#\big\{u\sim v | \psi_u\big(-H_{u,v}\big)\psi_v < 0\big\}. \tag{35}$$

It counts the number of edges on which the function changes sign. It is quite analogous to the number of zeros.

**Theorem 14.** *Let $H$ be a generalised Schrödinger operator, $\Gamma$ a connected graphs. Let $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \dots$ with corresponding eigenfunctions. If $\lambda_k$ is simple and $(\psi_k)_v \neq 0$ for all $v \in V$. Then:*

$$k-1 \leq \phi_H(\psi_k) \leq k-1+\beta_1 \tag{36}$$

*with $\beta_1 = |E| - |V| + 1 = \#$cycles the first Betti number (generalisations for Betti numbers seem not to exist).*

For $\beta = 0$ it is known since Fiedler, 1975. There was in independent proof by Biyikoglu in 2003. For $\beta > 0$, see Berkolaiko, 2008. One can drop some assumptions, see H. Xu, S.-T. Yau, 2012 and two articles in 2023 by C. Ge, S. Lin. See also Deidda-Putti-Tudisco-Hein for $p$-Laplacians.

Define the nodal surplus $\sigma(H,k) := \phi_H(\psi_k) - (k-1)$. Here is a really beautiful inverse result.

**Theorem 15** (Band, 2014)**.**

$$\sigma(H,k) = 0, \text{ for all } k, \text{ then } H \sim \text{a tree graph.} \tag{37}$$

Here is a converse result based on the two following lemmas.

**Lemma 16.** *Assume $\Gamma$ is a tree graph, $\psi$ an eigenvector of eigenvalue $\lambda$ of $H$ with $\psi_u \neq 0$ for all $u \in V$. Then $\lambda$ is simple, i.e. of multiplicity one.*

*Proof.* By induction on $n = |V|$. The $n = 1$ case is obvious because there is only one eigenvalue. For the induction: pick $u$ such that $\deg(u) = 1$ (it is always possible because we consider finite graphs; choosing a leaf is maybe not absolutely mandatory for the sake of the proof). Consider the perturbation: $\tilde{H}_{u,v} = 0$, $\tilde{H}_{v,u} = 0$, $\tilde{H}_{u,u} = H_{u,u} + \frac{\psi_v}{\psi_u} H_{u,v}$, $\tilde{H}_{v,v} = H_{v,v} + \frac{\psi_u}{\psi_v} H_{v,u}$. It has been built such that $\tilde{H}\psi$ is still equal to $\lambda\psi$ and $\tilde{H}$ is a rank one perturbation of $H$ (could be positive or negative but at this point we don't care).

Since $\lambda \in \text{spec}(\tilde{H})$ is of multiplicity two (no more than two by induction hypothesis; not understood this part). Assume $\lambda$ is not simple for $H$. Then, by interlacing theorem (the dimensional equality):

$$E(\tilde{H}, \lambda) \subset E(H, \lambda). \tag{38}$$

Note that $E(\tilde{H}, \lambda)$ contains a "strange" eigenvector :

$$\tilde{\psi} = \begin{cases} 1 & \text{on } u \\ 0 & \text{otherwise} \end{cases} \tag{39}$$

But, we have:

$$0 = (\lambda\tilde{\psi})_v = (H\tilde{\psi})_v = \sum_{w \sim v} H_{v,w}\psi_w = H_{v,u}. \tag{40}$$

This is a contradiction since $H_{v,u}$ cannot be 0. So $\lambda$ is simple. □

**Lemma 17.** *Assume $\Gamma$ is a tree ($\beta = 0$), $\psi$ an eigenvector with $\psi_u \neq 0$ for all $u \in V$. Then:*

$$\phi_H(\psi_k) = k - 1 = N(H, \lambda) \tag{41}$$

*where*

$$N(H,\lambda) := \#\{\lambda' \in \text{spec}(H) \mid \lambda' < \lambda\}. \tag{42}$$

*Proof.* We also proceed by induction on $n = |V|$. The proof is omitted since the author did not understood it. □

**Lecture 3. Transversal variation and magnetic characterisation of the nodal count.**

> **Overview.** While eigenvalue interlacing deals with a single rank-r perturbation to the graph operator, more precise information is available by going sideways: allowing the rank-r perturbation to vary in a small neighborhood and viewing the eigenvalue as a real-valued function on the space of rank-r perturbations. This idea allows us to compute the number of zeros of the graph eigenfunction as a Morse index of the corresponding eigenvalue with respect to magnetic perturbations of the operator, opening up the problem to tools from Morse theory and, more widely, algebraic topology.

