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Spectral theory, clustering problems and differential equations on metric graphs

“ Documento Definitivo”

Doutoramento em Matemática

Especialidade de Análise Matemática

Matthias Hofmann

Tese orientada por:

James Bernard Kennedy

Hugo Ricardo Nabais Tavares

Documento especialmente elaborado para a obtenção do grau de doutor

2021

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- Doutor James Bernard Kennedy, Professor Auxiliar da Faculdade de Ciências da Universidade de Lisboa (Orientador).

Documento especialmente elaborado para a obtenção do grau de doutor

Fianciado pela bolsa PD/BD/128412/2017 da Fundação para a Ciência e Tecnologia

2021

Acknowledgements

While the past few years have not always been easy, I am glad to have went this path towards a PhD. I feel that I learned a lot during this time, especially through hardships, and I am happy to say that I feel that I could finally give back a little to the mathematical community as I always wanted. On this path I had many people around me that supported and guided me which I would like to thank.

My deepest gratitude goes towards my advisors, James Kennedy and Hugo Tavares. I thank both of them for guiding me with their immense experience throughout these years. This includes their mentoring, providing me with plenty of literature and also teaching. James Kennedy especially has been always a great support and it was a pleasure to be working with him in several joint projects. But his help goes really beyond that, I want to thank him for always looking out for me and his commitment in making sure I stayed on track.

Naturally, I want to thank all the people that I was working together in forms of collaborations that I would like to mention. I thank Marvin Plümer and Delio Mugnolo that received me at the University of Hagen and for all the fruitful discussions that lead to several joint publications. I also would like to thank Andrea Serio and Francesco Tudisco whom I am still curently working on a project.

Furthermore, I would like to thank all my professors during my undergraduate studies, but also during my time at the University of Lisbon whose efforts became the founding for my mathematical background. There are many people, like colleagues and staff, at the university I want to thank for all the pleasant conversations, be it of mathematical nature or not.

During the course of the PhD I had the opportunity to be invited to speak at several events, whose organizers I would like to thank. Thanks to Paula Cerejeiras, Uwe Kähler, Pavel Kurasov, Delio Mugnolo, Jens Wirth, Dmitry Pelinovsky and Gregory Berkolaiko. Special thanks especially to Paula Cerejeiras and Uwe Kähler for providing me such a pleasant and uncomplicated stay at the University of Aveiro. Also a big thanks to Delio Mugnolo and Pavel Kurasov for their invitation to the workshop at the ZiF in Bielefeld, where I got to know my collaborators Andrea Serio and Francesco Tudisco.

Last but not least I would like to thank the people in my immediate surroundings that helped me throughout this time. Most notably, I want to thank Sandra Moreira, who I met only shortly after I started to live in Lisbon, and we actually soon after moved together. Thank you for always being there for me through all this time. I also would like to thank my family who always

supported me in my aspirations and despite being so far away always cared about me. *Danke, Obrigado!*

This work was supported by the Fundação para a Ciência e a Tecnologia (FCT) through the grant PD/BD/128412/2017, which I gratefully acknowledge.

Resumo

A presente tese aborda diferentes tópicos sobre teoria espectral, problemas de agrupamento e equações diferenciais em grafos métricos. Na primeira parte, provamos uma teoria de existência geral para problemas de minimização condicionada para funcionais definidos em espaços métricos de medida $(\mathcal{M}, d, \mu)$. Aplicamos esta teoria a funcionais definidos em grafos métricos $\mathcal{G}$, em particular problemas L^2 de minimização condicionada para funcionais da forma

$$E(u) = \frac{1}{2}a(u,u) - \frac{1}{q}\int_{\mathcal{K}} |u|^q \,\mathrm{d}x,$$

onde $q > 2$, $a(\cdot,\cdot)$ é uma forma sesquilinear simétrica adequada, definida num espaço de funções em $\mathcal{G}$ e $\mathcal{K} \subset \mathcal{G}$. Mostramos como a existência de soluções pode ser obtida por meio de métodos de decomposição, usando propriedades espectrais do operador A associadas à forma $a(\cdot,\cdot)$, e discutimos as quantidades espectrais envolvidas. Um exemplo que consideramos é a variante de ordem superior do funcional de energia NLS (Schrödinger não linear) estacionário com potencial $m \in L^2 + L^\infty(\mathcal{G})$

$$E^{(k)}(u) = \frac{1}{2}\int_{\mathcal{G}} |u^{(k)}|^2 + m(x)|u|^2 \,\mathrm{d}x - \frac{1}{p}\int_{\mathcal{K}} |u|^q \,\mathrm{d}x$$

definido num domínio denso. Tratamos em particular o caso em que $\mathcal{K}$ é um subgrafo limitado, que sua vez corresponde a ter uma não linearidade localizada. Quando $k = 1$ também consideramos gráficos métricos com um número infinito de arestas, bem como potenciais magnéticos. Neste sentido, o operador A associado à forma linear é um operador de Schrödinger e, no caso L^2-subcrítico $2 < q < 6$, obtemos generalizações de resultados de existência para o funcional NLS obtidos por Adami , Serra e Tilli [JFA 271 (2016), 201-223], e Cacciapuoti, Finco e Noja [Nonlinearity 30 (2017), 3271-3303], entre outros.

Na segunda parte da tese, lidamos principalmente com grafos métricos compactos com um número finito de arestas. Neste caso a existência de estados fundamentais é uma consequência imediata do método direto de cálculo das variações. Estudamos partições espectrais mínimas no âmbito de Kennedy et al [CVPDE 60 (2021), 61], ou seja, estudamos partições no grafo que minimizam uma quantidade espectral do tipo

$$\inf_{\mathcal{P}} \Lambda(\mathcal{P}). \tag{0.1}$$

Neste ponto, consideramos dois exemplos principais. Primeiramente, como motivação, consideramos os problemas de estado fundamental de Nehari relacionados com a mistura de condensados de Bose–Einstein. Estendemos os resultados de Chang et al [Physica D 196 (2004) 341–361] e Conti, Terracini, Verzini [AHIP 19 (2002), 871-888], [JFA 198 (2003), 160-196] para grafos

quânticos; as respectivas soluções dos sistemas penalizados convergem num sentido apropriado separando os suportes das soluções no limite, que ainda definem uma partição no grafo que minimiza um problema de partição mínima da forma (0.1). Quando $k = 2$ mostramos que existe $\lambda \in \mathbb{R}$ tal que

$$-\Delta u + (m + \lambda)u = \mu|u|^2 u, \qquad u \in D(-\Delta)$$

tem uma solução de troca de sinal.

Em segundo lugar, estudamos a partição espectral mínima associada aos funcionais Λ_p com $p \in [1, \infty]$ consistindo na p-média dos valores próprios dos respectivos elementos de partição com o primeiro valor próprio de Dirichlet, com pontos de Dirichlet nos pontos de fronteira da partição, ou o primeiro valor próprio não trivial de Neumann. Respetivamente,

$$\Lambda_{k,p}^N(\mathcal{P}) = \begin{cases} \left(\frac{1}{k}\sum_{i=1}^k (\mu_2(\mathcal{G}_i))^p\right)^{1/p} & 1 \le p < \infty \\ \max\{\mu_2(\mathcal{G}_1), \dots, \mu_2(\mathcal{G}_k)\} & p = \infty \end{cases},$$

$$\Lambda_{k,p}^D(\mathcal{P}) = \begin{cases} \left(\frac{1}{k}\sum_{i=1}^k (\lambda_1(\mathcal{G}_i))^p\right)^{1/p} & 1 \le p < \infty \\ \max\{\lambda_1(\mathcal{G}_1), \dots, \lambda_1(\mathcal{G}_k)\} & p = \infty \end{cases}.$$

Investigamos as propriedades das energias espectrais mínimas $\mathcal{L}_{k,p}^N(\mathcal{G})$ e $\mathcal{L}_{k,p}^D(\mathcal{G})$ associadas a $\Lambda_{k,p}^N$ e $\Lambda_{k,p}^D$ respectivamente. Em particular, mostramos estimativas inferiores e superiores óptimas para as energias de partição mínima e, para $p = \infty$, fornecemos desigualdades entrelaçadas entre $\mathcal{L}_{k,\infty}^D(\mathcal{G})$ e $\mathcal{L}_{k,\infty}^N(\mathcal{G})$, que envolvem grandezas topológicas tais como o número de ciclos independentes no grafo ou o número de vértices de grau 1 do grafo, uma reminiscência de estimativas e desigualdades entrelaçadas para os valores próprios do Laplaciano de todo o grafo. Em particular, obtemos uma desigualdade entre essas energias e os valores próprios do Laplaciano, válidos para todos os grafos compactos, que complementam uma versão para grafos de árvore das desigualdades de Friedlander entre valores próprios de Dirichlet e Neumann de um domínio de $\mathbb{R}^N$. Combinando essas estimativas com os limites obtidos para as energias espectrais mínimas, inferimos uma estimativa superior dos valores próprios do Laplaciano padrão, que em alguns casos resulta em melhores estimativas de valores próprios do Laplaciano do que aquelas obtidos anteriormente em Berkolaiko et al [J. Phys. A 50 (2017), 365201].

Na terceira parte da dissertação, estabelecemos as versões para grafos métricos do teorema de Pleijel sobre comportamento assintótico do número de domínios nodais ν_n da n-ésimas função própria de uma ampla classe de operadores em gráficos métricos compactos, incluindo operadores de Schrödinger com potenciais L^1 e uma variedade de condições de vértice, bem como o p-Laplaciano com condições naturais de vértice, e sem quaisquer suposições sobre os comprimentos das arestas, a topologia do gráfico ou o comportamento dos funções próprias nos vértices. Entre outras coisas, esses resultados caracterizam os pontos de acumulação da sucessão $(\frac{\nu_n}{n})_{n\in\mathbb{N}}$, que formam um subconjunto finito de $(0, 1]$. Consequentemente, estes resultados estendem em várias direções o resultado anteriormente conhecido de que, *genericamente,* $\nu_n \sim$

n, para certas realizações do Laplaciano. Em particular, nos casos especiais do Laplaciano com condições naturais, mostramos que para grafos com comprimentos de aresta racionalmente dependentes, podemos encontrar funções próprias para as quais $\nu_n \not\sim n$; mas, neste caso, mesmo o conjunto de pontos de acumulação pode depender da escolha da base própria.

Concluímos a tese com algumas desigualdades numéricas sobre os valores próprios do Laplaciano padrão num grafo. Com base no teorema de von Below, propomos uma técnica para aproximar os valores próprios de Kirchhoff–Neumann de um grafo métrico geral. A técnica mencionada envolve um processo com três etapas. Primeiro, para um grafo métrico geral $\mathcal{G}$, consideramos o grafo métrico equilátero que "melhor" aproxima $\mathcal{G}$. Desta forma, podemos usar esta aproximação para criar uma sequência de grafos discretos $\{G_N\}$ com N vértices que convergem para $\mathcal{G}$ no sentido de Hausdorff. Finalmente, provamos estimativas de erros a priori e a posteriori para os valores próprios do Laplaciano em $\mathcal{G}$ usando as valores próprios de G_N. Essas estimativas de erro permitem-nos aproximar os valores próprios do Laplaciano em $\mathcal{G}$ para uma precisão desejada, usando os valores próprios do Laplaciano normalizado de um grafo discreto. Este é um problema de valor próprio de matriz semidefinida para o qual estão disponíveis ferramentas de álgebra linear numérica muito eficientes.

Os novos conteúdos da presente tese irão aparecer nos seguintes artigos de investigação, que foram desenvolvidos durante o doutoramento:

- M. Hofmann. "An existence theory for nonlinear equations on metric graphs via energy methods". *arXiv preprint* arXiv:1909.07856 (2019).

- M. Hofmann, J. B. Kennedy, D. Mugnolo, and M. Plümer. "Asymptotics and Estimates for Spectral Minimal Partitions of Metric Graphs". *Integral Equations and Operator Theory* 93 (3) (2021), 1–36.

- M. Hofmann, J. B. Kennedy, D. Mugnolo, and M. Plümer. "On Pleijel's Nodal Domain Theorem for Quantum Graphs". *Annales Henri Poincaré* (2021), 1–30.

- M. Hofmann and J. B. Kennedy. "Interlacing and Friedlander-type inequalities for spectral minimal partitions of metric graphs". *Letters in Mathematical Physics* 111 (4) (2021), 1–30.

Palavras-Chave. Teoria espectral, cálculo de variações, análise de EDPs, grafos quânticos, partições espectrais mínimas.

Abstract

In the first part we prove a general existence theory for constrained minimization problems for functionals defined on function spaces on metric measure spaces $(\mathcal{M}, d, \mu)$. We apply this theory to functionals defined on metric graphs $\mathcal{G}$. We show how the existence of solutions can be obtained via decomposition methods using spectral properties of the operator A associated with the form $a(\cdot, \cdot)$ and discuss the spectral quantities involved. Concrete examples considered include higher order NLS functionals and metric graphs with infinite edge set and magnetic potentials. This generalizes results obtained by Adami, Serra and Tilli [JFA 271 (2016), 201-223], and Cacciapuoti, Finco and Noja [Nonlinearity 30 (2017), 3271-3303], among others.

In the second part we consider spectral minimal partitions of compact metric graphs. We motivate their study through Nehari ground state problems and certain penalized systems. We relate a class of minimal partitions to eigenvalues of the Laplacian and show sharp lower and upper estimates for the associated spectral minimal energies $\mathcal{L}_{k,\infty}^D$ and $\mathcal{L}_{k,\infty}^N$, estimates between these energies and eigenvalues of the Laplacian, which in some cases result in better estimates than the ones previously obtained in Berkolaiko et al [J. Phys. A 50 (2017), 365201]

In the third part we establish metric graph counterparts of Pleijel's theorem on the asymptotics of the number of nodal domains ν_n of the n-th eigenfunction(s) of a broad class of operators on compact metric graphs. Among other things, these results characterize the accumulation points of the sequence $(\frac{\nu_n}{n})_{n\in\mathbb{N}}$, which are shown always to form a finite subset of $(0, 1]$.

In the final part we introduce a numerical method for calculating the eigenvalues of the standard Laplacian based on a discrete graph approximation and von Below's theorem.

Keywords. Spectral theory, calculus of variations, analysis of PDE, quantum graphs, spectral minimal partitions.

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Symbol	Decription/name	See
$\mathcal{G}$, $\mathcal{G}(G, \boldsymbol{\ell})$	Metric graph, ur-graph	§2.1.1
$(\mathcal{M}, d, \mu)$	Metric measure space	Def. 3.2.1
$\mathcal{K}$	Subgraph, subset of $\mathcal{G}$ or $\mathcal{M}$	§3.3.1, §3.4.1
K	Core of a finite graph/ bounded subset	Equ. (2.28)
K_R	Expansion of K with radius R	Equ. (2.23), (3.11)
$\mathcal{E}$	Edge set	§2.1.1
$\mathcal{E}_\infty$	Set of rays/half-lines	§2.1.1
$\mathcal{V}$	Vertex set	§2.1.1
$\mathcal{V}_\infty$	Vertex set at infinity	§2.1.1
G	Underlying discrete graph	Def. 2.1.1
$\boldsymbol{\ell}$	Associated length vector	§2.1.1
$d_\mathcal{E}$	Pseudo-distance on $\mathcal{E}$	§2.1.1
$d_\mathcal{G}$	Metric on $\mathcal{G}$	Equ. (2.3), (2.4)
d_G	Hausdorff distance between two graphs	Equ. (2.1)
$C(\mathcal{G})$	Space of continuous functions	§2.2
$W^{1,p}(\mathcal{G})$, $H^1(\mathcal{G})$, $W_0^{1,p}(\mathcal{G}, \mathcal{V}^D)$, $H_0^1(\mathcal{G}, \mathcal{V}^D)$, $W^{1,p}(G)$, $H^1(G)$, $W_0^{1,p}(G, V^D)$, $H_0^1(G, V^D)$; $H_0^1(\mathcal{G})$, $H_w^1(\mathcal{G})$	First order Sobolev spaces; weighted first order Sobolev spaces	§2.2.1; §5.1
$\widetilde{W^{k,p}}(\mathcal{G})$, $\widetilde{W_0^{k,p}}(\mathcal{G})$, $\widetilde{W_c^{k,p}}$,$\widetilde{H}^k(\mathcal{G})$, $W^{k,p}(\mathcal{G})$, $H^k(\mathcal{G})$	Higher-order Sobolev spaces	§2.2.2
$\widetilde{C}^\infty(\mathcal{G})$, $\widetilde{C}_b^\infty(\mathcal{G})$, $\widetilde{C}_0^\infty(\mathcal{G})$	Smooth test function spaces	Equ. (2.7)
$-\Delta$, $(-\Delta)^k$	Laplacian, Polylaplacian	Equ. (2.12)