Some new notations:

- $H$ is the Laplacian associated with the graph $\Gamma = (V, E)$,
- $S(\Gamma; \mathbf{R})$ is the set of real symmetric $H$ supported on $\Gamma$,

- $S(H)$ is the set of all "signings" of $H$:

$$S(H) = \left\{ H' \in S(\Gamma; \mathbf{R}) \;\middle|\; |H'_{u,v}| = |H_{u,v}|, H'_{u,u} = H_{u,u} \right\}. \tag{43}$$

**Conjecture 18** (Berkolaiko and collaborators, see Alon-Goresky, 2022)**.** *Let $H \in S(\Gamma; \mathbf{R})$ be "generic" (technical meaning, not important here). Consider $\sigma(H', k)$ as a random variable with $k$ uniform in $\{1, \dots, n\}$, $H' \in S(H)$ uniform.*

*Then $\sigma(H', k)$, standardised (subtract mean and divide by variance), converges to $\mathcal{N}(0, 1)$ as $\beta \to +\infty$ uniformly on $\Gamma$ (pick a sequence of graph with $\beta \to +\infty$, uniformly means the choice of graphs is not taken into consideration).*

For Berkolaiko it sounds a little bit too good to be true, but:

**Theorem 19** (Alon-Goresky, 2024)**.** *Let $\Gamma$ have disjoint cycles, $H \in S(\Gamma; \mathbf{R})$ "generic". For any fixed $k$ (the result is the same of uniformly distributed $k$), $H' \in S(H)$, then the distribution is* $\mathrm{Bin}(1/2, \{0, \dots, \beta\})$.

Note that if $\beta \to +\infty$, it converges to the gaussian!

The conjecture was inspired by work of Alon-Band-Berkolaiko on quantum graphs. The tools used to prove the theorem are eigenvalue perturbations and Morse theory (counts number of critical points of a given index on a compact manifold).

***What is a transversal variation ?*** We want to compare $\mathrm{spec}(A + L(0))$ with $\mathrm{spec}(A)$, where $A$ is a selfadjoint matrix and $L(0)$ is a perturbation maybe depending on parameters, for instance: $\mathrm{spec}(A + tL)$. We want to vary $t$ and track the eigenvalues!

**Definition 20.** *Let $\mathcal{U} \subset \mathbf{R}^d$ a neighbourhood of $0$, let $L(x)$ with $x \in \mathcal{U}$ a family of operators on $\mathcal{H}$, let $g_0 \in \ker(L_0)$. Then $L(x)$ is a transversal variation of $L(0)$ with respect to $g_0$ if:*

- *the range of $L(x)$ is smooth in $x$,*
- *$\chi : \mathcal{U} \to \mathcal{H}$, $x \mapsto L(x)g_0$ is transversal to $\ker(L(0))^* = (\mathrm{range} L(0))^\perp$.*

**Theorem 21** (Berkolaiko, Kuchment; work in progress Berkolaiko, Latushkin, Sukhtaiev)**.** *Let $A$ be a selfadjoint operator on $\mathcal{H}$, $Ag_0 = \lambda_0 g_0$ and assume $\lambda_0$ is simple. The family of operators $L(x)$ is a transversal variation of $L(0)$ with respect to $g_0 \in \ker L_0$. Assume $\lambda_0 \in \mathrm{spec}(A + L(0))$ is simple, let $\Lambda(x) \in \mathrm{spec}(A + L(x))$ (thus $\Lambda(0) = \lambda_0$). Then: $d\Lambda(0) = 0$ and*

$$n_-(d^2\Lambda(0)) = \underbrace{n_-(A - \lambda_0) - n_-(A + L(0) - \lambda_0)}_{\text{the spectral shift}} + n_-(L(0)) \tag{44}$$

*where $n_-(\cdot)$ counts the number of negatives eigenvalues, $d^2$ is the hessian. We are thus computing the Morse index of $\Lambda$ at the critical point $x = 0$.*

The hypothesis $Ag_0 = \lambda_0 g_0$ can be dropped and it would be natural to drop the hypothesis of simplicity of $\lambda$. Note that the key ingredient is operators sharing the same eigenvector.

Fun fact, and that's why Berkolaiko finds this formula beautiful, if we open the brackets, then everything disappears and simplifies.

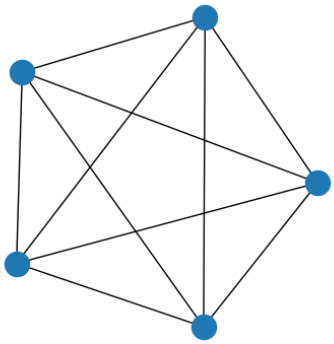
Here is a former result who motivated a little this work. Berkolaiko sent a mail to Y. Colin de Verdière and no more than two days later, he replied with a more beautiful proof (but Berkolaiko preferred his proof) using de Rham cohomology.