Continued on next page

Symbol	Description/name	See
$\lambda_k, \lambda_k(\mathcal{G}, \mathcal{V}^D)$	k-th eigenvalue of a Schrödinger operator/ Laplace	Equ. (2.19)
$\lambda_k^D(\mathcal{G})$	k-th eigenvalue of Dirichlet Laplacian/ Schrödinger operator	Equ. (2.20)
$\mu_k, \mu_k(\mathcal{G})$	Eigenvalues of the standard Laplacian (Laplacian with Kirchhoff–Neumann conditions) / Schrödinger operator	Equ. (2.18)
$\mu_k(G)$	Eigenvalues of the normalized Laplacian	Equ. (6.1)
$\lambda_{k,p}^D(\mathcal{G})$	Variational eigenvalues of the p-Laplacian with standard vertex conditions	Equ. (5.6)
$A^m, A^{M,m}$, $A(q, \mathcal{B}, w)$	Schrödinger operators	§2.3.1, §2.3.2, §5.1
$a^m, a^{M,m}, a_{q,\mathcal{B},w}$	Form associated to Schrödinger operators	Equ. (2.11), (2.14), (5.2)
$\Sigma_0^m, \Sigma_0^{M,m}$	Ground state energy of $A^{M,m}$, A^m	Equ. (2.29), (2.32); §5.1
$\Sigma^m, \Sigma^{M,m}$	Threshold energy for $A^{M,m}$, A^m	Equ. (2.30), (2.32)
NLS	Nonlinear Schrödinger	
$E_{\text{NLS}}(\mathbb{R}^N)$	NLS ground state energy associated on $\mathbb{R}^N$	Equ. (3.15)
E_{NLS}, $E_{\text{NLS}}^{(\mathcal{K})}$, $E^{(k)}$	NLS functional/ ground state energy	Equ. (3.20), (3.21), (3.32), (3.33), (3.35), (3.36)
$E_{\text{NLS}}(\cdot, \mathcal{G})$, $E_{\text{NLS}}^{(\mathcal{K})}(\cdot, \mathcal{G})$, $E_{\text{NLS}}(\mathcal{G})$, $E_{\text{NLS}}^{(\mathcal{K})}(\mathcal{G})$	NLS ground state functional/ energy	Equ. (3.8), (3.9)
$\widetilde{E}^{(k)}$, $\widetilde{E}_{\text{NLS}}$, $\widetilde{E}_{\text{NLS}}^{(\mathcal{K})}$	NLS threshold energy	Equ. (3.22), (3.37), (3.34)
$\mathcal{G}'$	Cut graph of $\mathcal{G}$	Def. 2.1.4
$\mathcal{C}(\mathcal{G}' : \mathcal{G})$	Cut set on $\mathcal{G}$	Def. 2.1.5
$\mathcal{C}_v(\mathcal{G}')$	Cut set associated to $v \in C(\mathcal{G}' : \mathcal{G})$ in $\mathcal{G}'$	Def. 2.1.5
$\operatorname{rank}(\mathcal{G}' : \mathcal{G})$	Rank of cut $\mathcal{G}'$	Def 2.1.6
$\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$	k-partition	Def. 2.1.12
$\mathcal{G}_{\mathcal{P}}$	Canonical cut graph	Def. 2.1.13
$\partial\mathcal{G}_i$	Boundary of partition element $\mathcal{G}_i$	Def. 2.1.17
$\partial\mathcal{P}$	Boundary set of partition	Def. 2.1.17

Continued on next page

Symbol	Description/name	See
$\mathfrak{C}$, $\mathfrak{C}(\mathcal{G})$, $\mathfrak{C}_k$, $\mathfrak{C}_k(\mathcal{G})$	Set of connected k-partitions	Def. 2.1.12, Rmk. 2.1.19
$\mathfrak{R}$, $\mathfrak{R}(\mathcal{G})$, $\mathfrak{R}_k$, $\mathfrak{R}_k(\mathcal{G})$	Set of rigid k-partitions	Def. 2.1.18, Rmk. 2.1.19
S_q	Optimal Sobolev constant/ quotient	(4.8)
$\Lambda^D_{k,p}(\mathcal{P})$, $\Lambda^D_{k,q,p}(\mathcal{P})$, $\Lambda^N_{k,p}(\mathcal{P})$, $\Lambda^N_{k,q,p}(\mathcal{P})$	Dirichlet, Neumann partition energy	Equ. (4.4), (4.9), (4.3), (4.11)
$\mathcal{L}^D_{k,q,p}$, $\mathcal{L}^D_{k,p}(\mathcal{G})$	Dirichlet (spectral) minimal partition	Equ. (4.6), (4.10)
$\mathcal{L}^N_{k,q,p}$, $\mathcal{L}^N_{k,p}(\mathcal{G})$, $\mathcal{L}^{N,c}_{k,p}(\mathcal{G})$,$\mathcal{L}^{N,r}_{k,p}(\mathcal{G})$	Connected/rigid Neumann (spectral) minimal energy	Equ. (4.5), (4.12)
J_β	Functional associated to k-mixtures of Bose–Einstein condensate equation	Equ. (4.14), (4.15)
$\mathcal{N}_\beta$	Nehari manifold associated to J_β	Equ. (4.16), (4.17)
$\mathcal{A}_\beta$	Nehari admissible set to J_β	Equ. (4.18)
S^β_4	Sobolev type functional associated to the Nehari ground state energy	Equ. (4.19)
c_β	Nehari ground state energy to J_β	Equ. (4.20)
ν_k	Number of nodal components of the k-th eigenfunction	Def. 5.3.1
$\mathfrak{E}_p$	Functional associated to p-Laplacian	Equ.(5.21)

Chapter 1

Introduction

1.1 Extended Abstract

In the first part of the thesis we deal with different topics on spectral theory, clustering problems and differential equations on metric graphs. We prove a general existence theory for constrained minimization problems for functionals defined on function spaces on metric measure spaces $(\mathcal{M}, d, \mu)$. We apply this theory to functionals defined on noncompact metric graphs $\mathcal{G}$, in particular L^2-constrained minimization problems for functionals of the form

$$E(u) = \frac{1}{2}a(u,u) - \frac{1}{q}\int_{\mathcal{K}} |u|^q \,\mathrm{d}x,$$

where $q > 2$, $a(\cdot,\cdot)$ is a suitable symmetric sesquilinear form on some function space on $\mathcal{G}$ and $\mathcal{K} \subset \mathcal{G}$ is given. We show how the existence of solutions can be obtained via decomposition methods using spectral properties of the operator A associated with the form $a(\cdot,\cdot)$ and discuss the spectral quantities involved. An example that we consider is the higher-order variant of the stationary NLS (nonlinear Schrödinger) energy functional with potential $m \in L^2 + L^\infty(\mathcal{G})$

$$E^{(k)}(u) = \frac{1}{2}\int_{\mathcal{G}} |u^{(k)}|^2 + m(x)|u|^2 \,\mathrm{d}x - \frac{1}{p}\int_{\mathcal{K}} |u|^q \,\mathrm{d}x$$

defined on a densely defined domain, that we further specify. When $\mathcal{K}$ is a bounded subgraph one has localized nonlinearities, which we treat as a special case. When $k = 1$ we also consider metric graphs with infinite edge set as well as magnetic potentials. Then the operator A associated to the linear form is a Schrödinger operator, and in the L^2-subcritical case $2 < q < 6$, we obtain generalizations of existence results for the NLS functional as for instance obtained by Adami, Serra and Tilli [JFA 271 (2016), 201-223], and Cacciapuoti, Finco and Noja [Nonlinearity 30 (2017), 3271-3303], among others. In the rest of the thesis we deal mainly with compact metric graphs with finitely many edges. Note that for such graphs existence of ground states of the energies we consider is typically an immediate consequence by the direct method of calculus of variation.

In the second part of the thesis, we study spectral minimal partitions within the framework of Kennedy et al [CVPDE 60 (2021), 61] , i.e. for $k \in \mathbb{N}$ we study k-partitions on the graph that minimize a spectral quantity

$$\inf_{\mathcal{P}} \Lambda(\mathcal{P}). \tag{1.1}$$

Here we consider two principal examples. Firstly, for a motivation we consider Nehari ground state problems related to k-mixtures of Bose–Einstein condensate equations. We extend results from Chang et al [Physica D 196 (2004) 341–361] and Conti, Terracini, Verzini [AHIP 19 (2002), 871-888], [JFA 198 (2003), 160-196] to quantum graphs; the respective solutions of the penalized systems converge in an appropriate sense separating the supports of the solutions in the limit, which yet define a partition on the graph that minimizes a spectral minimal partition problem of the form (1.1).

Secondly, we study spectral minimal partitions associated with functionals Λ_p with $p \in [1, \infty]$ consisting of the p-mean of eigenvalues of the respective partition elements with either the first Dirichlet eigenvalue with Dirichlet points at the boundary points of the partition or the first nontrivial Neumann eigenvalue

$$\Lambda^N_{k,p}(\mathcal{P}) = \begin{cases} \left(\frac{1}{k}\sum_{i=1}^k (\mu_2(\mathcal{G}_i))^p\right)^{1/p} & 1 \le p < \infty \\ \max\{\mu_2(\mathcal{G}_1), \dots, \mu_2(\mathcal{G}_k)\} & p = \infty \end{cases},$$

$$\Lambda^D_{k,\infty}(\mathcal{P}) = \begin{cases} \left(\frac{1}{k}\sum_{i=1}^k (\lambda_1(\mathcal{G}_i))^p\right)^{1/p} & p < \infty \\ \max\{\lambda_1(\mathcal{G}_1), \dots, \lambda_1(\mathcal{G}_k)\} & 1 \le p = \infty \end{cases}.$$

We investigate properties of the minimal spectral energies $\mathcal{L}^N_{k,p}(\mathcal{G})$ and $\mathcal{L}^D_{k,p}(\mathcal{G})$ associated to $\Lambda^N_{k,p}$ and $\Lambda^D_{k,p}$ respectively. In particular, we show sharp lower and upper estimates for the minimal partition energies and for $p = \infty$ provide interlacing inequalities between $\mathcal{L}^D_{k,\infty}(\mathcal{G})$ and $\mathcal{L}^N_{k,\infty}(\mathcal{G})$, which involve topological quantities as the number of independent cycles in the graph or the number of degree one vertices of the graph, reminiscent to estimates and interlacing inequalities for the Laplacian eigenvalues of the whole graph. In particular, we obtain an inequality between these energies and the actual Dirichlet and standard Laplacian eigenvalues, valid for all compact graphs, which complements a version for tree graphs of Friedlander's inequalities between Dirichlet and Neumann eigenvalues of a domain. Combining these estimates with the bounds obtained for the spectral minimal energies, we infer an upper estimate on the eigenvalues of the standard Laplacian, which in some cases result in better Laplacian eigenvalue estimates than those obtained previously, such as by Berkolaiko et al [J. Phys. A 50 (2017), 365201].

In the third part of the thesis we establish metric graph counterparts of Pleijel's theorem on the asymptotics of the number of nodal domains ν_n of the n-th eigenfunction(s) of a broad class of operators on compact metric graphs, including Schrödinger operators with L^1-potentials and a variety of vertex conditions as well as the p-Laplacian with standard vertex conditions, and without any assumptions on the lengths of the edges, the topology of the graph, or the behavior of the eigenfunctions at the vertices. Among other things, these results characterize the accumulation points of the sequence $(\frac{\nu_n}{n})_{n\in\mathbb{N}}$, which are shown always to form a finite subset of $(0,1]$. This extends the previously known result that $\nu_n \sim n$ *generically*, for certain realizations of the Laplacian, in several directions. In particular, in the special cases of the Laplacian with standard conditions, we show that for graphs with rationally dependent edge lengths, one can find eigenfunctions thereon for which $\nu_n \not\sim n$; but in this case even the set of points of accumulation may depend on the choice of eigenbasis.

We conclude the thesis with some inequalities and numerics on the eigenvalues of the standard Laplacian on a graph. Based on von Below's theorem, we propose a technique for approximating the Kirchhoff–Neumann eigenvalues of a general metric graph. This involves a three step process. First, for a general metric graph $\mathcal{G}$, we consider an equilateral metric graph that 'best' approximates $\mathcal{G}$. Thus, we may use this approximation to create a sequence of discrete graphs $\{G_N\}$ with N vertices that converges to $\mathcal{G}$ in the Hausdorff sense. Finally, we prove a-priori and a-posteriori error estimates on the eigenvalues of the Laplacian on $\mathcal{G}$ obtained using those of G_N. These error estimates allow us to approximate the eigenvalues of the Laplacian on $\mathcal{G}$ to a desired precision, using the eigenvalues of the normalized Laplacian of a discrete graph. This is a semi-definite matrix eigenvalue problem for which very efficient numerical linear algebra tools are available.

1.2 Motivation

Metric graphs, and *quantum graphs*, have been appearing as early as the 1930s in the context of molecule models, and were studied in various areas, including chemistry, physics, and mathematics. A metric graph is essentially a collection of intervals joint together in a network like fashion (see [BK13], [Mug19])) In recent years differential operators on metric graphs, in this context we call metric graphs also *quantum graphs*, were studied in various contexts and we present in the following some areas of interest on metric graphs as a motivation to place it in context with the main results of this thesis, which will be presented in §1.3.

1.2.1 On network analysis and relationship to metric graphs

On given networks, be it social networks or otherwise linked structures, detecting clusters, i.e. the grouping of items in a network, is an essential task. There are several quantities to determine the "importance" of an item in a network and to determine clusters (c.f. e.g. [OG12], [TPFG18]) and there are several interdisciplinary approaches at network analysis and we refer to [Pre12] for an overview and history on the area of research. Note that applications can be found in everyday instances, for example through Google web search feature, which is based on the PageRank algorithm (c.f. [PBMW99]), which revolves around a simple eigenvalue problem to determine the relevance of web pages given a search term.

A viable approach of clustering is based on the study of eigenvalues of the discrete Laplacian on a given network. Let $G = (V, E)$ be a combinatorial graph, then we define the discrete or normalized Laplacian $L \in \mathbb{R}^{|V|\times|V|}$ via the linear map

$$(L\boldsymbol{u})_v = \sum_{\widetilde{v}:(\widetilde{v},v)\in E} \frac{u_v - u_{\widetilde{v}}}{d_v},$$

where $d_v = \deg(v)$ is the degree of the vertex $v \in V$. The eigenvector of the smallest nontrival eigenvalue changes sign and the graph can be divided in two subgraphs of similar "spectral" size via the subgraphs restricted to where the eigenvector is positive and negative respectively. This is referred to as *spectral clustering*. The corresponding eigenvalue can be variationally described with the discrete Rayleigh quotient

$$\mathcal{R}_G(\boldsymbol{f}) = \frac{\sum_{(u,v)\in E} |f(u) - f(v)|^2}{\sum_{v\in V} d_v f(v)^2}$$

via

$$\mu_2(G) = \min_{\substack{\boldsymbol{f}\in\mathbb{R}^{|V|}\setminus\{0\} \\ \sum_{v\in V} f(v)=0}} \mathcal{R}_G(\boldsymbol{f}).$$

The other eigenvalues can be then characterized via the minmax principle

$$\mu_k(G) = \min_{\substack{\boldsymbol{f}_1,\dots,\boldsymbol{f}_k\in\mathbb{R}^{|V|}\setminus\{0\} \\ \boldsymbol{f}_i\cdot\boldsymbol{f}_j=0 \text{ for all } i\neq j}} \max_{\boldsymbol{f}\in\operatorname{span}(\boldsymbol{f}_1,\dots,\boldsymbol{f}_k)\setminus\{0\}} \mathcal{R}_G(f).$$

A related concept from spectral geometry on manifolds involves partitioning the graph into connected subsets $S_1, \dots, S_k \subset V$ of similar conductance

$$\varphi_G(S) := \frac{|E(S)|}{|S|},$$

where $E(S)$ denotes the subset of edges that connect S with its complement in S and $|S| = \sum_{v\in S} \deg(v)$ is the volume of the graph. A Cheeger cut is a configuration $(S_1, \dots, S_k)$, that attains the infimum

$$h_k(G) = \min_{S_1,\dots,S_k} \max_i \varphi_G(S_i),$$

also called k-th Cheeger constant of G, where the minimum is taken over k-partitions of k nonempty vertex sets.

An adaptation of Cheeger's original result from [LGT14] for combinatorial graphs is given by the following:

Theorem 1.2.1 (Cheeger inequalities)**.** *Let $G = (V, E)$ be a combinatorial graph, then there* *exists* $C > 0$ *such that for all* $k \in \mathbb{N}$

$$\frac{\mu_k(G)}{2} \leq h_k(G) \leq Ck^4\sqrt{\mu_k(G)}.$$

In fact, this result was used this result on combinatorial graphs in [Mic15] to prove higher-order Cheeger inequalities for manifolds.

Similarly to the combinatorial Laplacian, for metric graphs $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ (see §2.1) we can define the standard Laplacian as the operator $-\Delta$ associated to the form

$$Q(u) = \int_{\mathcal{G}} |u'|^2 \, \mathrm{d}x$$

with $D(Q) = H^1(\mathcal{G}) \subset L^2(\mathcal{G})$. Then as a consequence of the spectral theory (see also §2; in particular, we define the relevant function spaces on metric graphs therein) the discrete eigenvalues of $-\Delta$ are given by the minimax principle

$$\mu_k(\mathcal{G}) = \min_{\substack{u_1,\dots,u_k \in H^1(\mathcal{G})\setminus\{0\} \\ \int_{\mathcal{G}} u_i u_j \, \mathrm{d}x = 0 \text{ for all } i \neq j}} \max_{u \in \operatorname{span}(u_1,\dots,u_k)\setminus\{0\}} \frac{Q(u)}{\|u\|_{L^2}}. \tag{1.2}$$

Eigenvalues between metric graphs and combinatorial graphs can be related through von Below's Theorem. In [Bel85] was shown (see for details §6.4)

Theorem 1.2.2 (von Below)**.** *Let* $\mathcal{G}$ *be an equilateral compact metric graph*[1] *such that each edge has length* $\ell > 0$. *For any eigenvalue* $\mu \neq 0, 2$ *of the Laplacian* L *of the underlying discrete graph* G, *there is an eigenvalue* λ *of* $-\Delta$ *on* $\mathcal{G}$, *such that* $\ell\sqrt{\lambda}/\pi \notin \mathbb{Z}$ *and*

$$1 - \cos \ell\sqrt{\lambda} = \mu\,.$$

Furthermore, the multiplicities of the two eigenvalues λ *and* μ *coincide and the values of the associated eigenvectors and eigenfunctions can be chosen such that their values coincide at the corresponding vertices.*

In particular we have the simple relation between the first nontrivial eigenvalues of the Laplacian on an equilateral metric graph $\mathcal{G}$ with basis length ℓ and underlying metric graph G

$$1 - \cos \ell\sqrt{\mu_2(\mathcal{G})} = \mu_2(G). \tag{1.3}$$

In [KKMM16] this was used for instance to show estimates and surgery principles for the first nontrivial eigenvalue of the Laplacian and the results were extended to the first nontrivial eigenvalue of the Laplacian on the underlying combinatorial graph via (1.3).

[1] We always assume compact metric graphs to only consist of finitely many edges throughout the thesis.

In fact, there is a natural connection between spectral clusters of metric graphs and combinatorial graphs due to Theorem 1.2.2. There are several similarities that combinatorial and metric graphs share. For example, it was shown in [KM16] (see also the references therein) that Cheeger type inequalities can be also shown for (1.2). In the context of spectral clustering of the Laplacian in [KKLM21] the spectral quantity

$$\mathcal{L}^D_{k,\infty}(\mathcal{G}) = \min_{\mathcal{G}_1,\dots,\mathcal{G}_k} \max\{\lambda_1(\mathcal{G}_1,\partial\mathcal{G}_1),\dots,\lambda_1(\mathcal{G}_k,\partial\mathcal{G}_k)\} \tag{1.4}$$

minimized over all connected k-partitions on the graph, where $\lambda_1(\mathcal{G}_i,\partial\mathcal{G}_i)$ denote the first nontrivial Dirichlet eigenvalue with Dirichlet points at the boundary set $\partial\mathcal{G}_i$ to be understood as the topological boundary of $\mathcal{G}_i$ as a subset of $\mathcal{G}$. Relationships to (1.4) were already initially investigated in [KKLM21] and in fact it was shown

$$\mathcal{L}^D_{k,\infty}(\mathcal{G}) \geq \mu_k(\mathcal{G}) \tag{1.5}$$

for all $k \in \mathbb{N}$ with $\mu_k(\mathcal{G})$ given as in (1.2). This will be one of the topics of study in the present thesis: we will discuss properties of the associated spectral minimizers and spectral minimal energies in §4 and our main results can be found in §1.3.2. In fact, von Below's theorem can be used to compute the eigenvalues of an equilateral graph and is essential in our approach in §6 to approximate eigenvalues of a Laplacian, and we will further elaborate on the approach in §1.2.5.

In the context of spectral clustering it is natural to study the number of so called *nodal partitions* of eigenfunctions of the Laplacian as defined as follows:

Definition 1.2.3. Let $\mathcal{G}$ be a metric graph and $u \in C(\mathcal{G})$, then we define the nodal set of u as

$$N(u) = \{x \in \mathcal{G} | u(x) = 0\}$$

and we define the connected components of $\mathcal{G} \setminus N(u)$ as the nodal components of u. The nodal partition associated to u is the partition on $\mathcal{G}$ consisting of the connected components of $\mathcal{G} \setminus N(u)$.

On euclidean domains, Courant's theorem guarantees the k-th eigenfunction to have at most k nodal domains. For graphs only a weaker version of this result holds (from [KKLM21, Proposition 8.6])

Theorem 1.2.4 (Weak Courant Theorem)**.** *Given an eigenvalue $\mu_k(\mathcal{G})$ and an associated eigenfunction ψ, denote by $\kappa(\mu_k(\mathcal{G}))$ the integer*

$$\kappa(\mu_k(\mathcal{G})) := \max\{j \in \mathbb{N} : \mu_j(\mathcal{G}) = \mu_k(\mathcal{G})\}$$

and by $\nu(\psi)$ the number of nodal domains of ψ. Then $\nu(\psi) \leq \kappa(\mu_k(\mathcal{G}))$.

In other words, the k-th eigenfunction, up to algebraic multiplicities, partitions the graph in at most k spectral clusters. Every eigenfunction restricted to its nodal domain is the first eigenfunction of the Dirichlet Laplacian with Dirichlet vertices at the respective cut vertices of the nodal partition. Similarly, given a Dirichlet vertex set $\mathcal{V}^D$, the eigenvalues of the corresponding Dirichlet Laplacian can be characterized via the minmax principle

$$\lambda_k(\mathcal{G}, \mathcal{V}^D) = \min_{\substack{u_1,\ldots,u_k \in H_0^1(\mathcal{G},\mathcal{V}^D)\setminus\{0\} \\ \int_{\mathcal{G}} \overline{u_i} u_j \,\mathrm{d}x = 0 \text{ for all } i \neq j}} \max_{u \in \operatorname{span}(u_1,\ldots,u_k)\setminus\{0\}} \frac{Q(u)}{\|u\|_{L^2}^2}.$$

In particular, suppose $\mathcal{G} = (\mathcal{G}_1, \ldots, \mathcal{G}_{k'})$ with $k' \leq k$ is a nodal partition associated to the k-th eigenfunction with eigenvalue μ_k, then (see for notation §2)

$$\mu_k = \max\{\lambda_1(\mathcal{G}_1, \partial\mathcal{G}_1), \ldots, \lambda_1(\mathcal{G}_{k'}, \partial\mathcal{G}_{k'})\}.$$

In [KKLM21] a related partitioning problem was studied. Namely, let $\mathfrak{C}_k$ be the set of connected k-partitions on $\mathcal{G}$, then we minimize

$$\Lambda_{k,\infty}^D(\mathcal{P}) = \max\{\lambda_1(\mathcal{G}_1, \partial\mathcal{G}_1), \ldots, \lambda_1(\mathcal{G}_{k'}, \partial\mathcal{G}_{k'})\} \tag{1.6}$$

among all k-partitions $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k) \in \mathfrak{C}_k$ and we define

$$\mathcal{L}_{k,\infty}^D(\mathcal{G}) = \inf_{\mathcal{P} \in \mathfrak{C}_k} \max\{\lambda_1(\mathcal{G}_1, \partial\mathcal{G}_1), \ldots, \lambda_1(\mathcal{G}_{k'}, \partial\mathcal{G}_{k'})\}.$$

This quantity is closely related to the k-th eigenvalue of the Laplacian (see also [BB18; BHH17; BL17c; HHT09] for domain counterparts). In fact, if the k-th eigenfunction has exactly k nodal domains, then we have equality in (1.5)

$$\mu_k(\mathcal{G}) = \mathcal{L}_{k,\infty}^D(\mathcal{G}).$$

In this case one says the k-th eigenfunction is Courant-sharp and the nodal partition associated to the eigenfunction minimizes (1.6). Minimizers of (1.6) are an example of spectral minimal partition problems that we will discuss in §4. In particular, we discuss relations to solutions of eigenvalue problems for the linear but also the nonlinear eigenvalue problem.

1.2.2 Ground states of nonlinear Schrödinger energy functional

In recent years, there has been a growth of interest in functionals on metric graphs $\mathcal{G}$ of the stationary NLS (Nonlinear Schrödinger) energy functional

$$E_{\mathrm{NLS}}(u, \mathcal{G}) = \frac{1}{2}\int_{\mathcal{G}} |u'|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \qquad u \in H^1(\mathcal{G}),\ \|u\|_{L^2}^2 = 1,\ q > 2,\ \mu > 0 \tag{1.7}$$

and associated ground states of the stationary NLS energy functional, i.e. minimizers for the constrained minimization problem

$$E_{\mathrm{NLS}}(\mathcal{G}) := \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} E_{\mathrm{NLS}}(u, \mathcal{G}), \qquad 2 < q < 6. \tag{1.8}$$

Minimizers of (1.8) are solutions to the stationary nonlinear Schrödinger equation on $\mathcal{G}$ given by

$$\begin{cases} -u'' + \lambda u = \mu |u|^{q-2} u & \text{edgewise,} \\ u \text{ is continuous on } \mathcal{G} \text{ and satisfies the Kirchhoff condition} \\ \displaystyle\sum_{e \in \mathcal{E}: e \succ \mathsf{v}} \frac{\partial u}{\partial \nu}\Big|_e(\mathsf{v}) = 0, \qquad \forall \mathsf{v} \in \mathcal{V}, \end{cases}$$

where $\lambda \in \mathbb{R}$ is a lagrange multiplier, $\mu > 0$, $e \succ \mathsf{v}$ denotes the relation that the edge e is adjacent to the vertex $\mathsf{v} \in \mathcal{V}$ and $\frac{\partial u}{\partial \nu}|_e(\mathsf{v})$ denotes the inward pointing derivative at v towards the interior of the edge e. For compact graphs, due to the compact imbedding of $H^1(\mathcal{G})$ in $L^2(\mathcal{G})$ and $L^q(\mathcal{G})$ and Gagliardo–Nirenberg inequality, existence of minimizers is a consequence of the direct method of the calculus of variations. For noncompact graphs the existence of minimizers is not necessarily guaranteed. Existence of ground states of (1.8) was researched extensively throughout the last few years.

Among the physical motivations for this problem, the most notable one is given by the Bose-Einstein equation from solid-state physics (see e.g. [DGPS99]; and [BK14] for some discussion in the context of many-particle quantum graphs). Under a critical low temperature, a boson gas is forced in a large number of N particles in the same quantum state given by the minimizer of the Gross-Pitaevski functional

$$E(\varphi) = \frac{1}{2}\|\varphi'\|_{L^2}^2 + 8\pi\alpha\|\varphi\|_{L^4}^4$$

under the normalization $\|\varphi\|_{L^2}^2 = N$ and $\alpha \in \mathbb{R}$ being the scattering length associated with the two-body interaction between the particles in the gas. In general, the importance of quantum graphs, i.e. metric graphs associated with differential operators, comes from being simplified models in ramified structures appearing in molecule physics or chemistry. Specifically, in the context of ramified traps, Bose-Einstein condensate equations on quantum graphs were previously considered as a theoretical model in [KFTK03] and [VLL11].

For the real line or even the half line, existence of ground states in (1.7) is known[2]. For general metric graphs, however, [AST15] shows that graphs of a particular topological structure, such as the graph of two half-lines joint together with a double bridge (see Figure 1.1), do not admit ground states. For graphs satisfying a certain threshold condition (as discussed in [AST16]) one can show existence of ground states however:

[2] See [AA11, §13] for a proof based on rearrangement techniques.

Figure 1.1: Double bridge graph. The double bridge (left) as an example for which NLS ground states do not exist. However, the graph consisting of two half-lines and a pendant satisfies the threshold condition (1.9) and we have existence of NLS ground states as discussed in [AST15].

Theorem 1.2.5 ([AST16])**.** *Let $\mathcal{G}$ be a noncompact metric graph with finitely many edges and $2 < q < 6$. Assume*

$$E_{NLS}(\mathcal{G}) < E_{NLS}(\mathbb{R}), \tag{1.9}$$

then there exists a minimizer for $E_{NLS}(\mathcal{G})$.

Theorem 1.2.5 provides an existence principle based on an energy threshold condition and we will in fact prove several generalizations in term of the considered functional and even the underlying function spaces in §3. Thresholdestimates like (1.9) allow to deduce existence of minimizers in certain situations as shown in [Ten16] and [AST17].

A variant of this problem with potential was considered in [CFN17] and [Cac18], where the energy functional was given by

$$E^m_{\text{NLS}}(u) = \frac{1}{2}\int_{\mathcal{G}} |u'|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \qquad \|u\|^2_{L^2} = 1 \tag{1.10}$$

with $m \in L^1 + L^\infty(\mathcal{G})$, i.e. there exist $m_1 \in L^1(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ such that $m = m_1 + m_\infty$. In [CFN17] the existence of minimizers of (1.10) was related to the existence of eigenvalues of the Schrödinger operator $-\Delta + m$ below the essential spectrum:

Theorem 1.2.6 ([CFN17])**.** *Let $\mathcal{G}$ be a noncompact metric graph with finitely many edges and $m \in L^1 + L^\infty(\mathcal{G})$ with $m_- = \min\{0, m\} \in L^r(\mathcal{G})$ for $r \in [1, 1 + \frac{2}{q-2}]$ and $2 < q \leq 6$. Assume*

$$\Sigma_0 := \inf \sigma(-\Delta + m) < \inf \sigma_{ess}(-\Delta + m_-) = 0. \tag{1.11}$$

Then there exists $\mu^* > 0$ such that for $\mu \in (0, \mu^*)$ the functional (1.10) *is bounded below and the associated constrained minimization problem*

$$E^m_{NLS} := \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|^2_{L^2} = 1}} E^m_{NLS}(u)$$

admits a minimizer.

In a sense the inequality (1.11) replaces the inequality (1.9) in Theorem 1.2.5 to achieve the existence results.

Remark 1.2.7. [Cac18] quantifies the result in Theorem 1.2.6: given the stationary NLS ground state energy on the real line

$$\gamma_q := \inf_{\substack{u\in H^1(\mathbb{R})\\ \|u\|_{L^2}^2=1}} \frac{1}{2}\int_{\mathbb{R}} |u'|^2 \,\mathrm{d}x - \frac{1}{q}\int_{\mathbb{R}} |u|^q \,\mathrm{d}x < 0$$

and $\Sigma_0 = \inf \sigma(-\Delta + m) < 0$ as in (1.11) one can choose $\mu^* > 0$ as

$$\mu^* = (\Sigma_0/\gamma_q)^{\frac{3}{2}-\frac{q}{4}}.$$

In §3 we consider an abstract theory to recover these results (see also §1.3.1 for the statement of the main results). Firstly, we develop a general existence theory in a far more abstract setting which can be applied to a variety of problems as for example E_{NLS} and E_{NLS}^m, providing in particular a unified approach to these problems. However, this theory is not limited to metric graphs, and may be also applied to functionals defined on function spaces on metric measure spaces, such as combinatorial graphs or general domains in $\mathbb{R}^N$. Secondly, we use the flexibility of this existence theory to obtain generalizations of the results in [AST16], [CFN17] and [Cac18] in several directions by considering more general graphs and higher-order derivatives in the functionals. We also tackle different variants of the problems, including the case of decaying potentials and localized nonlinearities, i.e. we replace the set of integration in the term corresponding to the nonlinearity by a bounded subgraph $\mathcal{K} \subset \mathcal{G}$, as well as a variant with magnetic potential and higher-order derivatives. Thirdly, we provide a spectral theoretical foundation for this type of existence theory.

1.2.3 Spectral minimal partitions and Bose-Einstein condensate equations

Let $\mathcal{G}$ be a compact metric graph. We already discussed the importance of spectral minimal partitions in connection with spectral clustering in §1.2.1. There are also connections between spectral minimal partition problems and the study of functionals as considered in §1.2.2 as we will see in the following in the context of limiting profiles of k-mixtures of Bose-Einstein condensate equations. Consider the coupled system of stationary Bose-Einstein condensate equations

$$\begin{cases} -u_i''(x) + (m_i(x) + \lambda_i)u_i(x) = \mu_i |u_i|^2 u_i - \beta \sum_{j\neq i} u_j^2 u_i \\ \sum_{e\succ v} \frac{\partial}{\partial \nu} u_i\big|_e(v) = 0, \qquad i = 1, \dots, k. \end{cases} \tag{1.12}$$

with $m_i \in L^\infty(\mathcal{G})$, $\lambda_i \in \mathbb{R}$, $\mu_i > 0$ for all $i = 1, \dots, k$, and $\beta > 0$. An analogue of the system of differential equations in (1.12) was proposed as a mathematical model for multispecies Bose–Einstein condensation in k different hyperfine spin states (see [CLLL04] and references therein) and experimentally such a condensation was observed in so-called triplet states (see [Rüe+03]).

We search for existence of solutions in $H^1(\mathcal{G})$ to (1.12) via the study of critical points of the functional

$$J_\beta(u_1,\dots,u_k)=\sum_{i=1}^{k}\left[\frac{1}{2}\int_{\mathcal{G}}|u_i'|^2+(m_i+\lambda_i)|u_i|^2\,\mathrm{d}x-\frac{\mu}{4}\int_{\mathcal{G}}|u_i|^4\,\mathrm{d}x\right]+\frac{\beta}{4}\sum_{\substack{i,j=1\\ i\neq j}}^{k}\int_{\mathcal{G}}u_i^2u_j^2\,\mathrm{d}x.$$

For $\beta=\infty$ we define

$$J_\infty(u_1,\dots,u_k)=\begin{cases}\displaystyle\sum_{i=1}^{k}\left[\frac{1}{2}\int_{\mathcal{G}}|u_i'|^2+m_i|u_i|^2\,\mathrm{d}x-\frac{\mu}{4}\int_{\mathcal{G}}|u_i|^4\,\mathrm{d}x\right], & \begin{array}{c}u_i\cdot u_j=0 \text{ a.e.}\\ \text{for all } i\neq j\end{array}\\ \infty, & \text{otherwise.}\end{cases}$$

Critical points can be obtained via the study of minimizers on the Nehari manifolds

$$\begin{aligned}\mathcal{N}_\beta&=\{U=(u_1,\dots,u_k)\in(H^1(\mathcal{G})\setminus\{0\})^k:\partial_{u_i}J_\beta(U)u_i=0, i=1,\dots,k\}\\ &=\Big\{U=(u_1,\dots,u_k)\in(H^1(\mathcal{G})\setminus\{0\})^k:\\ &\qquad\int_{\mathcal{G}}|u_i'|^2+(m_i+\lambda_i)|u_i|^2\,\mathrm{d}x=\mu\int_{\mathcal{G}}u_i^4-\int_{\mathcal{G}}\beta u_i^2\sum_{\substack{j=1\\ i\neq j}}^{k}u_j^2, i=1,\dots,k\Big\}.\end{aligned}$$

for $\beta\in[1,\infty)$ and for $\beta=\infty$

$$\begin{aligned}\mathcal{N}_\infty&=\{U=(u_1,\dots,u_k)\in(H^1(\mathcal{G})\setminus\{0\})^k:u_i\cdot u_j=0 \text{ a.e. for all } i\neq j,\\ &\qquad\partial_{u_i}J_\infty(U)u_i=0, i=1,\dots,k\}\\ &=\Big\{U=(u_1,\dots,u_k)\in(H^1(\mathcal{G})\setminus\{0\})^k:u_i\cdot u_j=0 \text{ a.e. for all } i\neq j\\ &\qquad\int_{\mathcal{G}}|u_i'|^2+(m_i+\lambda_i)|u_i|^2\,\mathrm{d}x=\mu\int_{\mathcal{G}}u_i^4, i=1,\dots,k\Big\}.\end{aligned}$$

for the minimization problem

$$\inf_{U\in\mathcal{N}_\beta}J_\beta(U). \tag{1.13}$$

Existence of a minimizer in (1.13) was already previously considered for domains (see e.g. [Tav10, Part I §1], [CTV02], [CTV03]). We show in §4 existence of minimizers of (1.13) on compact metric graphs. As in the case of domains, as $\beta\to\infty$, we obtain minimizers for the problem $\beta=\infty$, and the supports of the minimizer $u_1,\dots,u_k$ of (1.13) define a partition on $\mathcal{G}$; we will see (c.f. Example 4.3.1) that it solves the minimization problem

$$\mathcal{L}^D_{k,4,4}=\inf_{\mathcal{P}}\Lambda^D_{k,4,4}(\mathcal{P})$$

minimized among k-partitions as defined in §4.1. We will in fact study different minimization problems of the form

$$\inf_{\mathcal{P}} \Lambda(\mathcal{P})$$

where the minimum is taken among k-partitions and refer to minimizers of the respective quantity as spectral minimal partitions.