**Theorem 22** (Berkolaiko, Colin de Verdière, 2013)**.** *Let $\lambda_k$ be a simple eigenvalue, $\psi_k \neq 0$ on vertices. Consider $\Lambda(x) := \lambda_k(H(\vec{x}))$, where $H(\vec{x})$ is the discrete magnetic Schrödinger operator. Then $\Lambda(x)$ has a critical point at $\vec{x} = \vec{0}$ with Morse index $\sigma(H, k)$.*

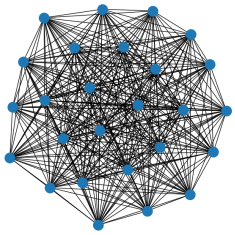
For Berkolaiko, there is magic in constant rank operators!

## Appendix: A glimpse into graph theory

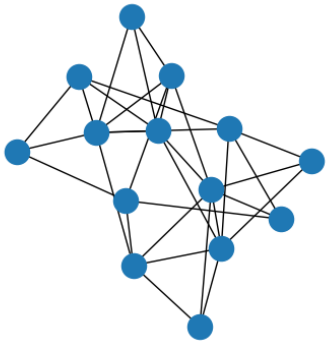
**Graph theory.** Graph are what we usually expect to model system of discrete interactions between various objects. The key idea is to link (by edges) two states (i.e. vertices) in a sense depending on the context. The next plots presents some possible configurations (that may be deterministic or random):



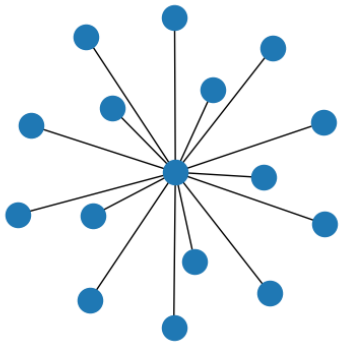
(A) Complete graph (5 vertices)



(B) Complete graph (26 vertices)



(C) Random graph (14 vertices)



(D) Star graph (16 vertices)

It is worth noting that we use *rustworkx* [Tre+22] with *Matplotlib* [Hun07] to generate graphs and plots.

**Definition 23.** *An undirected graph $G$ is a couple $(V, E)$ where $V$ is the set of vertices and $E$ is the set of edges. Vertices are points of the graph and edges are unordered pairs of vertices.*

We write an edge as $\{e_1, e_2\}$, for $(e_1, e_2) \in V^2$. If $e_1 = e_2$, we simply note an edge as $\{e_1\}$. For an undirected graph, the relation *being connected* (i.e. there exists an edge between selected vertices) is reflexive, symmetric and transitive, then graph connectedness is an equivalence relation. This relation induces a partition of the the set of vertices in connected component classes. We express the transitivity in the following way: if $\{e_1, e_2\}$ and $\{e_2, e_3\}$ are two edges, then:

$$\{e_1, e_2\} + \{e_2, e_3\} := \{e_1, e_2, e_3\}.$$

If the order is relevant (i.e. $\{e_1, e_2\} \neq \{e_2, e_1\}$ for some vertices) the graph is said to be directed.

Before introducing families or types of graphs, we introduce the general vocabulary of graphs.

*Vocabulary.* The most important notion is the one of neighbourhood.

**Definition 24.** *Two vertices $x$ and $y$ are said to be neighbours, noted $x \sim y$, if there exists an edge linking directly $x$ to $y$.*

An example of the talk of Brian Winn (June 24, 2024; *Quantum ergodicity for large quantum graphs*, MAQM, Toulouse) made the author think that one could use equivalence relations to build non-trivial graphs to study.

**Definition 25.** *The set of all direct neighbours of a vertex $x$ is denoted $\overline{\mathrm{B}}(x,1)$ or $\overline{\mathrm{B}}(x)$ when the context is clear. Thus:*

$$\overline{\mathrm{B}}(x,1) := \{y \in V \mid \{x,y\} \in E\}.$$

As a first observation, the neighbourhood of $x$ is never empty because it always contains the vertex $x$ itself. In case $\overline{\mathrm{B}}(x)$ is reduced to $x$ we say $x$ is an isolated point. Here is an example of such a point:

(A) Isolated point on the left

More generally we introduce the closed balls of "radius" $n \in \mathbf{N}_{\geq 2}$:

$$\overline{\mathrm{B}}(x,n) := \{y \in V \mid \exists (z_1,\dots,z_{n-1}) \in V^{n-1}, \{x,z_1,z_2,\dots,z_{n-1},y\} \in E\}$$

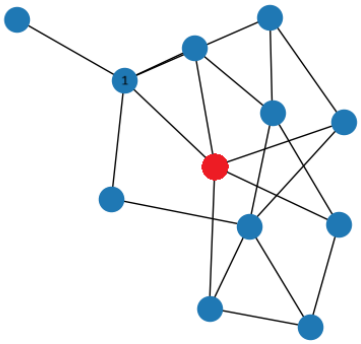
where the case of $n = 1$ is defined as previously. In the above definition, the vertices $z_i$ can be equals. If not, we would **not** have the following inclusion $\overline{\mathrm{B}}(x,n-1) \subset \overline{\mathrm{B}}(x,n)$, for $n \in \mathbf{N}^*$ (for an example, think to a straight line graph).