The theory on spectral minimal partitions from [KKLM21], strongly motivated from existence theory on the plane (see [CTV05], [HHT09]), allows the consideration of a broad class of spectral clustering problems. Another spectral minimal partition problem we consider in the thesis are Neumann partitions. More exactly, we minimize

$$\Lambda_{k,\infty}^{N}(\mathcal{P}) = \max\{\mu_2(\mathcal{G}_1), \ldots, \mu_2(\mathcal{G}_k)\}$$

among all connected k-partitions $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ (see §2 for more details) and define

$$\mathcal{L}_{k,\infty}^{N}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda_{k,\infty}^{N}(\mathcal{P}).$$

In fact we will differ between different types of partitions. The most natural notion, is a partition of a graph in closed subgraphs, so called *faithful* partitions. These inherit all possible connections from the original graph and reflect its topology as closely as possible. Any other partition where we are still only altering the connectivity of our clusters at separating points we call *rigid*; this is, in particular, the case of the partition in Figure 1.3 (though it is also true of the faithful partition from Figure 1.2.

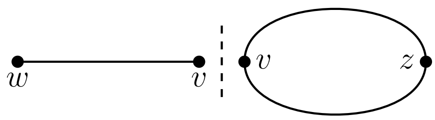


Figure 1.2: Faithful partition on the lasso graph. A faithful 2-partition of the lasso $\mathcal{G}$; the only cut vertex is v. (c.f [KKLM21, Figure 3])

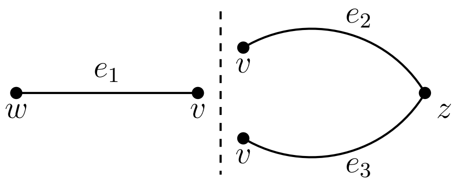


Figure 1.3: Rigid partition on the lasso graph. A rigid 2-partition of the lasso $\mathcal{G}$; again, the only cut vertex is v. (c.f. [KKLM21, Figure 4])

Rigid partitions may appear less natural than faithful ones. However, the spaces of graph partitions with respect to rigid partitions is not closed (in the sense explained in c.f. §2.1; see [KKLM21] for details). This decisive topological feature is the main reason it is appropriate to consider them. We conclude by considering a further relaxation, which also explains the use of the term *rigid*: namely, we may allow cuts not only at the points separating clusters but also at interior points of clusters (note that these points are not necessarily interior points on some edges: these points could be vertices lying inside clusters), as long as each cluster stays connected. We shall refer to partitions which may involve cuts in interior points as *connected* (see also Figure 1.4 for an example).

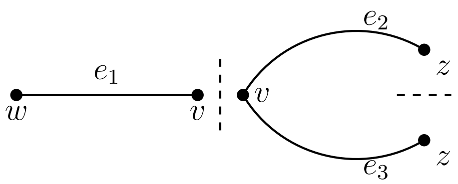


Figure 1.4: Connected partition on the lasso graph. A connected 2-partition of the lasso $\mathcal{G}$; in this case, the only boundary vertex of the partition is v but we are additionally cutting through z (c.f. [KKLM21, Figure 5]).

Under this distinguishment let $\mathfrak{C}_k$ be the set of connected k-partitions and $\mathfrak{R}_k$ be the set of rigid k-partitions. Then more specifically we define

$$\begin{gathered}\mathcal{L}^D_{k,\infty}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{R}_k} \Lambda^D_{k,\infty}(\mathcal{P}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda^D_{k,\infty}(\mathcal{P}),\\ \mathcal{L}^{N,r}_{k,\infty}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{R}_k} \Lambda^N_{k,\infty}(\mathcal{P}), \quad \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda^N_{k,\infty}(\mathcal{P}),\end{gathered} \tag{1.14}$$

where we have equality in the first quantity since cutting a partition element does not decrease the eigenvalues due to the variational characterization (c.f. [KKLM21, Lemma 4.3]) and without loss of generality we can restrict ourselves to faithful partitions.

In §4 we discuss the relations between these quantities and the eigenvalues of the Dirichlet Laplacian. In particular, we establish interlacing inequalities, which remind of the interlacing inequalities between eigenvalues, obtained via finite rank perturbations and establish the Weyl asymptotics of the quantities (see also [BK13, §3] for basic properties of the operators considered). We refer to our results in §1.3.2. The results are based on the joint works [HKMP21a] and [HK21].

1.2.4 Pleijel's theorem

The classical Sturm Oscillation Theorem, first proved in Sturm's paper [Stu36], states that the n-th eigenfunction ψ_n of a Sturm–Liouville operator with continuous coefficients and separated boundary conditions on a compact interval has $n-1$ zeros in the interior of the interval, that is, $\nu_n = n$ nodal domains. We refer to [Hin05] for a historical overview of the generalisations of this result, including more general coefficients and boundary conditions.

The counterpart in higher dimensions, Courant's Nodal Domain Theorem [Cou23], states that the number ν_n of nodal domains of the eigenfunction ψ_n associated with the n-th eigenvalue of the Dirichlet Laplacian on a bounded domain in $\mathbb{R}^d$ is no larger than n. Pleijel's theorem [Ple56], which establishes an asymptotic bound on the quotient ν_n/n, sharpens Courant's result by implying that the number of eigenvalues for which equality may hold is finite if $d = 2$. In fact, Pleijel's argument can be extended to the case $d \geq 3$ (see [BM82]) and the same conclusion holds for $d \geq 2$.

In the case of quantum graphs which may have cycles, the Courant–Pleijel theory was first obtained – again, only under the genericity assumptions (generic in the sense of [BL17b]) that

- the spectrum is simple,
- no eigenfunction vanishes at any vertex

– by Gnutzmann, Smilansky and Weber in [GSW04]; their proof mirrors the original one by Pleijel but, unlike in Pleijel's result, it only yields that the number ν_n of nodal domains associated with the n-th eigenfunction is *generically* bounded from above by n. Under the same assumptions, the nodal deficiency $n - \nu_n$ has since been studied by Band, Berkolaiko and their co-authors in several papers since [BBRS12] (see, e.g., [ABB18; BW14] and the references therein).

In the joint work [HKMP21b] we showed Pleijel type results for general graphs without any additional assumption of genericity of the eigenvalues, which we present in §5 (see also §1.3.3 for our main results). With the aim of showing the flexibility of our approach – which, unlike that of [GSW04] does not rely on global linear algebraic manipulations, but rather on isoperimetric inequalities applied locally to the nodal domains – we turn to an important *nonlinear* operator. §5.5 is devoted to the theory of p-Laplacian, and to obtaining a Pleijel-type theorem in this context. Closely related, we obtain Pleijel type theorems for a broad class of differential operators of second order. In particular, this will include the important special cases of Schrödinger operators with smooth (or even zero) potential and (possibly) delta couplings, or else any of the usual vertex conditions, at the vertices.

In §5 given a sequence of the k-th eigenfunctions ψ_n we present the behavior of the sequence ν_n/n for quantum graphs and explore the validity, or lack thereof, of Pleijel's theorem. In this context, we prove

$$\frac{\nu_n}{n} \sim \frac{|\{\psi_n \neq 0\}|}{|\mathcal{G}|} \qquad (n \to \infty).$$

Refer to §1.3.2 for the precise statement and consequences of this result for Schrödinger operators with standard vertex conditions and the p-Laplacian.

1.2.5 Finite element methods on metric graphs

Via introduction dummy vertices (see §2.1.2) in $\mathcal{G}$ to obtain so called extended graphs $\mathcal{G}_h$, in [AB18] a finite element method was developed and a discretization for eigenvalue problems of differential operators derived, which reduces to a generalized algebraic eigenvalue problem

$$Au_h = \lambda M u_h$$

with a discretization parameter $h \to 0$ and numerical approximations of eigenvalues were computed for some examplary graphs. For such a discretization an *extended graph* is considered, i.e. the edges are partitioned and without loss of generality the discretization points can be considered as dummy vertices. However, if we consider the Kirchhoff–Neumann eigenvalue problem

$$\begin{cases} -\Delta u &= \lambda u \\ \sum\limits_{\mathsf{e} \text{ incident to } \mathsf{v}} \dfrac{\partial}{\partial \nu_{\mathsf{e}}} u(x) &= 0, \qquad \forall \mathsf{v} \in V, \end{cases} \tag{1.15}$$

then its eigenvalues can be related to the eigenvalues of the corresponding normalized Laplacian of the underlying combinatorial graph for equilateral graphs due to Theorem 1.2.2 as discussed in §1.2.1. We will evolve this result to general graphs, that we review in detail in §6.4 for graphs with pairwise rational edge lengths, and present a technique for approximating the Kirchhoff–Neumann eigenvalues of a general metric graph based on the joint work [HST].

To this end, our approach is three-fold. First, for a general metric graph $\mathcal{G}$, we consider an equilateral metric graph that 'best' approximates $\mathcal{G}$. Thus, we use this approximation to create a sequence of discrete graphs $\{G_N\}$ with N vertices that converges to $\mathcal{G}$ in the Hausdorff sense. Finally, we prove a-priori and a-posteriori error estimates on the eigenvalues of $\mathcal{G}$ obtained using those of G_N. These error estimates allow us to approximate the eigenvalues of $\mathcal{G}$ to a desired precision, using the eigenvalues of the normalized Laplacian of a discrete graph. This is a semi-definite matrix eigenvalue problem for which very efficient numerical linear algebra tools are available.

More precisely, given a metric graph $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$, i.e. the metric graph with underlying combinatorial graph $G = (V, E)$ and associated length vector $\boldsymbol{\ell} \in \mathbb{R}^{|E|}$, with rationally dependent edges, i.e. for all $i \neq j$ $\frac{\ell_i}{\ell_j} \in \mathbb{Q}$, we show in §6 how one can compute the eigenvalues of the Laplacian. Given two metric graphs $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ and $\widetilde{\mathcal{G}} = \widetilde{\mathcal{G}}(G, \widetilde{\boldsymbol{\ell}})$ we define the distance

$$\operatorname{dist}(\mathcal{G}_n, \mathcal{G}) = \max_{\mathsf{e} \in E} |\ell_{\mathsf{e}} - \widetilde{\ell}_{\mathsf{e}}|$$

and we say a sequence of graphs $\mathcal{G}_n$ with same underlying graph converge towards G if

$$\operatorname{dist}(G_n, G) \qquad (n \to \infty).$$

We then introduce an approximation technique based on the SDAP-Algorithm (c.f. §6.5) to approximate a graph $\mathcal{G}$ by graphs $\mathcal{G}_n$ with rational dependent edge lengths such that

$$\operatorname{dist}(\mathcal{G}_n, \mathcal{G}) \to 0 \qquad (n \to \infty).$$

Then by analytic dependence of the eigenvalues with respect to the edge length for each k one has

$$|\lambda_k(\mathcal{G}_n) - \lambda_k(\mathcal{G})| \to 0 \qquad (n \to \infty).$$

More specifically we show bounds for the relative error

$$\operatorname{rel\,err}(\lambda_k) := \left| \frac{\lambda_k(\mathcal{G}) - \lambda_k(\widetilde{\mathcal{G}})}{\lambda_k(\mathcal{G})} \right|.$$

using spectral bounds obtained previously in [BKKM17].

1.3 Main results

In this section we summarize the main results of the thesis. In §1.3.1 we have the results from [Hof19] on the existence of ground states of the NLS energy functional, in §1.3.2 the results from [HK21] and [HKMP21a] on interlacing inequalities, estimates and asymptotics involving spectral minimal partitions, in §1.3.3 we formulate Pleijel type theorems for the eigenfunctions of the considered operators from [HKMP21b], and in §1.3.4 our results regarding approximation estimates and a-priori/a-posteriori estimates for the Laplacian on metric graphs from [HST].

1.3.1 Existence principles for Ground states of NLS energy functionals

Let $\mathcal{G}$ be a finite metric graph. In §1.2.2 (for $k = 1$) we introduced the minimization problem

$$E^{(k)} = \inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \tag{1.16}$$

for $\mu > 0$ and $2 < q < 6$ and the development of existence principles for (1.16) with $k \in \mathbb{N}$ is subject of §3. Our general existence principle will be developed in §3.2 and then applied to general NLS type energy functionals in §3.3. While it would be not feasible to reproduce the definitions and main abstract results here, we present here our principal applications:

Theorem 1.3.1. *Let $\mathcal{G}$ be a noncompact metric graph with finitely many edges. Assume that either*

(i) there exists $m = m_2 + m_\infty$ such that $m_2 \in L^2(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ and

$$m_\infty(x) \to 0 \qquad (x \to \infty)$$

on all edges of infinite length, or

(ii) $A = (-\Delta)^k + m$ admits a ground state, i.e. $\inf \sigma(A)$ is an eigenvalue.

Then $E^{(k)}$ is strictly subadditive, i.e.

$$t \mapsto E_t := \inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_{L^2}^2 = t}} \frac{1}{2} \int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathcal{G}} |u|^q \,\mathrm{d}x$$

satisfies $E_1 < E_t + E_{1-t}$ *for all* $t \in (0,1)$*, and if additionally*

$$E^{(k)} < \widetilde{E^{(k)}} := \sup_{K \Subset \mathcal{G}} \inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1,\, \operatorname{supp} u \subset \mathcal{G} \setminus K}} E^{(k)}(u), \tag{1.17}$$

then $E^{(k)}$ *admits a minimizer.*

Analogously to (1.8) and (1.10), we will refer to the minimizers of $E^{(k)}$ as ground states. Theorem 1.3.1 generalizes Theorem 1.2.5 since (1.7) satisfies the prerequisites of Theorem 1.3.1. Indeed, one can show with a test function argument (see Example 3.4.13) that if $\mathcal{G}$ is a metric graph with finitely many edges then

$$\widetilde{E_{\text{NLS}}} := \sup_{K \Subset \mathcal{G}} \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1,\, \operatorname{supp} u \subset \mathcal{G} \setminus K}} E_{\text{NLS}}(u) = E_{\text{NLS}}(\mathbb{R})$$

and we recover Theorem 1.2.5.

Under the assumption that eigenvalues exist below the essential spectrum, i.e.

$$\inf \sigma((-\Delta)^k + m) < \inf \sigma_{\text{ess}}((-\Delta)^k + m),$$

by a perturbation argument one can ensure that (1.17) is satisfied for small nonlinearities and deduce a generalization of Theorem 1.2.6:

Theorem 1.3.2. *Let* $\mathcal{G}$ *be a noncompact metric graph with finite edge set. Let* $m \in L^2 + L^\infty(\mathcal{G})$*. Then* $(-\Delta)^k + m : D((-\Delta)^k + m) \subset L^2(\mathcal{G}) \to L^2(\mathcal{G})$ *is a self-adjoint operator. Furthermore, if*

$$\inf \sigma((-\Delta)^k + m) < \inf \sigma_{ess}((-\Delta)^k + m)$$

then (1.16) *admits a ground state for sufficiently small* $\mu > 0$*.*

Note that Theorem 1.2.6 also includes the critical case $q = 6$, which is considered as a special case, since the functional is bounded below only for sufficiently small $\mu > 0$. It is reasonable to expect that a similar result as in Theorem 1.3.2 holds in this particular case.