Notice that this definition can easily be adapted for general metric graphs, but we won't consider them.

This can be rephrased using the notion of path.

**Definition 26.** *A path from vertex $x$ to vertex $y$ is a sequence of vertices $\{z_k\}_{k=0}^{n}$ such that $z_0 = x$, $z_n = y$ and $z_k \sim z_{k+1}$ for $k \in [\![0, n-1]\!]$. A path is said closed if moreover $z_n \sim z_0$. The number $n$ of edges is referred as the length of the path.*

Then, $\overline{\mathrm{B}}(x,n)$ represents all the vertices linked to $x$ by a path of length at most $n$. The open ball $\mathrm{B}(x,n)$ is thus $\overline{\mathrm{B}}(x,n-1)$. Nevertheless, the frontier of $\overline{\mathrm{B}}(x,n)$ can't be defined as the set vertices linked to $x$ by a path of length exactly $n$. For instance, starting from the red node $x$:




(A)

the point labelled 1 should not be in the frontier of $\overline{\mathrm{B}}(x,2)$ since the left top extremal point is already inside the frontier. This point is inside the what we naively call the *frontier* of the closed ball $\overline{\mathrm{B}}(x,2)$ and belongs to the open ball $\mathrm{B}(x,2)$. This is problematic. This example is just here to give an idea how careful one shall be when dealing with topology on graphs. We do not talk that more of this subject. See CW-complexes ([Hat02, § 1.A]) to be more rigorous.

**Definition 27.** *A graph is connected if there exists a path between every vertices.*

One naturally can generalize this definition to subparts of the graphs.

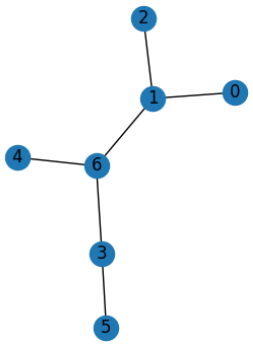
A path minimizing the distance between two vertices is called a **geodesic**. A geodesic is not necessarily unique. We use the convention to set the length of the path between two vertices to $+\infty$ if they are not linked. Such a convention is in accordance with the fact that the minimal length linking the two vertices is never attained.

*Degree and weight.* Attached to a vertex, its degree counts the number of its neighbours.

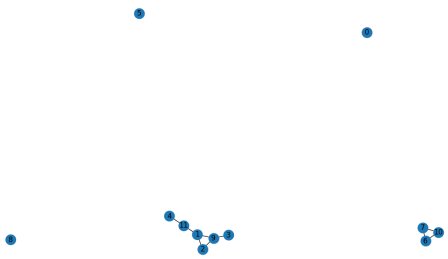
**Definition 28.** *The degree of a vertex is:*

$$\deg(x) := \left|\overline{\mathrm{B}}(x)\right|.$$

We show two examples of the degree map for two different random graphs.




(A) 7 vertices



(B) 12 vertices

For the first one, we have $\deg(\{0,1,2,3,4,5,6\}) = \{1,3,1,2,1,1,3\}$ and for the second, we have $\deg(\{0,1,2,3,4,5,6,7,8,9,10,11\}) = \{0,3,2,1,1,0,2,2,0,3,2,2\}$.

**Definition 29.** *If the degree of every vertices is finite, then the graph is said to be locally finite.*

Obviously a finite graph is locally finite but the contrary is (also obviously) false (see $\mathbf{Z}^d$ as a graph).

One can then naturally introduce the quantities $\deg_n(x) := \left|\overline{\mathrm{B}}(x,n)\right|$, for integers $n \geq 1$. But, this definition is a little bit too restrictive: all the vertices may have not the same importance depending on the context. That is why we want to balance / regulate the weight a vertex can have on others.

**Definition 30** ([Gri18])**.** *A weight on $G = (V,E)$ is a non-negative function defined on $V \times V$ such that $(x,y) \mapsto \mu_{xy}$ and*

- $\mu_{xy} = \mu_{yx}$,
- $\mu_{xy} > 0$ *if and only if* $x \sim y$.

Notice that the weight function space cannot generally be a vector space (the zero function belongs to it only for totally disconnected graph, i.e. constituted only of isolated point).

The symmetry property non necessarily holds for undirected graphs. Note than on a locally finite graph, every weight function is finitely supported. A graph is said to be **weighted** if it is endowed with a weight $\mu$, we note it $G = (V,E,\mu)$. We can introduce our first function defined over the vertices of a graph:

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

for $x \in V$. This is not a weight (because of its domain) but we will abuse and call it the weight of the vertex $x$. In the special case where the weight is simple, i.e. $\mu_{xy} = 1$ if and only if $x \sim y$, we find back the degree of $x$.

In [MP23] and [GMP24], a seemingly more interesting viewpoint is adopted. They introduce, for $G$ a countably infinite set, a measure $\mu$ satisfying $\mu(\{x\}) < +\infty$ for every $x \in G$. A weight is replaced by a symmetric, zero-diagonal and finite sum function $\omega$. They then have defined a weighted graph as the triplet $(G,\omega,\mu)$, where $\omega$ and $\mu$ are the so-called edge weight and node measure, respectively.

## Appendix: The discrete Laplacian (a first encounter)

Everyone is well-aware of the definition of the Laplacian (the author is not able to make any link with differential geometry, Riemannian manifolds and the so-called *Laplace-Beltrami operator*). Let $f$ be a twice differentiable multi-variable function, we then define the Laplace operator:

$$\Delta f = \sum_{i=1}^{n} \partial_i^2 f, \text{ for instance, if } n = 3\text{: } \Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}. \tag{45}$$

This definition can be motivated from different perspectives. For instance, the Laplace operator in all respects is equal to $\mathrm{Tr}(\mathrm{Hess}(f))$ or even $\mathrm{div}(\overrightarrow{\mathrm{grad}} f)$. Using the appropriate definition may sometime be fruitful. That is why, even if we'll be inclined to use a « canonical » discrete Laplacian, we'll construct in many ways the discrete Laplacian operator such that we mimic the definition and properties of the Laplacian in a graph-theoretic context.

How to derive a discrete version of the Laplace operator ? More generally, is there limits to expectations from going to global to local (or local to global) ? We have some evidences that graphs are limit objects of continuous ones. Thus, we expect to proceed the following way : starting from the definition of the derivative operator, one discretizes it and combines adequately to get a discretized Laplacian operator. We won't discuss in which manner a graph can serve as a mesh for a manifold and scaling limits.

Recall the usual real derivative definition. Let $f$ be one-variable differentiable function. We then have for some real number $x$ :

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}. \tag{46}$$

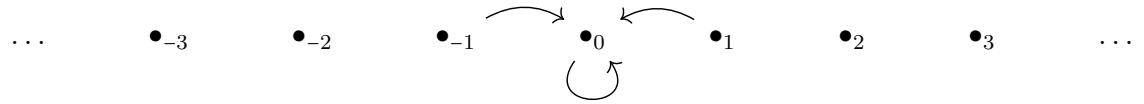
To compute a one-variable Laplace operator, we need the second derivative. It expresses as (for a twice-differentiable function):

$$\begin{aligned} f''(x) &= \lim_{h \to 0} \frac{f'(x+h) - f'(x)}{h} \\ &= \lim_{h \to 0} \frac{f(x+2h) - f(x+h) - (f(x+h) - f(x))}{h^2} \\ &= \lim_{h \to 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2}. \end{aligned}$$

Moreover, if $f$ is twice continuously differentiable, we find that the second derivative is more or less a *mean* between its neighbouring points:

$$f''(x) = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = \lim_{h \to 0} \frac{2}{h^2} \left( \frac{f(x+h) + f(x-h)}{2} - f(x) \right). \tag{47}$$

On a discrete graph, we would like to reproduce this situation : the discrete Laplacian should be a function of its neighbouring points. For instance, the set $\mathbf{Z}$ can be endowed by a graph structure where each vertex is an integer coordinate points of the real line. The action of the discrete Laplacian on 0 shall depend of the point itself, 1 and −1:




A natural question arise: at the time, the Laplacian varies only with neighbouring points, can one asks more? For instance, (a modified discrete) Laplacian at 0 could be a function of $0, 1, -1, 2, -2$ or $0, 1, -1, 2, -2, 3, -3$... We will call such operator an *unscreened Laplacian operator or order* $r$, where $r$ is the size of the neighbourhood. A study will be made in the next part. The name has been chosen having in mind the Slater screening effect on electrons.

For the sake of completeness, we need to derive a similar expression for a multi-variable function. The partial derivative is then, for some $\mathbf{x}$ in $\mathbf{R}^d$ and $i \in [\![1, d]\!]$:

$$\partial_i f(\mathbf{x}) = \lim_{h\to 0} \frac{f(\mathbf{x}+h) - f(\mathbf{x})}{h} = \lim_{h\to 0} \frac{f(x_1, \dots, x_i + h, \dots, x_d) - f(x_1, \dots, x_d)}{h}. \tag{48}$$

The second partial derivative is:

$$\begin{aligned}
\partial_i^2 f(\mathbf{x}) &= \lim_{h\to 0} \frac{\partial_i f(\mathbf{x}+h) - \partial_i f(\mathbf{x})}{h} \\
&= \lim_{h\to 0} \frac{f(\mathbf{x}+2h) - f(\mathbf{x}+h) - \big(f(\mathbf{x}+h) - f(\mathbf{x})\big)}{h^2} \\
&= \lim_{h\to 0} \frac{f(\mathbf{x}+2h) - 2f(\mathbf{x}+h) + f(\mathbf{x})}{h^2}
\end{aligned}$$

Nothing changes (so, we expect the dimension changes only computations not the way the Laplacian behaves).