Let now $\mathcal{G}$ be a locally finite graph, i.e. we consider a broader class of graphs, the NLS ground state problem with magnetic potential, but second order in place of k-th order. Namely, we consider the minimization problem

$$E_{\text{NLS}}^{(\mathcal{K})} = \min_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i \frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{p} \int_{\mathcal{K}} |u|^q \,\mathrm{d}x,$$

with $\mu > 0$, $m \in L^2 + L^\infty(\mathcal{G})$ and $2 < q < 4k + 2$. The following theorem is an analog of Theorem 1.3.2. Interestingly, if one considers localized nonlinearities, i.e. $\mathcal{K}$ is a bounded subgraph of $\mathcal{G}$, then the existence result can be shown independent of the parameter $\mu > 0$ in the nonlinearity:

Theorem 1.3.3. *Let $\mathcal{G}$ be a noncompact locally finite metric graph and $\mathcal{K} \subseteq \mathcal{G}$ a connected subgraph. Let $V \in L^2 + L^\infty(\mathcal{G})$ and $M \in H^1 + W^{1,\infty}(\mathcal{G})$. Suppose $A^M = (i\frac{\mathrm{d}}{\mathrm{d}x} + M)^2 + m$ admits a ground state that does not vanish identically on $\mathcal{K}$.*

(i) If $\inf \sigma(A^M) < \inf \sigma_{ess}(A^M)$, then

$$E_{NLS}^{(\mathcal{K})} := \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i \frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathcal{K}} |u|^q \,\mathrm{d}x$$

admits a minimizer for sufficiently small $\mu > 0$.

(ii) If $\mathcal{K}$ is a bounded subgraph of $\mathcal{G}$, then minimizers exist for all $\mu > 0$.

In §3.4.4 we are going to show that for a tree graph $\mathcal{G}$ the ground states of Schrödinger operators with magnetic potential do not vanish anywhere on $\mathcal{G}$. Then, given a *decaying potential* $m \in L^2 + L^\infty(\mathcal{G})$ with $m = m_2 + m_\infty$, such that $V_2 \in L^2(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ satisfying

$$\sup_{x \in \mathcal{G} \setminus K} |m_\infty(x)| \to 0 \qquad (n \to \infty), \tag{1.18}$$

we show:

Theorem 1.3.4. *Let $\mathcal{G}$ be a noncompact locally finite tree graph with finitely many vertices of degree* 1*. Suppose $M \in H^1 + W^{1,\infty}(\mathcal{G})$ and $V \in L^2 + L^\infty(\mathcal{G})$ that satisfies* (1.18)*. Then* (3.6) *admits a minimizer if*

$$E_{NLS}^{(\mathcal{K})} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i \frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathcal{K}} |u|^q \,\mathrm{d}x < E_{NLS}(\mathbb{R}).$$

In particular, if

$$\inf \sigma \left(\left(i \frac{\mathrm{d}}{\mathrm{d}x} + M \right)^2 + m \right) < 0,$$

then we have existence of minimizers of $E_{NLS}^{(\mathcal{K})}$ for $0 < \mu \le (\Sigma_0/\gamma_q)^{\frac{3}{2} - \frac{p}{4}}$ with Σ_0, γ_q defined as in Remark 1.2.7.

1.3.2 Estimates and Asymptotics of Spectral minimal partitions

Given a compact metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with (first) Betti number $\beta = |\mathcal{E}| - |\mathcal{V}| + 1$, which is the number of independent cycles on the graph, and $|N|$ vertices of degree one. Recall the expressions $\mathcal{L}_{k,p}^{N,r}$, $\mathcal{L}_{k,p}^{N,c}$, and $\mathcal{L}_{k,p}^{D}$ from (1.14). First of all we get the following estimates on the quantities:

Theorem 1.3.5. *For all $k \in \mathbb{N}$ such that $k \geq \beta$ we have*

$$\left(\mathcal{L}^{N,r}_{k,\infty}(\mathcal{G}) \geq\right) \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^{D}_{k+1-\beta,\infty}(\mathcal{G}).$$

Theorem 1.3.6. *For all $k \in \mathbb{N}$ such that $k \geq \beta + |N|$ we have*

$$\mathcal{L}^{D}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k+1-\beta-|N|,\infty}(\mathcal{G}).$$

A consequence of these inequalities is that we can relate these spectral minimal energies with the eigenvalues of the Laplacian on the whole graph, both with standard conditions at all vertices and with Dirichlet conditions at all vertices. Indeed, recall that $\mu_k(\mathcal{G})$ denotes the k-th eigenvalue of the Laplacian with standard conditions on $\mathcal{G}$ (starting at $\mu_1(\mathcal{G}) = 0$ and counting multiplicities) and let $\lambda_k(\mathcal{G}, \mathcal{V}^D)$ be the k-th eigenvalue of the Laplacian with Dirichlet conditions at a distinguished set $\mathcal{V}^D$ of Dirichlet vertices and standard conditions on the rest, which we abbreviate to $\lambda_k(\mathcal{G}) := \lambda_k(\mathcal{G}, \mathcal{V})$ for when *all* vertices are Dirichlet vertices. Then the following result is a fairly direct consequence of Theorem 1.3.5.

Corollary 1.3.7. *Let $\mathcal{G}$ be a (connected, compact, finite) metric graph with first Betti number $\beta \geq 0$. Then for all $k \geq \beta + 1$ we have*

$$\lambda_k(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^{D}_{k+1-\beta,\infty}(\mathcal{G}) \geq \mu_{k+1-\beta}(\mathcal{G}). \tag{1.19}$$

Due to Weyl's asymptotics (c.f. Lemma 5.3.5) we have

$$\lambda_k(\mathcal{G}), \mu_k(\mathcal{G}) = \frac{\pi^2 k^2}{|\mathcal{G}|^2} + O(k) \qquad (k \to \infty)$$

and in particular, by (1.19) Weyl asymptotics holds for the spectral minimal partitions

$$\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}), \mathcal{L}^{N,r}_{k,\infty}(\mathcal{G}), \mathcal{L}^{D}_{k+1-\beta,\infty}(\mathcal{G}) = \frac{\pi^2 k^2}{|\mathcal{G}|^2} + O(k) \qquad (k \to \infty). \tag{1.20}$$

In §4.4 we study spectral estimates, and recover the Weyl asymptotics independently. Denote with (ℓ_{e}) the lengths of the edges and let $\ell_{\min}$ be the length of the shortest edge and $L = \operatorname{sum}(\ell_{\mathsf{e}})$ be the total length of the graph. We show the following:

Theorem 1.3.8. *Let $p \in [1, \infty]$. Then*

$$\frac{\pi^2}{4kL^2}\left(k^3 + 3(k - \beta - |N|)^3\right) \leq \mathcal{L}^{D}_{k,p}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\left(k + \left(|\mathcal{E}| - 1 - \left\lfloor \frac{|N|}{2} \right\rfloor\right)\right)^2$$

for all sufficiently large $k \geq 2$, in particular for

$$k \geq \max\left\{\beta + |N|, \frac{L}{\ell_{\min}} + |\mathcal{E}| - 1\right\}.$$

In particular,

$$\mathcal{L}^D_{k,p}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty. \tag{1.21}$$

Theorem 1.3.9. *Let* $p \in [1, \infty]$. *Then*

$$\frac{\pi^2}{L^2}k^2 \leq \mathcal{L}^{N,c}_{k,p}(\mathcal{G}) \leq \mathcal{L}^N_{k,p}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\big(k + (|\mathcal{E}| - 1)\big)^2.$$

for all $k \geq 1$ *in the case of the lower bound, and for all sufficiently large* k *in the case of the upper bound, in particular for* $k \geq 5|\mathcal{E}| - 1$. *In particular,*

$$\mathcal{L}^{N,c}_{k,p}(\mathcal{G}),\, \mathcal{L}^N_{k,p}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty. \tag{1.22}$$

Theorem 1.3.8 and Theorem 1.3.9 give an estimate for a second term in the asymptotics, if it exists. The sequences

$$\frac{\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}), \mathcal{L}^N_{k,\infty}(\mathcal{G}), \mathcal{L}^D_{k+1-\beta,\infty}(\mathcal{G}) - \frac{\pi^2 k^2}{|\mathcal{G}|^2}}{k}$$

are then bounded by (1.21) and (1.22). Unlike on the interval for a general metric graph the sequence we may have mixing properties in the corresponding sequence. In fact, dynamical systems on graphs are known to be able to admit mixing dynamics due to the existence of ramification as shown in the context of a discrete scattering system introduced in [GS06]. Unlike on intervals due to the junctions in a metric graph, we see in §4.4.6 that no second term in the Weyl asymptotics in (1.20) exists in general. In other words, the sequence

$$\frac{\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}), \mathcal{L}^N_{k,\infty}(\mathcal{G}), \mathcal{L}^D_{k+1-\beta,\infty}(\mathcal{G}) - \frac{\pi^2 k^2}{|\mathcal{G}|^2}}{k}$$

may not converge. For simple examples we study the dynamics of the sequence c_k, and categorize when the sequence either contain finitely many limit points, or have as a limit set whole intervals.

1.3.3 Pleijel's theorem on metric graphs

As mentioned in §1.2.4 we consider second order differential operator with a possible relaxation of the continuity condition at the vertices (see §5.1). In particular, suppose $\nu_n \in \mathbb{N}$ is the nodal count of the n-th eigenfunction ψ_n of the Schrödinger operator $-\Delta + q$ with real-valued $q \in L^1(\mathcal{G})$ potential. Then we have:

Theorem 1.3.10. *The nodal count* $(\nu_n)_{n\in\mathbb{N}}$ *satisfies*

$$\operatorname{acc}\left\{\tfrac{\nu_n}{n} : n \in \mathbb{N}\right\} = \operatorname{acc}\left\{\frac{|\mathit{supp}\,\psi_n|}{|\mathcal{G}|} : n \in \mathbb{N}\right\} \subset \left\{\frac{\sum_{\mathsf{e}\in E_0}\ell_{\mathsf{e}}}{|\mathcal{G}|} : E \supset E_0 \text{ is a nonempty set of edges}\right\}.$$

In particular, $\operatorname{acc}\left\{\frac{\nu_n}{n} : n \in \mathbb{N}\right\}$ *is a finite set, and*

$$0 < \frac{\ell_{\min}}{|\mathcal{G}|} \le \liminf_{n\to\infty} \frac{\nu_n}{n} \le \limsup_{n\to\infty} \frac{\nu_n}{n} \le 1.$$

We show that, this result in fact even holds for the p-Laplacian on metric graphs, i.e. the Fréchet derivative of the functional

$$\mathfrak{E}_p : u \mapsto \int_{\mathcal{G}} |u'|^p \,\mathrm{d}x, \qquad u \in D(\mathfrak{E}_p) := W^{1,p}(\mathcal{G}).$$

In the particular case ($p = 2$) of the free Laplacian with standard conditions at all vertices, we can say somewhat more. The following, our second main result, is a complement to the main result in [GSW04], whose scope we also extend by removing the genericity condition therein. Note, that the first statement in the following theorem is simply an immediate consequence of Theorem 1.3.10 and [BL17b], [GSW04] (see also §5.4).

Theorem 1.3.11. *Suppose* $\nu_n \in \mathbb{N}$ *is the nodal count of the* n*-th eigenfunction of the Laplacian with standard vertex conditions. Then the following assertions hold.*

1. *If* $\mathcal{G}$ *does not contain any loops, then the set of edge length vectors in* $\mathbb{R}_+^{|E|}$ *for which, for the corresponding graph with the given topology and these edge lengths, all eigenvalues are simple and* $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$*, is of the second Baire category (i.e., is a countable intersection of open dense sets).*

2. *If* $\mathcal{G}$ *contains a loop of length* ℓ*, then* $\frac{\ell}{|\mathcal{G}|}$ *is a point of accumulation of* $\frac{\nu_n}{n}$*. In particular, the lower estimate of* (5.10) *is sharp whenever* $\ell_{\min}$ *is realized by a loop.*

3. *If all edge lengths of* $\mathcal{G}$ *are rationally dependent, then* $\limsup_{n\to\infty} \frac{\nu_n}{n} = 1$*. If* $\mathcal{G}$ *contains a cycle, and is not a loop, then the basis may be chosen so that additionally* $\liminf_{n\to\infty} \frac{\nu_n}{n} < 1$ *holds.*

1.3.4 Approximation of eigenvalues of the Laplacian

To specify the metric graphs we also denote a metric graph via $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ to emphasize its dependence on the underlying combinatorial graph $G = (V, E)$ and length vector $\boldsymbol{\ell}$, which we introduce in this subsection to emphasize the dependence of the length of the given graph. In particular, for the Laplacian with standard vertex conditions and its k-th eigenvalues λ_k we have the following approximation theorem:

Theorem 1.3.12. *Let* $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ *and* $\widetilde{\mathcal{G}} = \mathcal{G}(G, \widetilde{\boldsymbol{\ell}})$ *be metric graphs with* $\operatorname{sum}(\boldsymbol{\ell}) = \operatorname{sum}(\widetilde{\boldsymbol{\ell}})$*, then*

$$\operatorname{rel\,err}(\lambda_k) := \left|\frac{\lambda_k(\mathcal{G}) - \lambda_k(\widetilde{\mathcal{G}})}{\lambda_k(\mathcal{G})}\right| \le C_k \max_{\mathsf{e}\in E} \frac{|\ell_e - \widetilde{\ell}_e|}{\min\{\ell_e, \widetilde{\ell}_e\}}$$

where β is the Betti number of G, $|N|$ is the number of pendants, i.e. vertices of degree 1, and

$$C_k := \left(\frac{k - 2 + \frac{3\beta+N}{2}}{\min\{k - \frac{\beta+N}{2}, 2k\}} \right)^2 \leq \max\{8, (3\beta + |N| - 1)^2\}$$

Moreover, we have the following asymptotic estimate:

Corollary 1.3.13. *Suppose $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ and $\mathcal{G}^{(n)} = \mathcal{G}^{(n)}(G, \boldsymbol{\ell}^{(n)})$ with $\operatorname{sum}(\boldsymbol{\ell}) = \operatorname{sum}(\boldsymbol{\ell}^{(n)})$, and*

$$\operatorname{dist}_G(\mathcal{G}^{(n)}, \mathcal{G}) := \|\boldsymbol{\ell}^{(n)} - \boldsymbol{\ell}\|_\infty \to 0$$

as $n \to \infty$, then for sufficiently large n, there exists $C > 0$ independent of k such that

$$\operatorname{rel\,err}(\lambda_k) \leq C \operatorname{dist}(\mathcal{G}^{(n)}, \mathcal{G}).$$

In this flavor, we show also a-posteriori and a-priori bounds (see §6.3) and regarding converging speed we have the following result, which guarantees the existence of graphs that approximate $\mathcal{G}$ arbitrarily exactly:

Theorem 1.3.14. *Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ be a metric graph with $\langle \boldsymbol{\ell}, \mathbf{1} \rangle = 1$, then for all $q \in \mathbb{N}$ there exists a metric graph $\mathcal{G}_q = \mathcal{G}_q(G, \boldsymbol{n}_q/q)$ with $\boldsymbol{n}_q \in \mathbb{N}^{|E|}$ such that*

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_q) \leq \frac{C_1}{q}$$

for some $C_1 > 0$. Furthermore, for every $q \in \mathbb{N}$ there exists $Q > q$, such that

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_Q) \leq \frac{C_2}{Q^{\frac{N}{N-1}}}$$

for some $C_2 > 0$.

1.4 Structure of the Thesis

Let us briefly summarize the structure of this work. §2 is a preliminary chapter devoted to collecting definitions and basic results and fixing notation – even if a number of basic results are actually, in principle, new on metric graphs, being graph versions of known results on domains. In §2.1 we introduce the notation for metric graph, combinatorial graphs and partitions. In §2.2 we introduce the function spaces, show imbedding inequalities and prove basic properties of the function spaces considered. In §2.3 we discuss the spectral theory of the operators to be considered. In §2.4 we characterize the infimum of the spectrum and essential spectrum, also known as Persson theory. In §2.5 we show some rearrangement inequalities for graphs and use them to prove Sobolev inequalities on graphs. In §2.6 we discuss the analytic dependence of eigenvalues of the operators considered with respect to the lengths.

In §3 we prove the general existence result motivated in 1.2.2 and summarized in 1.3.1 for constrained minimization problems of the form (3.1) and apply it to the stationary NLS energy functional for domains and metric graphs. In §3.2 we prove the general existence theory that we will use throughout §3. In §3.3 we prove general results for abstract NLS type functionals. The results obtained in §3.3 apply in particular for metric graphs and the stationary NLS energy functional, and we recover results obtained in the literature. For metric graphs however additional results can be shown in this case, which are discussed in §3.4.

In §4 we formally introduce and motivate spectral minimal partitions and study their basic properties, and their relations to limiting profiles of k-mixtures of Bose–Einstein condensate equations. In §4.1 we provide an overview of the topic and formally introduce the notion of spectral minimal partitions. In §4.2 we prove existence results of spectral minimal partitions as limiting profiles of solutions of k-mixtures of Bose–Einstein condensate equations. In §4.4 we show spectral estimates for $\mathcal{L}_{k,p}^N, \mathcal{L}_{k,p}^D$ as defined in (1.14). In §4.5 we show interlacing inequalities between $\mathcal{L}_{k,\infty}^N$ and $\mathcal{L}_{k,\infty}^D$ and discuss some consequences of the interlacing inequalities obtained from §4.5.4 and §4.5 in §4.5.4.

In §5 we discuss Pleijel-type (non-)theorems for metric graphs. We give the general setting, i.e. the forms of the operators considered, in §5.1. We prove an estimate on the first eigenvalue of the operators considered in §5.2.1. In §5.3 we show Pleijel type theorems for general Schrödinger operators and give a stronger Pleijel's theorem for the Laplacian with standard vertex conditions in §5.4. In §5.5 we show Pleijel's theorem for the p-Laplacian by adapting the proofs in the previous sections to the setting, this involves the discussion of Weyl's law in §5.2.2.