For the same reason as before, if $f$ is a twice continuously differentiable function, we find:

$$\partial_i^2 f(\mathbf{x}) = \lim_{h\to 0} \frac{f(\mathbf{x}+h) - 2f(\mathbf{x}) + f(\mathbf{x}-h)}{h^2} = \lim_{h\to 0} \frac{2}{h^2}\left( \frac{f(\mathbf{x}+h) + f(\mathbf{x}-h)}{2} - f(\mathbf{x}) \right). \tag{49}$$

The Laplacian now writes as:

$$\Delta f = \sum_{i=1}^{d} \partial_i^2 f(\mathbf{x}) = \lim_{h\to 0} \frac{2}{h^2} \sum_{i=1}^{d} \left( \frac{f(\mathbf{x}+h) + f(\mathbf{x}-h)}{2} - f(\mathbf{x}) \right) \tag{50}$$

(the inversion of the sum and the limit is possible because the sum is finite). Writing the coordinates, we obtain:

$$\Delta f = \lim_{h\to 0} \frac{2}{h^2} \sum_{i=1}^{d} \left( \frac{f(x_1, \dots, x_i + h, \dots, x_d) + f(x_1, \dots, x_i - h, \dots, x_d)}{2} - f(x_1, \dots, x_d) \right). \tag{51}$$

For instance, for $d = 3$, we get:

$$\begin{aligned}
\Delta f = \lim_{h\to 0} \frac{2}{h^2} \Bigg( & \frac{f(x_1+h, x_2, x_3) + f(x_1-h, x_2, x_3)}{2} \\
& + \frac{f(x_1, x_2+h, x_3) + f(x_1, x_2-h, x_3)}{2} \\
& + \frac{f(x_1, x_2, x_3+h) + f(x_1, x_2, x_3-h)}{2} - 3f(x_1, x_2, x_3) \Bigg)
\end{aligned}$$

$$\begin{aligned}
\Delta f = \lim_{h\to 0} \frac{6}{h^2} \Bigg( & \frac{f(x_1+h, x_2, x_3) + f(x_1-h, x_2, x_3)}{6} \\
& + \frac{f(x_1, x_2+h, x_3) + f(x_1, x_2-h, x_3)}{6} \\
& + \frac{f(x_1, x_2, x_3+h) + f(x_1, x_2, x_3-h)}{6} - f(x_1, x_2, x_3) \Bigg).
\end{aligned}$$

Up to a scalar constant, the definition of the discrete Laplacian operator can be modelled on equation 51 with a parameter $h$ equal to 1. For an arbitrary $d$, one would obtain:

$$\Delta_{\text{discretized}} f = \sum_{i=1}^{d} \left( \frac{f(x_1, \dots, x_i + 1, \dots, x_d) + f(x_1, \dots, x_i - 1, \dots, x_d)}{2d} \right) - f(x_1, \dots, x_d).$$

A major problem on a graph is the following: a vertex can have more (or less) than two neighbours. That is why we will care about this aspect in next section by considering the size of the neighbourhood of a vertex. (Need to be done.)

## References


[Hüc31] E. Hückel. ***Quantentheoretische Beiträge zum Benzolproblem***. 1931.

[Pac91] B.G. Pachpatte. ***On Lieb and Thirring type discrete inequalities***. 1991. URL: https://journals.math.tku.edu.tw/index.php/TKJM/article/view/4587/1614.

[Ver98] Y.C. de Verdière. ***Spectres de graphes***. Collection SMF: Cours spécialisés. Société mathématique de France, 1998. ISBN: 9782856290682. URL: https://books.google.fr/books?id=TffuAAAAMAAJ.

[Hat02] A. Hatcher. ***Algebraic topology***. 2002.

[FT04] Joel Friedman and Jean-Pierre Tillich. ***Calculus on Graphs***. 2004. arXiv: cs/0408028 [cs.DM]. URL: https://arxiv.org/abs/cs/0408028.

[Dod05] J. Dodziuk. ***Elliptic operators on infinite graphs***. 2005. arXiv: math/0509193 [math.SP]. URL: https://arxiv.org/abs/math/0509193.

[DM05] Jozef Dodziuk and Varghese Mathai. ***Kato's inequality and asymptotic spectral properties for discrete magnetic Laplacians***. 2005. arXiv: math/0312450 [math.SP]. URL: https://arxiv.org/abs/math/0312450.

[LT05] Elliott H. Lieb and Walter E. Thirring. ***Inequalities for the Moments of the Eigenvalues of the Schrödinger Hamiltonian and Their Relation to Sobolev Inequalities***. Ed. by Walter Thirring. Berlin, Heidelberg, 2005. DOI: 10.1007/3-540-27056-6_16. URL: https://doi.org/10.1007/3-540-27056-6_16.

[Pra06] Karel Pravda-Starov. ***Etude du pseudo-spectre d'opérateurs non auto-adjoints***. 2006. URL: https://theses.hal.science/tel-00109895.

[Hun07] J. D. Hunter. ***Matplotlib: A 2D graphics environment***. 2007. DOI: 10.1109/MCSE.2007.55.

[Sjo08] Johannes Sjoestrand. ***Some results on non-self-adjoint operators, a survey***. 2008. arXiv: 0804.3701 [math.SP]. URL: https://arxiv.org/abs/0804.3701.

[DHK09] Michael Demuth, Marcel Hansmann, and Guy Katriel. ***On the discrete spectrum of non-selfadjoint operators***. 2009. arXiv: 0908.2188 [math.SP]. URL: https://arxiv.org/abs/0908.2188.

[JP09] Palle Jorgensen and Erin Pearse. ***Operator theory and analysis of infinite networks***. 2009.

[Agm10] S. Agmon. ***Lectures on Elliptic Boundary Value Problems***. AMS Chelsea Publishing Series. AMS Chelsea Pub., 2010. ISBN: 9780821849101. URL: https://books.google.fr/books?id=FKoJBAAAQBAJ.

[Bre10] H. Brezis. ***Functional Analysis, Sobolev Spaces and Partial Differential Equations***. Universitext. Springer New York, 2010. ISBN: 9780387709130. URL: https://books.google.fr/books?id=GAA2XqOIIGoC.

[BH11] A.E. Brouwer and W.H. Haemers. ***Spectra of Graphs***. Universitext. Springer New York, 2011. ISBN: 9781461419396. URL: https://books.google.fr/books?id=F98THwYgrXYC.

[Gol11] Sylvain Golenia. ***Hardy inequality and Weyl asymptotic for discrete Laplacians***. 2011. URL: https://hal.science/hal-00598054.

[Sal12] Justin Salomon. ***PDE Approaches to Graph Analysis***. 2012.

[Bog13] Beni Bogosel. ***Theory behind patterns formed on Chladni plates?*** Physics Stack Exchange. 2013. URL: https://physics.stackexchange.com/q/90021.

[Hen13] Raphaël Henry. ***Spectre et pseudospectre d'opérateurs non-autoadjoints***. 2013. URL: https://theses.hal.science/tel-00924425.

[Rob14] Didier Robert. ***Sur les traces d'opérateurs (De Grothendieck à Lidskii)***. Apr. 2014. URL: https://hal.science/hal-01015295.

[SCV14] Justin Salomon, Keenan Crane, and Etienne Vouga. ***Laplace-Beltrami: the swiss aarmy knife of geometry processing***. 2014.

[GLY15] Alexander Grigor'yan, Yong Lin, and Yunyan Yang. ***Yamabe type equations on finite graphs***. 2015.

[Vog15] Martin Vogel. ***Propriétés spectrales des opérateurs non-auto-adjoints aléatoires***. 2015. URL: http://www.theses.fr/2015DIJOS018/document.

[KR16] Oliver Knill and Annie Rak. ***Differential equations on graphs***. 2016.

[Bal18] Marwa Balti. ***Non self-adjoint laplacians on a directed graph***. 2018. arXiv: 1801.04088 [math.SP]. URL: https://arxiv.org/abs/1801.04088.

[Gri18] A. Grigor'yan. ***Introduction to Analysis on Graphs***. University Lecture Series. American Mathematical Society, 2018. ISBN: 9781470443979. URL: https://books.google.fr/books?id=dJVqDwAAQBAJ.

[Cot19] Francesca Cottini. ***Random evolution operator on combinatorial and metric graphs***. 2019. URL: https://www.fernuni-hagen.de/analysis/docs/masterarbeit_cottini.pdf.

[Pra19] Karel Pravda-Starov. ***Estimations de résolvante et localisation du spectre pour certaines classes d'opérateurs pseudo-différentiels semi-classiques non autoadjoints, d'après Dencker, Sjöstrand et Zworski***. 2019. URL: https://hal.science/hal-02372329.

[BST20] Olivier Bourget, Diomba Sambou, and Amal Taarabt. ***On the spectral properties of non-selfadjoint discrete Schrödinger operators***. 2020. arXiv: 1807.01282 [math.SP]. URL: https://arxiv.org/abs/1807.01282.

[PG20] Mircea Petrache and Matias Gomez. ***Sharp discrete isoperimetric inequalities in periodic graphs via discrete PDE and Semidiscrete Optimal Transport***. 2020. arXiv: 2012.11039 [math.MG]. URL: https://arxiv.org/abs/2012.11039.