In §6 we consider Approximation techniques for metric graphs for computation of eigenvalues of the Laplacian via von Below's theorem. In §6.1 we fix the notation and introduce basic results. In §6.2 we give an overview of the operators considered and discuss the results summarized in 1.3.4. In §6.3 we prove estimates on the relative error given for the k-th eigenvalue of two metric graphs with same underlying combiantorial graphs. In §6.4 we discuss how given a rational metric graph one can find the eigenvalues of the Laplacian with standard vertex conditions and give a concrete function that evaluates the eigenvalues. In §6.5 we elaborate on the Simulataneous Dirichlet Approximation (SDAP) Theorem and prove an adapted version of the SDAP Theorem to approximate graphs by equilateral metric graphs. Based on the algorithm from the SDAP Theorem in §6.5 we summarize a method to approximate the spectrum given a tolerance for the relative error and give a few examples regarding efficiency of the algorithms in §6.6.

Chapter 2

Spectral Theory on Graphs for Schrödinger Operators

In this preliminary section we set the notation and discuss aspects regarding the operators involved including self-adjointness and spectral theory of the operators considered. We adopt the framework from [BK13] and [Mug19] for metric graphs and [KKLM21] and [HK21] for cuts of graphs and partitions in the following in §2.1. In §2.2 we introduce the function spaces we consider and show basic properties, such as density and can also be found in [Hof19]. In §2.3 we discuss the self-adjointness of Schrödinger operator and characterize the infimum of the spectrum and essential spectrum in §2.4 via Persson theory for the operators considered, adapted from [HS96, §14.4], for metric graphs and can also be found in [Hof19].

2.1 Metric Graphs, Combinatorial Graphs and Partitions

2.1.1 Basic assumptions

For us, a *metric graph* $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ will consist of a union $\mathcal{E} = \{[x_1, x_2], [x_3, x_4], \ldots\}$ of closed intervals in $\mathbb{R}$, turned into a metric space by gluing the intervals at the *endpoint set* $\mathcal{X} = \{x_1, x_2, x_3, \ldots\}$, via a partition $\mathcal{V} = \{v_1, v_2, \ldots\}$ on $\mathcal{X}$,

$$\mathcal{X} = \bigcup_i v_i.$$

We call each element of $\mathcal{V}$, which is formally a set of endpoints, a *vertex* of $\mathcal{G}$; we call $\mathcal{V}$ the *vertex set* of $\mathcal{G}$ and $\mathcal{E}$ the *edge set* of $\mathcal{G}$.

We turn $\mathcal{G}$ into a metric space by identifying each vertex with a point, treating each edge $e \in \mathcal{E}$ as a subset of $\mathcal{G}$, and introducing paths between pairs of points on the graph in accordance with this identification (cf. [Mug19]). The length of an edge e, i.e., the length of the interval to which it corresponds, will be denoted by $|e|$ or $\ell_e \in (0, \infty]$, and we say e is a *ray* or *lead* if

$|e| = \infty$; the *total length* of $\mathcal{G}$ will be denoted by

$$L := |\mathcal{G}| = \sum_{e \in \mathcal{E}} |e|.$$

Given a metric graph $\mathcal{G}$ we define its underlying combinatorial graph G:

Definition 2.1.1. The underlying combinatorial graph $G = (V, E)$ of a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is the graph where we identify every vertex

$$\mathsf{v} \in V$$

with an element $v \in \mathcal{V}$ and the edges $e \in \mathcal{E}$ with an edge $e \in E$ consisting of a pair of vertices

$$e = \{v, \widetilde{v}\} \in E$$

with $v, \widetilde{v} \in \mathcal{V}$ in which their correspondent endpoints are contained in $v, \widetilde{v}$ respectively.

We say $\mathcal{G}$ is connected if it is connected as a metric space. We assume that the corresponding underlying combinatorial graph is locally finite, i.e. $\deg(v) = |v| < \infty$ for all $v \in \mathcal{V}$, and that

$$\inf_{e \in \mathcal{E}} |e| > 0.$$

In particular, any precompact set intersects with at most a finite number of edges. We refer to such graphs also as *locally finite graphs* in contrast to *finite graphs*, which we call graphs that have a finite edge set. Note that under these assumptions a metric graph is compact if and only if it is finite and does not contain any rays.

We can define an equivalence relation on the class of all such metric graphs via isometrically isomorphisms, bijective mappings between graphs which preserve the metric; if two graphs are isometrically isomorphic to each other, then we are in one or both of the following situations:

(i) the edge and vertex sets of one graph are permutations (i.e. a relabelling) of the edge and vertex set of the other;

(ii) the graphs differ by the presence of dummy vertices, i.e. vertices of degree 2 that can be added at will essentially subpartitioning an interval in two intervals of total length of the original interval (see §2.1.2 for details).

We will always identify graphs that are isometrically isomorphic, and choose a convenient representative of the corresponding equivalence classes (called *ur-graphs* in [KKLM21]) in any given context, without further comment.

This way the graphs $G = (V, E)$ are undirected graphs, such that $e = \{\mathsf{v}_i, \mathsf{v}_j\}$ connects the vertices v_i and v_j. Then e is always associated to the two bonds, i.e. directed edges, that is the pairs

$$b_e = (\mathsf{v}_i, \mathsf{v}_j), \bar{b}_e = (\mathsf{v}_j, \mathsf{v}_i).$$

Given a bond

$$b_e = (\mathsf{v}_i, \mathsf{v}_j)$$

we associate $e = \{\mathsf{v}_i, \mathsf{v}_j\}$ with the interval $I_e = (0, \ell_e)$, such that $(0, b_e)$ is associated to v_i and (ℓ_e, b_e) is associated to v_j and we identify the points on the intervals on the two bonds associated to e via the relationship

$$x_{b_e} = \ell_e - x_{\bar{b}_e}.$$

Naturally, if $\ell_e = \infty$ we assume the graph to be connected back to the rest of the graph and only consider the bond b_e such that $(0, b_e)$ refers to the vertex, which we refer to as *rays* or *half-lines*, which is not a vertex at infinity, i.e. (∞, b_f) associated to such a vertex for any $f \in \mathcal{E}$; we denote the set of vertices at infinity with $\mathcal{V}_\infty$. In particular, we do not consider graphs with edges between vertices at infinity.

In other words, we can characterize a graph by associating the edges with a length vector

$$\boldsymbol{\ell} = (\ell_1, \ell_2, \ldots)$$

and we will sometimes write $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ to specify the dependence of a graph on their underlying combinatorial graph G and the edge lengths $\boldsymbol{\ell}$, which we will mostly use in §6. In particular, a metric graph is uniquely determined by associating intervals $\mathcal{I}_e = (0, \ell_e)$ for a choice of bonds b_e. Given two graph with the same underlying combinatorial graph we can then define the Hausdorff distance:

Definition 2.1.2. Given two graphs $\mathcal{G}_1(G; \boldsymbol{\ell}^{(1)}), \mathcal{G}_2(G; \boldsymbol{\ell}^{(2)})$ with underlying combinatorial graph $G = (V, E)$ we define the Hausdorff distance

$$d_G(\mathcal{G}_1, \mathcal{G}_2) := \sup_{e \in E} |\ell_e^{(1)} - \ell_e^{(2)}|. \tag{2.1}$$

We say a sequence of graphs $\mathcal{G}^{(n)} = \mathcal{G}(G, \boldsymbol{\ell}^{(n)})$ converges to $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$, and write $\mathcal{G}^{(n)} \to \mathcal{G}$, if and only if

$$\lim_{n \to \infty} d_G(\mathcal{G}^n, \mathcal{G}) = 0.$$

If we want to describe the graph locally at a vertex $v \in V \setminus \mathcal{V}_\infty$, i.e. restricted to edges incident to v, then we can choose the bonds b_e associated to the edge e, such that

$$0_{e,\mathsf{v}} := (0, b_e)$$

is associated to the vertex v. If e is incident to v, we also write $e \succ v$ and we say

$$\mathcal{D}_\mathsf{v} := v = \{x_{i_1}, \ldots, x_{i_{\deg v}}\} \tag{2.2}$$

is the incidence set of endpoints associated to a vertex $\mathsf{v} \in V$. In this manner we define

$$\widetilde{\mathcal{E}} := \bigoplus_{e\in\mathcal{E}} \mathcal{I}_e = \bigsqcup_{e\in\mathcal{E}} \bigcup_{x\in\mathcal{I}_e} (x, e)$$

endowed with the disjoint union topology. This topology is induced by the pseudo-metric

$$d_{\mathcal{E}}((x,e),(y,f)) = \begin{cases} |x-y|, & e = f \\ \infty, & \text{otherwise.} \end{cases}$$

Then a metric graph $\mathcal{G}$ as a metric structure can be characterized by

$$\mathcal{G} = \widetilde{\mathcal{E}}/\sim,$$

where

$$x \sim y \overset{\text{def}}{\iff} x = y \ \text{ or } x, y \in \mathcal{D}_v \text{ for some } \mathsf{v} \in \mathcal{V}.$$

Then $\mathcal{G}$ becomes a topological space with the quotient topology. Edges $e \in \mathcal{E}$ are then by identification given by

$$e_\sim := \bigcup_{x\in I_e} [(x,e)]_\sim \simeq I_e$$

and for each $\xi \in e_\sim$ there exists a canonical representative $x_\xi \in I_e$. Vertices $\mathsf{v} \in V$ are identified via $\mathcal{D}_\mathsf{v}$ as defined in (2.2) and we identify V with $\mathcal{V} \subset \mathcal{G}$.

We also endow $\mathcal{G}$ with the quotient pseudo-metric

$$d_{\mathcal{G}}(\xi,\theta) = \inf \sum_{i=1}^{k} d_{\mathcal{E}}(\xi_i,\theta_i) \tag{2.3}$$

where the infimum is taken over all $k \in \mathbb{N}$ and all pairs of k-tuples $(\xi_1,\dots,\xi_k)$ and $(\theta_1,\dots,\theta_k)$ with $\xi_1 = \xi$, $\theta_k = \theta$ and $\theta_i \sim \xi_{i+1}$ for $i = 1,\dots,k-1$. When $\mathcal{G}$ is connected, then $d = d_{\mathcal{G}}$ defines a metric on $\mathcal{G}$ and $(\mathcal{G}, d_{\mathcal{G}})$ becomes a metric space. Moreover, suppose $\gamma : [0,1] \to \mathcal{G}$ is a simple curve with bounded variation, i.e.

$$L(\gamma) := \sup_{\delta} \sum_{i=0}^{n_\delta-1} d_{\mathcal{G}}(\gamma(t_i),\gamma(t_{i+1})) < \infty$$

where the supremum is taken over all partitions $\delta = (t_i)_{i=0}^{n_\delta}$ with

$$0 = t_0 < t_1 < \cdots < t_{n_\delta-1} < t_{n_\delta} = 1,$$

then equivalently

$$d_{\mathcal{G}}(\xi,\theta) = \inf_{\substack{\gamma \text{ simple curve} \\ \gamma(0)=\xi,\ \gamma(1)=\theta}} L(\gamma). \tag{2.4}$$

2.1.2 Dummy vertices and isometries on graph

By definition, given a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, we have

$$|v| = \deg v$$

for all $v \in \mathcal{G}$. Suppose $\deg v = 2$, then suppose w.l.o.g. $e_1, e_2 \succ \mathsf{v}$. Suppose e_1 is connecting $\mathsf{v}^{(1)}$ and v and e_2 is connecting $\mathsf{v}^{(2)}$ and v. Consider the metric graph $\widehat{\mathcal{G}} = (\widehat{\mathcal{E}}, \widehat{\mathcal{V}}))$ given by

$$\widehat{\mathcal{E}} = \{\widehat{e}, e_3, \ldots\}, \quad \widehat{\mathcal{V}} = V \setminus \{v\}, \qquad \widehat{e} = (\mathsf{v}^{(1)}, \mathsf{v}^{(2)}),$$

such that

$$I_e = \begin{cases} [0, \ell_{e_1} + \ell_{e_2}], & e = \widehat{e} \\ [0, \ell_e], & \text{otherwise.} \end{cases}$$

Proposition 2.1.3. *The metric graphs $\mathcal{G}$ and $\widehat{\mathcal{G}}$ are isometrically isomorphic, i.e. there exists a isomorphism $\Phi : \mathcal{G} \to \widehat{\mathcal{G}}$, such that*

$$d_{\widehat{\mathcal{G}}}(\Phi(x), \Phi(y)) = d_{\mathcal{G}}(x, y)$$

for all $x, y \in \mathcal{G}$.

Proof. Suppose $[(x, e)]_\sim \in \mathcal{G}$. Then given a choice of directed bonds $(b_e)_{e \in \mathcal{E}}$, such that $b_{e_1} = (\mathsf{v}_1, \mathsf{v})$ and $b_{e_2} = (\mathsf{v}, \mathsf{v}_2)$, i.e. v is associated to $(0, b_e)$ for each $e \succ \mathsf{v}$, consider a choice of directed bonds $(\widehat{b}_e)_{e \in \widehat{E}}$, such that

$$\widehat{b}_e = b_e, \qquad \text{for all } e \in \widehat{E} \setminus \{\widehat{e}\}$$

and $\widehat{b}_{\widehat{e}} = (\mathsf{v}^{(1)}, \mathsf{v}^{(2)})$, i.e $(0, \widehat{b}_{\widehat{e}})$ is associated with $\mathsf{v}^{(1)}$ and $(\ell_{e_1} + \ell_{e_2}, \widehat{b}_{\widehat{e}})$ is associated with $\mathsf{v}^{(2)}$. Then we define the map $\Phi : \mathcal{G} \to \widehat{\mathcal{G}}$ via

$$\Phi([(x, b_e)]) = \begin{cases} [(\ell_{e_1} - x, \widehat{b}_{\widehat{e}})]_\sim, & e = e_1 \\ [(\ell_{e_1} + x, \widehat{b}_{\widehat{e}})]_\sim, & e = e_2 \\ [(x, \widehat{b}_e)]_\sim, & \text{otherwise.} \end{cases} \tag{2.5}$$

One easily checks, that the map is invertible and the inverse is given by

$$\Phi^{-1}([y, b_f]) = \begin{cases} [(x, (\mathsf{v}, \mathsf{v}^{(1)}))]_\sim, & f = \widehat{e} \text{ and } 0 \le y \le \ell_{e_1} \\ [(x - \ell_1, (\mathsf{v}, \mathsf{v}^{(2)}))]_\sim, & f = \widehat{e} \text{ and } \ell_1 \le x \le \ell_1 + \ell_2 \\ [(x, b_f)]_\sim, & \text{otherwise.} \end{cases}$$

It only is required to show that the distance is preserved under Φ. From (2.4) we have

$$d_{\widehat{\mathcal{G}}}(\Phi(x),\Phi(y)) = \inf_{\substack{\gamma \text{ simple path} \\ \gamma(0)=\Phi(x),\, \gamma(1)=\Phi(y)}} L(\gamma)$$

Suppose γ is a simple path connecting x and y, then $\Phi\circ\gamma$ is a simple path connecting x and y. Then it is sufficient to prove a local property, that is suppose $\xi,\theta\in e_\sim$ for some $e\in\mathcal{E}$, such that

$$d_{\mathcal{E}}(x_e,y_e) < \inf_{e\in E}\ell_e,$$

then

$$d_{\widehat{\mathcal{G}}}(\Phi(x),\Phi(y)) = d_{\widehat{\mathcal{E}}}(\xi_e,\theta_e) = |\Phi(x)_e - \Phi(y)_e| = |x_e - y_e| = d_{\mathcal{G}}(x,y).$$

We infer

$$\begin{aligned} L(\gamma) &= \sup_\delta \sum_{i=0}^{n_\delta -1} d_{\mathcal{G}}(\gamma(t_i),\gamma(t_{i+1})) \\ &= \sup_\delta \sum_{i=0}^{n_\delta -1} d_{\widehat{\mathcal{G}}}(\Phi\circ\gamma(t_i),\Phi\circ\gamma(t_{i+1})) = L(\Phi\circ\gamma). \end{aligned}$$

and conclude

$$d_{\widehat{\mathcal{G}}}(\Phi(x),\Phi(y)) = d_{\mathcal{G}}(x,y).$$

□

For our purposes we will not distinguish between metric graphs that are isometrically isomorphic to each other. As a consequence of Proposition 2.1.3 given any metric graph $\mathcal{G}=(\mathcal{V},\mathcal{E})$, there exists a *canonical representative* in the category of metric graphs (so called *(ur-)graphs* according to [KKLM21]), which are isometrically isomorphic to $\mathcal{G}=(\mathcal{V},\mathcal{E})$, by removing all dummy vertices, also referred to as *clean graphs* in the literature. On the other hand, suppose $x\notin\mathcal{V}$ and w.l.o.g $x\in(v_1,v_2)_\sim$. there exists a representative $\widehat{\mathcal{G}}=(\widehat{\mathcal{V}},\widehat{\mathcal{E}})$ given by

$$\widehat{\mathcal{E}} = (\mathcal{E}\setminus\{(\mathsf{v}_1,\mathsf{v}_2)\})\cup\{(\mathsf{v}_1,\mathsf{v}),(\mathsf{v},\mathsf{v}_2)\}, \quad \widehat{\mathcal{V}} \ = \mathcal{V}\cup\{\mathsf{v}\}$$

such that

$$I_e = \begin{cases} [0, d_{\mathcal{E}}(0_{\mathsf{v}_1,(\mathsf{v}_1,\mathsf{v}_2)},x)], & e=(\mathsf{v}_1,\mathsf{v}) \\ [0, d_{\mathcal{E}}(0_{\mathsf{v}_2,(\mathsf{v}_1,\mathsf{v}_2)},x)] & e=(\mathsf{v},\mathsf{v}_2) \\ I_e, & \text{otherwise.} \end{cases}$$

Given a choice of bonds $(b_e)_{e\in E}$, as constructed in (2.5) $\Phi: G\to\widehat{G}$ defines an isometrically isomorphism between G and $\widehat{G}$. By construction, $\Phi^{-1}(x)=\mathcal{D}_{\mathsf{v}}$ and we can construct for each finite set of $\widetilde{\mathcal{V}}\subset\mathcal{G}$ a representative $\widehat{G}=(\widehat{E},\widehat{V})$ among the category of metric graphs isometrically isomorphic with each other, such that

$$\widehat{\mathcal{V}} = \mathcal{V} \cup \widetilde{\mathcal{V}}.$$

Important quantities that are invariant with respect to isometric isomorphisms are the first Betti number β, i.e. the number of independent cycles of a graph, and the number of

2.1.3 Cuts of Graphs

The notion of *cutting a graph* will be used extensively. While it is by no means new – among other things it has appeared frequently in the context of spectral geometry of graphs as a prototypical "surgery principle" (see, for example, [BKKM19] and the references therein) and was also used in [KKLM21] as the basis for defining partitions of graphs – we will need to study this notion far more carefully than in those works, and introduce a number of new concepts around it. We thus start with the basic definition.

Definition 2.1.4. Let $\mathcal{G}$ and $\mathcal{G}'$ be metric graphs. Then $\mathcal{G}'$ is a *cut* (or *cut graph*) of $\mathcal{G}$ if

(i) $\mathcal{G}$ and $\mathcal{G}'$ have a common edge set, and

(ii) for all $v' \in \mathcal{V}'$ there exists $v \in \mathcal{V}$ such that $v' \subset v$.

In this context we define cut vertices and their corresponding cut set.

Definition 2.1.5. Suppose $\mathcal{G}'$ is a cut graph of $\mathcal{G}$. We say $v \in \mathcal{V}$ is a *cut vertex* if there exists $v' \in \mathcal{V}'$ such that $v' \subsetneq v$, and denote the set of cut vertices, the *cut set*, by $\mathcal{C}(\mathcal{G}' : \mathcal{G})$, which we treat as a subset of $\mathcal{G}$. If $\mathcal{C}(\mathcal{G}' : \mathcal{G}) = \{v\}$, then we say $\mathcal{G}$ has been cut at v. For $v \in \mathcal{C}(\mathcal{G}' : \mathcal{G})$ we define

$$\mathcal{C}_v(\mathcal{G}') = \{v' \in \mathcal{V} | v' \subset v\} \subset \mathcal{G}',$$

which we refer to as the cut set at v.

In practice this definition allows for cutting through the interior of edges of $\mathcal{G}$, as in accordance with our observation in §2.1.2 we may always insert dummy vertices at the cut locations before making the cut. The process of "undoing" a cut, i.e., reverting to $\mathcal{G}$ from $\mathcal{G}'$, will as usual be called gluing. In particular, we say $\mathcal{G}$ has been obtained from $\mathcal{G}'$ by gluing the vertices $v_1, \ldots, v_n \in \mathcal{V}(\mathcal{G}')$ if $\mathcal{G}'$ is a cut of $\mathcal{G}$ such that $\mathcal{C}(\mathcal{G}' : \mathcal{G}) = \{v\}$, where $v = v_1 \cup \ldots \cup v_n$.

The next notion will be central for all our interlacing results in the proofs of our results in §1.3.2; in what follows we will adapt from [HK21, §2].

Definition 2.1.6. Let $\mathcal{G}$, $\mathcal{G}'$ be compact metric graphs. Suppose $\mathcal{G}'$ is a cut of $\mathcal{G}$, such that the graphs have vertex sets $\mathcal{V}'$ and $\mathcal{V}$, respectively, then we say

(i) $\mathcal{G}'$ is a cut of $\mathcal{G}$ of rank

$$\operatorname{rank}(\mathcal{G}' : \mathcal{G}) := |\mathcal{V}'| - |\mathcal{V}|.$$

(ii) $\mathcal{G}'$ is a simple cut if

$$\operatorname{rank}(\mathcal{G}' : \mathcal{G}) = 1,$$

i.e. there exists a unique $v \in \mathcal{V}$ and $v_1', v_2' \in \mathcal{V}'$ such that $v = v_1' \cup v_2'$ (see also [KKLM21, Definition 2.7(1) with $k = 1$]).

The rank, thus defined, is invariant under relabeling of the edges and insertion or removal of dummy vertices in $\mathcal{G}$ (which by definition of a cut must then also be inserted or removed simultaneously in $\mathcal{G}'$), and is hence invariant under isometrically isomorphisms of the graph.

Lemma 2.1.7. *Let $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3$ be compact metric graphs with common edge set. Suppose $\mathcal{G}_1$ is a cut of $\mathcal{G}_2$ and $\mathcal{G}_2$ is a cut of $\mathcal{G}_3$, then*

(1) $\mathcal{G}_1$ is a cut of $\mathcal{G}_3$ and

$$\operatorname{rank}(\mathcal{G}_1 : \mathcal{G}_3) = \operatorname{rank}(\mathcal{G}_1 : \mathcal{G}_2) + \operatorname{rank}(\mathcal{G}_2 : \mathcal{G}_3);$$

(2) if $\operatorname{rank}(\mathcal{G}_1 : \mathcal{G}_3) = \operatorname{rank}(\mathcal{G}_2 : \mathcal{G}_3)$, then $\mathcal{G}_1 = \mathcal{G}_2$.

Proof. Suppose $\mathcal{G}_1, \mathcal{G}_2, \mathcal{G}_3$ have a common edge set, and vertex sets $\mathcal{V}_1, \mathcal{V}_2, \mathcal{V}_3$ respectively, then (1) follows immediately from the definitions of cut and rank. Now suppose that $\operatorname{rank}(\mathcal{G}_1 : \mathcal{G}_3) = \operatorname{rank}(\mathcal{G}_2 : \mathcal{G}_3)$, then $\operatorname{rank}(\mathcal{G}_1 : \mathcal{G}_2) = 0$ and so $k := |\mathcal{V}_1| = |\mathcal{V}_2|$. Let

$$\mathcal{V}_1 = \{v_1^{(1)}, \dots, v_k^{(1)}\}, \qquad \mathcal{V}_2 = \{v_1^{(2)}, \dots, v_k^{(2)}\}.$$

Since $\mathcal{G}_1$ is a cut of $\mathcal{G}_2$ we may assume, possibly after a relabeling, that $v_i^{(1)} \subset v_i^{(2)}$ for all $i = 1, \dots, k$. But since there is a bijection between the two vertex sets there must be equality, $v_i^{(1)} = v_i^{(2)}$ for all $i = 1, \dots, k$. □

A graph $\mathcal{G}_1$ being a cut of $\mathcal{G}_2$ defines a partial ordering on the set of metric graphs. Given a compact metric graph $\mathcal{G}$ (with a *fixed* vertex set, i.e., where we do not permit the insertion or removal of dummy vertices), the set of its cut graphs becomes a partially ordered family, and by Lemma 2.1.7 the rank is additive on this family.

Lemma 2.1.8. *Let $\mathcal{G}, \mathcal{G}'$ be compact metric graphs. Then $\mathcal{G}'$ is a cut of $\mathcal{G}$ of rank $k \in \mathbb{N}$ if and only if there exists a sequence of cuts of $\mathcal{G}$*

$$\mathcal{G} = \mathcal{G}^{(0)}\ ,\ \mathcal{G}^{(1)}\ ,\ \cdots\ ,\ \mathcal{G}^{(k-1)}\ ,\ \mathcal{G}^{(k)} = \mathcal{G}'$$

such that $\mathcal{G}^{(i+1)}$ is a simple cut of $\mathcal{G}^{(i)}$ for all $i = 0, \dots, k-1$.

Proof. Suppose $\mathcal{G}'$ is a cut of $\mathcal{G}$ of rank $k \in \mathbb{N}$, where the graphs have common edge set $\mathcal{E}$ and vertex sets $\mathcal{V}'$, $\mathcal{V}$, respectively. For the “only if” statement we give a constructive proof. Let

$v \in \mathcal{C}(\mathcal{G}' : \mathcal{G})$ and $v' \in \mathcal{V}'$ such that $v' \subsetneq v$, then we define

$$\mathcal{V}^{(1)} = \mathcal{V} \setminus \{v\} \cup \{v', v \setminus v'\}.$$

Then by construction $\mathcal{G}^{(1)} = (\mathcal{V}^{(1)}, \mathcal{E})$ is a simple cut of $\mathcal{G}$ and $|\mathcal{V}^{(1)}| = |\mathcal{V}| + 1$ and $\mathcal{G}^{(1)}$ is a simple cut of $\mathcal{G}$. One easily sees that $\mathcal{G}'$ is a cut of $\mathcal{G}^{(1)}$ and by Lemma 2.1.7 (1) we have

$$\operatorname{rank}(\mathcal{G}' : \mathcal{G}^{(1)}) = k - 1.$$

We sucessively construct metric graphs $\mathcal{G}^{(1)}, \dots, \mathcal{G}^{(k)}$ such that $\mathcal{G}^{(i+1)}$ is a simple cut of $\mathcal{G}^{(i)}$ and $\operatorname{rank}(\mathcal{G}^{(i)} : \mathcal{G}) = i$ for all $i = 1, \dots, k$. Then $\operatorname{rank}(\mathcal{G}' : \mathcal{G}) = \operatorname{rank}(\mathcal{G}^{(k)} : \mathcal{G})$ and so by Lemma 2.1.7 (2) we conclude that $\mathcal{G}^{(k)} = \mathcal{G}'$. The other direction is a direct consequence of the additivity of the rank in the sense of Lemma 2.1.7 (1). $\square$

Definition 2.1.9. Let $\mathcal{G}$ be a metric graph and $\mathcal{V}_0 \subset \mathcal{V}$ a distinguished vertex set. Then we call the graph $\mathcal{G}_1$ with common edge set and vertex set

$$\mathcal{V}_1 := \big(\mathcal{V} \setminus \mathcal{V}_0\big) \cup \bigcup_{v \in \mathcal{V}_0} \bigcup_{x \in v} \{x\}$$

the *total cut (graph)* of $\mathcal{G}$ at $\mathcal{V}_0$.

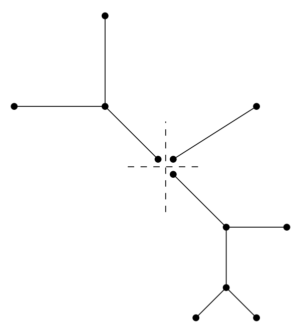


Figure 2.1: An example of a total cut of a graph at one vertex.

Example 2.1.10. Let $\mathcal{G}$ be the metric graph depicted in Figure 2.1. Then the total cut at the indicated vertex disconnects the graph into 3 components, and the corresponding cut is of rank 2.

We finish with the following notion, which also goes to the structure of the partial ordering of the set of all cuts of a fixed graph $\mathcal{G}$.

Definition 2.1.11. Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a metric graph. Suppose $\mathcal{G}_1, \mathcal{G}_2$ are cuts of $\mathcal{G}$ with vertex sets $\mathcal{V}_1$ and $\mathcal{V}_2$, respectively. We define the *common cut (graph)* $\mathcal{G}_3 = (\mathcal{V}_3, \mathcal{E})$ of $\mathcal{G}_1, \mathcal{G}_2$ via

$$\mathcal{V}_3 = \{v_1 \cap v_2 \subset \mathcal{X} : v_1 \in \mathcal{V}_1, v_2 \in \mathcal{V}_2 \text{ such that } v_1 \cap v_2 \neq \emptyset\}.$$

Equivalently, the common cut of two cut graphs $\mathcal{G}_1, \mathcal{G}_2$ of $\mathcal{G}$ is the cut $\mathcal{G}'$ of $\mathcal{G}$ of minimal rank such that $\mathcal{G}'$ is a cut graph of $\mathcal{G}_1$ and $\mathcal{G}_2$.

2.1.4 Partitions

We can now introduce partitions that are the central object of study in context of spectral minimal partitions in §4, and also are relevant in the context of nodal clustering in §5. The next definition follows [KKLM21, §2].

Definition 2.1.12. Let $k \geq 1$ and let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a metric graph. Then:

(i) $\mathcal{P} := (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ is a *connected k-partition* of $\mathcal{G}$, or *k-partition* for short, if there exists a cut $\mathcal{G}'$ such that $\mathcal{G}_1, \ldots, \mathcal{G}_k$ are connected components of $\mathcal{G}'$. We refer to the components $\mathcal{G}_1, \ldots, \mathcal{G}_k$ as *clusters* or *partition elements*;

(ii) $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ is an *exhaustive connected k-partition* if $\mathcal{G}' = \sqcup_{i=1}^k \mathcal{G}_i$ is a cut graph of $\mathcal{G}$ and $\mathcal{G}_1, \ldots, \mathcal{G}_k$ are its connected components.

Since we will only be interested in connected partitions, that is, partitions whose clusters are themselves connected metric graphs, we will drop the adjective "connected" and simply refer to connected partitions as partitions. In principle there could be multiple cuts of $\mathcal{G}$ which generate $\mathcal{P}$ if the latter is not exhaustive, cf. Figure 2.2. However, there will always be a cut of minimal rank which gives rise to $\mathcal{P}$; we will call this cut graph the *canonical cut graph*.

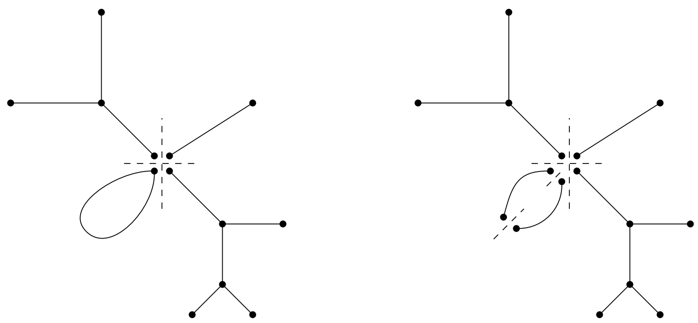


Figure 2.2: On canonical cut graphs. The clusters in Figure 2.1 are connected components of the two cut graphs presented. The cut graph on the left is the canonical cut graph associated with the partition, as any other cut giving rise to these three clusters would have higher rank (that is, it would involve cutting the original graph more), as is the case for the cut on the right. In fact, it is easy to see that the right cut graph is itself a cut of the left cut graph.

Definition 2.1.13. Let $k \geq 1$, $\mathcal{G}$ be a metric graph and $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ be a k-partition of $\mathcal{G} = (\mathcal{V}, \mathcal{E})$. Suppose $\mathcal{G}_1 = (\mathcal{V}_1, \mathcal{E}_1), \ldots, \mathcal{G}_k = (\mathcal{V}_k, \mathcal{E}_k)$ with disjoint subsets $\mathcal{E}_1, \ldots, \mathcal{E}_k$ and $\mathcal{V}_1, \ldots, \mathcal{V}_k$ of $\mathcal{E}$ and $\mathcal{V}$ respectively. Then we define the *canonical cut (graph) $\mathcal{G}_\mathcal{P}$* of $\mathcal{G}$ associated with the partition $\mathcal{P}$ as the unique cut graph of $\mathcal{G}$ of minimal rank such that $\mathcal{G}_1, \ldots, \mathcal{G}_k$ are connected components of the cut graph. We will refer to the quantity $\operatorname{rank}(\mathcal{G}_\mathcal{P} : \mathcal{G})$ as the *rank of the partition $\mathcal{P}$*.

Remark 2.1.14. Let $\mathcal{G}$ be a metric graph and let $\mathcal{P}$ be a k-partition, $k \geq 1$. Then, keeping the notation of Definition 2.1.13, the canonical cut graph $\mathcal{G}_{\mathcal{P}}$ can be constructed as the unique cut graph with the following properties:

(i) for any cut vertex $v \in \mathcal{C}(\mathcal{G}_{\mathcal{P}} : \mathcal{G})$ there exists at least one cluster $\mathcal{G}_i = (\mathcal{V}_i, \mathcal{E}_i)$ and $v_i \in \mathcal{V}_i$ such that $v_i \subset v$;

(ii) if a cut vertex $v \in \mathcal{C}(\mathcal{G}_{\mathcal{P}} : \mathcal{G})$ is not divided among vertices of the $\mathcal{G}_i$, that is, if $w := v \setminus \bigcup_{\widetilde{v} \in \bigcup_{i=1}^k \mathcal{V}_i}$ is non-empty, then there is exactly one connected component of $\mathcal{G}_{\mathcal{P}}$ such that w is a vertex of that connected component.