[BB21] L.W. Beineke and J.S. Bagga. ***Line Graphs and Line Digraphs***. Developments in Mathematics. Springer International Publishing, 2021. ISBN: 9783030813864. URL: https://books.google.fr/books?id=um1LEAAAQBAJ.

[Bög21] Sabine Bögli. ***Improved Lieb-Thirring type inequalities for non-selfadjoint Schrödinger operators***. 2021. arXiv: 2111.03938 [math.SP]. URL: https://arxiv.org/abs/2111.03938.

[Han21] Jakob Hansen. ***A gentle introduction to sheaves on graphs***. 2021.

[KX21] Christian Kuehn and Chuang Xu. ***Vlasov equations on digraph measures***. 2021. arXiv: 2107.08419 [math.AP]. URL: https://arxiv.org/abs/2107.08419.

[LX21] Yong Lin and Yuanyuan Xie. ***The existence of the solution of the wave equation on graphs***. 2021. arXiv: 1908.02137 [math.AP]. URL: https://arxiv.org/abs/1908.02137.

[BCK22] M. Brio, J.-G. Caputo, and H. Kravitz. ***Spectral solutions of PDEs on networks***. 2022. URL: https://www.sciencedirect.com/science/article/pii/S0168927421002750.

[Roy22] Julien Royer. ***The Damped Wave Equation and other Evolution Problems involving Non-selfadjoint Operators***. 2022. URL: https://hal.science/tel-03905989.

[Tre+22] M. Treinish et al. ***rustworkx: A High-Performance Graph Library for Python***. 2022. DOI: 10.21105/joss.03968. URL: https://doi.org/10.21105/joss.03968.

[JZ23] Jürgen Jost and Dong Zhang. ***Cheeger inequalities on simplicial complexes***. 2023. arXiv: 2302.01069 [math.CO]. URL: https://arxiv.org/abs/2302.01069.

[MP23] G. Meglioli and F. Punzo. ***Uniqueness in weighted $\ell^p$ spaces for the Schrödinger equation on infinite graphs***. 2023. arXiv: 2212.05928.

[SYZ23] Mengqiu Shao, Yunyan Yang, and Liang Zhao. ***Sobolev spaces on locally finite graphs***. 2023. arXiv: 2306.02262 [math.AP]. URL: https://arxiv.org/abs/2306.02262.

[CFS24] Lucrezia Cossetti, Luca Fanelli, and Nico M. Schiavone. ***Recent Developments in Spectral Theory for Non-self-adjoint Hamiltonians***. 2024.

[Gar24] Mathias Garnier. ***Méthode de Hückel simple pour*** $H_n$. 2024. URL: https://mathiasgarnier.github.io/HuckelHn.pdf.

[Gri24] Alexander Grigor'yan. ***Lectures on path homology and Hodge Laplacian on digraphs***. 2024.

[GMP24] G. Grillo, G. Meglioli, and F. Punzo. ***Blow-up and global existence for semilinear parabolic equations on infinite graphs***. 2024. arXiv: 2406.15069.

[MY24] Jicheng Ma and Yunyan Yang. ***A modified Ricci flow on arbitrary weighted graph***. 2024. arXiv: 2408.09435 [math.AP]. URL: https://arxiv.org/abs/2408.09435.

[Roy24a] Julien Royer. ***Séries de Fourier, PS Maths Licence 2***. 2024. URL: https://plmbox.math.cnrs.fr/f/6961fc954df14c39b3b8/.

[Roy24b] Julien Royer. ***Spectral theory, M2 RI. Chapter 5, Semigroups and evolution equations***. 2024. URL: https://www.math.univ-toulouse.fr/~jroyer/TD/2023-24-M2/M2-Ch5.pdf.

[Sun24] Linlin Sun. ***Sinh-Gordon equations on finite graphs***. 2024. arXiv: 2406.17166 [math.DG]. URL: https://arxiv.org/abs/2406.17166.

[YXZ24] Zhangyi Yu, Junping Xie, and Xingyong Zhang. ***Nontrivial solutions for a*** $(p,q)$***-Kirchhoff type system with concave-convex nonlinearities on locally finite graphs***. 2024. arXiv: 2408.02041 [math.AP]. URL: https://arxiv.org/abs/2408.02041.

[ZLY24a] Mengjie Zhang, Yong Lin, and Yunyan Yang. ***Fractional Laplace operator and related Schrödinger equations on locally finite graphs***. 2024. arXiv: 2408.02902 [math.AP]. URL: https://arxiv.org/abs/2408.02902.

[ZLY24b] Mengjie Zhang, Yong Lin, and Yunyan Yang. ***Fractional Laplace operator on finite graphs***. 2024. arXiv: 2403.19987 [math.AP]. URL: https://arxiv.org/abs/2403.19987.