Hence the canonical cut graph $\mathcal{G}_{\mathcal{P}}$ may be described formally as the metric graph with the same edge set as $\mathcal{G}$ and vertex set

$$\mathcal{V}_{\mathcal{P}} = \bigcup_{i=1}^k \mathcal{V}_i \cup \left\{ v \setminus \bigcup_{\widetilde{v} \in \bigcup_{i=1}^k \mathcal{V}_i} \widetilde{v} : v \in \mathcal{V} \setminus \bigcup_{i=1}^k \mathcal{V}_i \right\}.$$

We have the following concrete bounds on the rank of a partition:

Lemma 2.1.15. *Let $\mathcal{G}$ be a metric graph with first Betti number $\beta \geq 0$. Suppose $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ is an exhaustive k-partition of $\mathcal{G}$, $k \geq 1$. Then*

$$k - 1 \leq \operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) \leq k - 1 + \beta. \tag{2.6}$$

Proof. Assume without loss of generality that $\mathcal{G}_1 = (\mathcal{V}_1, \mathcal{E}_1)$ and $\mathcal{G}_2 = (\mathcal{V}_2, \mathcal{E}_2)$ are neighboring clusters. Suppose there exists $v_1 \in \mathcal{V}_1$, $v_2 \in \mathcal{V}_2$ and $v \in \mathcal{V}$ such that $v_1, v_2 \subset v$. We glue $\mathcal{G}_1$ and $\mathcal{G}_2$ at v, i.e. we obtain a graph $\mathcal{G}^{(1)}$ with edge set $\mathcal{E}^{(1)} = \mathcal{E}_1 \cup \mathcal{E}_2$ and vertex set $\mathcal{V}^{(1)} = \mathcal{V}_1 \cup \mathcal{V}_2 \cup \{v_1 \cup v_2\} \setminus \{v_1, v_2\}$. By construction $\mathcal{P}^{(1)} = \{\mathcal{G}^{(1)}, \mathcal{G}_3, \ldots, \mathcal{G}_k\}$ defines a $k-1$-partition and $\mathcal{G}_{\mathcal{P}}$ is a simple cut of $\mathcal{G}_{\mathcal{P}^{(1)}}$. Applying this procedure iteratively and invoking Lemma 2.1.8, we end up with an exhaustive 1-partition $\mathcal{G}^{(k-1)}$ such that $\mathcal{G}_{\mathcal{P}}$ is a cut of $\mathcal{G}^{(k-1)}$, $\mathcal{G}^{(k-1)}$ is a cut of $\mathcal{G}$, and $\operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}^{(k-1)}) = k - 1$. Lemma 2.1.7 now yields the lower bound in (2.6).

On the other hand, since $\mathcal{G}$ admits β independent cycles any cut of rank $\beta+1$ would necessarily disconnect $\mathcal{G}$; since $\mathcal{G}^{(k-1)}$ is a connected cut graph of $\mathcal{G}$ we thus have $\operatorname{rank}(\mathcal{G}^{(k-1)} : \mathcal{G}) \leq \beta$. Lemma 2.1.7 now yields the upper bound in (2.6). $\square$

Definition 2.1.16. Let $\mathcal{G}$ be a metric graph and let $\mathcal{P} = \{\mathcal{G}_1, \ldots, \mathcal{G}_k\}$ be a (non-exhaustive) k-partition of $\mathcal{G}$, $k \geq 1$, with edge sets $\mathcal{E}_1, \ldots, \mathcal{E}_k \subset \mathcal{E}$. We say that $\mathcal{P}' = \{\mathcal{G}_1', \ldots, \mathcal{G}_k'\}$ is an *exhaustive extension* of $\mathcal{P}$ if

(i) $\mathcal{G}_{\mathcal{P}}$ is a cut of $\mathcal{G}_{\mathcal{P}'}$

(ii) $\mathcal{E}_i \subset \mathcal{E}_i'$ for all $i = 1, \ldots, k$

(iii) $\bigcup_{i=1}^k \mathcal{E}_i' = \mathcal{E}$.

We next introduce the following notation for the boundary points of a partitions.

Definition 2.1.17. Let $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ be a (not necessarily exhaustive) k-partition of $\mathcal{G}$, $k \geq 1$, and let $\mathcal{G}_\mathcal{P}$ the canonical cut graph of $\mathcal{G}$ associated with $\mathcal{P}$.

(i) We say $\mathcal{G}_i = (\mathcal{V}_i, \mathcal{E}_i)$ and $\mathcal{G}_j = (\mathcal{V}_j, \mathcal{E}_j)$, $i \neq j$, are *neighboring clusters*, or just *neighbors*, if there exist $v_i \in \mathcal{V}_i$, $v_j \in \mathcal{V}_j$ and $v \in \mathcal{V}$ such that $v_i, v_j \subset v$. We call any such $v \in \mathcal{V}$ a *boundary vertex* (or *boundary point*) of $\mathcal{P}$, and define the *boundary set of* $\mathcal{P}$ to be the set of all such boundary points:

$$\partial\mathcal{P} := \{v \in \mathcal{V} : \exists v_i \in \mathcal{V}_i, v_j \in \mathcal{V}_j, i \neq j : v_i, v_j \subset v\}.$$

(ii) We define the *boundary set of the cluster* $\mathcal{G}_i = (\mathcal{V}_i, \mathcal{E}_i)$ by

$$\partial\mathcal{G}_i = \{v \in \mathcal{V}_i : \exists v' \in \mathcal{C}(\mathcal{G}_\mathcal{P} : \mathcal{G}) : v \subsetneq v'\}.$$

We consider besides connected partitions also rigid partition. We take the definition of *rigid partitions* from [KKLM21], where cuts can only be made at the boundary between neighbors; these can be characterized conveniently using the notion of canonical cut graphs.

Definition 2.1.18. We say a k-partiton $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ of $\mathcal{G}$ is *rigid* if its boundary set $\partial\mathcal{P}$ coincides with the cut set $\mathcal{C}(\mathcal{G}_\mathcal{P} : \mathcal{G})$.

Remark 2.1.19. We denote the class of all (connected) exhaustive k-partitions of $\mathcal{G}$ by $\mathfrak{C}_k(\mathcal{G})$ and the class of all rigid exhaustive k-partitions of $\mathcal{G}$ by $\mathfrak{R}_k(\mathcal{G})$. The set of connected partitions $\mathfrak{C} = \mathfrak{C}(\mathcal{G})$ and rigid partitions $\mathfrak{R} = \mathfrak{R}(\mathcal{G})$ we define then as as the disjoint union of the the sets of k-partitions

$$\mathfrak{C}(\mathcal{G}) = \bigcup_{k\geq 1} \mathfrak{C}_k(\mathcal{G}), \qquad \mathfrak{R}(\mathcal{G}) = \bigcup_{k\geq 1} \mathfrak{R}_k(\mathcal{G}).$$

Given a partition $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ by our definition each cluster is a metric graph themselves. However, often it will be useful to consider the subset of $\mathcal{G}$ which corresponds to the clusters; to this end we define:

Definition 2.1.20. Let $\mathcal{G}$ be a metric graph, $k \geq 1$ and let $\mathcal{P} = \{\mathcal{G}_1, \ldots, \mathcal{G}_k\}$ be a k-partition of $\mathcal{G}$ and let $\mathcal{G}_\mathcal{P}$ be the canonical cut graph such that $\mathcal{G}$ and $\mathcal{G}_\mathcal{P}$ have common edge set $\mathcal{E}$, then for each $i = 1, \ldots, k$ we denote by Ω_i the unique closed subset of $\mathcal{G}$ such that

$$\{e \in \mathcal{E} : e \subset \mathcal{G}_i\} = \{e \in \mathcal{E} : e \subset \Omega_i\}$$

and call the set Ω_i the *cluster support* (associated with the cluster $\mathcal{G}_i$), or just *support* for short.

In particular given a partition $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ with $\mathcal{D} = (\Omega_1, \dots, \Omega_k)$ is a partition on $\mathcal{G}$, such that

$$|\Omega_i \cap \Omega_j| = 0$$

for $i \neq j$. The best partition type to reflect its cluster support as closely as possible is a partition of a graph in closed subgraphs, so called *faithful* partitions, since they inherit all possible connections from the original graph:

Definition 2.1.21. We say a k-partition $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ is faithful if for all $v \in \mathcal{C}(\mathcal{G}_\mathcal{P} : \mathcal{G})$ the cut set of $C_v(\mathcal{G}_\mathcal{P})$ of v contains at most one element in any cluster support of $\mathcal{P}$.

In this context, we refer to Figure 1.2, 1.4 and 1.3 for a comparison of the different types of partitions for a graph with identical cluster supports.

2.2 Function spaces

2.2.1 Preliminaries: L^p spaces and first order Sobolev spaces

Given a metric graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ and $p \in [1, \infty)$, we define the function spaces

$$L^p(\mathcal{G}) := \left\{ u \in \bigoplus_{e \in \mathcal{E}} L^p(I_e) | \|u\|_p^p := \sum_{e \in \mathcal{E}} \|u_e\|_p^p < \infty \right\}$$
$$W^{1,p}(\mathcal{G}) := \left\{ u \in \bigoplus_{e \in \mathcal{E}} W^{1,p}(I_e) \cap C(\mathcal{G}) | \|u\|_{W^{1,p}}^p := \sum_{e \in \mathcal{E}} \|u_e\|_{W^{1,p}}^p < \infty \right\}.$$

and we also write $H^1(\mathcal{G}) = W^{1,2}(\mathcal{G}$. For $p = \infty$ we define

$$L^\infty(\mathcal{G}) = \left\{ u \in \bigoplus_{e \in \mathcal{E}} L^\infty(I_e) | \|u\|_\infty := \sup_{e \in \mathcal{E}} \|u_e\|_\infty < \infty \right\}$$
$$W^{1,\infty}(\mathcal{G}) = \left\{ u \in \bigoplus_{e \in \mathcal{E}} W^{1,\infty}(I_e) \cap C(\mathcal{G}) | \|u\|_{W^{1,\infty}} := \sup_{e \in \mathcal{E}} \|u_e\|_{W^{1,\infty}} < \infty \right\}$$

Since the isomorphism in §2.1.2 under removal and addition of dummy vertices preserves the measure, we have for all $p \in [1, \infty]$

$$\begin{aligned} L^p([0, \ell_1 + \ell_2]) &\simeq L^p([0, \ell_1]) \oplus L^p([\ell_1, \ell_1 + \ell_2]) \\ W^{1,p}([0, \ell_1 + \ell_2]) &\simeq W^{1,p}([0, \ell_1]) \oplus W^{1,p}([\ell_1, \ell_1 + \ell_2]) \cap C([0, \ell_1 + \ell_2]) \\ &:= \left\{ u \in C([0, \ell_1 + \ell_2]) \mid u\big|_{[0,\ell_1]} \in W^{1,p}([0, \ell_1]) \right. \\ &\qquad \left. \wedge\ u\big|_{[\ell_1, \ell_1 + \ell_2]} \in W^{1,p}([\ell_1, \ell_1 + \ell_2]])| \right\}. \end{aligned}$$

Indeed, the spaces $L^2(\mathcal{G})$ and $H^1(\mathcal{G})$ are isometrically isomorphic under addition or removal of dummy vertices and hence, do not dependant on the represantative of the metric graph. In particular we can define the imbeddings

$$i : \begin{array}{c} C(\mathcal{G}_2) \hookrightarrow C(\mathcal{G}_1) \\ [[x]_{\sim_2} \mapsto u([x]_{\sim_2})] \mapsto [[x]_{\sim_1} \mapsto u([x]_{\sim_2})] \end{array}$$

In a similar fashion we can also define imbeddings $L^p(\mathcal{G}_1) \hookrightarrow L^p(\mathcal{G}_2)$ and $W^{1,p}(\mathcal{G}_1) \hookrightarrow W^{1,p}(\mathcal{G}_2)$.

Proposition 2.2.1. *Let $\mathcal{G}_1$ be a cut of $\mathcal{G}_2$ of rank n and $p \in [1, \infty]$. Then*

$$\dim C(\mathcal{G}_1)/C(\mathcal{G}_2) = n$$
$$\dim W^{1,p}(\mathcal{G}_1)/W^{1,p}(\mathcal{G}_2) = n.$$

Proof. There exist representatives of $\mathcal{G}_1$ and $\mathcal{G}_2$, such that

$$\mathcal{G}_1 = \mathcal{E}/\sim_1, \qquad \mathcal{G}_2 = \mathcal{E}/\sim_2 .$$

Suppose $\mathsf{v} \in \mathcal{C}(\mathcal{G}_1 : \mathcal{G}_2)$, then for each $\mathsf{v}' \in \mathcal{C}_{\mathsf{v}}(\mathcal{G}_1)$ we can construct a function $u_{v'} \in H^1(\mathcal{G}_1)$ such that

$$u_{v'}(v) = \delta_{\mathsf{v},\mathsf{v}'},$$

for all $v \in \mathcal{V}_1$, where $\delta_{\mathsf{v},\mathsf{v}'}$ is the Kronecker delta. Then

$$\dim C(\mathcal{G}_1)/C(\mathcal{G}_2) = n, \qquad \dim W^{1,p}(\mathcal{G}_1)/W^{1,p}(\mathcal{G}_2) = n$$

since for each $u \in C(\mathcal{G}_2)$ and each $\mathsf{v} \in \mathcal{V}$ we can choose a linear combination of

$$|\mathcal{D}_{\mathsf{v}}| - 1$$

functions $u_{v'}$, such that

$$u - \sum \lambda_{\mathsf{v}'} u_{\mathsf{v}'}$$

coincides for all $\mathcal{D}_{\mathsf{v}} \subset \mathcal{G}_1$. Indeed, suppose $u(\mathsf{v}) = u_1$, then for each $u \in \mathcal{C}(\mathcal{G}_1)$ or $u \in W^{1,p}(\mathcal{G}_1)$ there exists a linear combination of $|\mathcal{D}_{\mathsf{v}}| - 1$ linearly independent functions $u_{v'}$ in $C(\mathcal{G}_1)/C(\mathcal{G}_2)$ and $W^{1,p}(\mathcal{G}_1)/W^{1,p}(\mathcal{G}_2)$ respectively such that

$$u - \sum \lambda_{\mathsf{v}'} u_{\mathsf{v}'}$$

coincide for all $\mathcal{D}_{\mathsf{v}} \subset \mathcal{G}_1$. Then by iteration we can construct such functions for each cut vertex and we conclude

$$\dim C(\mathcal{G}_1)/C(\mathcal{G}_2) = \dim W^{1,p}(\mathcal{G}_1)/W^{1,p}(\mathcal{G}_2) = \sum_{\mathsf{v}\in\mathcal{C}(\mathcal{G}_1:\mathcal{G}_2)} |\mathcal{D}_{\mathsf{v}}| - 1 = |\mathcal{V}_1| - |\mathcal{V}_2| = n.$$

□

For our purposes we also consider Dirichlet vertices. Given a set $\mathcal{V}^D$, referred to as Dirichlet set, we define

$$W_0^{1,p}(\mathcal{G},\mathcal{V}^D) = \{u \in W^{1,p}(\mathcal{G}) |\, u(x) = 0 \text{ for all } x \in \mathcal{V}^D\},$$
$$H_0^1(\mathcal{G},\mathcal{V}^D) = \{u \in H^1(\mathcal{G}) |\, u(x) = 0 \text{ for all } x \in \mathcal{V}^D\}.$$

For a function $u \in C(\mathcal{G})$ we define the support

$$\operatorname{supp} u = \overline{\{x \in \mathcal{G} | u(x) = 0\}}.$$

Then we define

$$W_c^{1,p}(\mathcal{G}) = \{u \in W^{1,p}(\mathcal{G}) |\, \operatorname{supp} u \text{ is compact}\},$$
$$H_c^1(\mathcal{G}) = \{u \in H^1(\mathcal{G}) |\, \operatorname{supp} u \text{ is compact}\}.$$

We introduce canonical spaces of first order Sobolev functions, since they become relevant in §4 and §6, given a combinatorial graph $G = (\mathcal{E},\mathcal{V})$ with Dirichlet vertex set $V^D \subset V$ which corresponds to the equilateral metric graph $\mathcal{G} = \mathcal{G}(G,\mathbf{1})$ with Dirichlet vertex set $\mathcal{V}^D \subset \mathcal{V}$ corresponding to $V^D \subset V$ and we write

$$W^{1,p}(G) = W^{1,p}(\mathcal{G}), \qquad H^1(G) = H^1(\mathcal{G}),$$
$$W_0^{1,p}(G,V^D) = W_0^{1,p}(\mathcal{G},\mathcal{V}^D), \qquad H_0^1(G,V^D) = W_0^{1,p}(\mathcal{G},\mathcal{V}^D).$$

2.2.2 Higher-order Sobolev spaces

In this section we introduce the notion of higher-order Sobolev spaces on graphs for $p \in [1,\infty]$. Let $\mathcal{G}$ be a locally finite metric graph. One naive way of doing so is simply defining it analogously as in $W^{1,p}(\mathcal{G})$

$$\widetilde{W^{k,p}}(\mathcal{G}) := \left\{ u \in \bigoplus_{e\in E} W^{k,p}(I_e) \cap C(\mathcal{G}) \middle| \|u\|^p_{W^{k,p}} := \sup_{\mathcal{E}'\subset\mathcal{E} \text{ is a finite subset}} \sum_{e\in\mathcal{E}'} \|u_e\|^p_{W^{k,p}(I_e)} < \infty \right\}$$

Then for $u \in \widetilde{W^{k,p}}(\mathcal{G})$ we always have $u_e \in C^{k-1}(I_e)$ for all $e \in \mathcal{E}$. However, we also want to specify a condition on the higher-order derivatives at the vertices. We define

$$\begin{aligned} W^{k,p}(\mathcal{G}) = \{u \in \widetilde{W^{k,p}}(\mathcal{G}) | u^{(j)} \in C(\mathcal{G}) \quad \forall j \leq k-1 \text{ even} \\ \wedge \quad \sum_{e: e \succ \mathsf{v}} \frac{\partial^j}{\partial \nu^j} u_e(\mathsf{v}) = 0 \quad \forall j \leq k-1 \text{ odd } \forall \mathsf{v} \in V\}, \end{aligned}$$

where $e : e \succ \mathsf{v}$ denotes the set of edges e adjacent to a vertex v.

In the thesis we will refer to the conditions at the odd derivatives as *Kirchhoff–Neumann*, or just *Kirchhoff* or *Neumann*, conditions. Otherwise the derivatives satisfy continuity conditions. In the context of operators we will also say that the operators with domains $W^{k,p}(\mathcal{G})$ satisfy *standard* conditions.

This definition is natural in the sense that if we consider a dummy vertex $\hat{v}$ of degree 2, i.e. subdividing an edge $e \in \mathcal{E}$ connecting two vertices v_1, v_2 into two edges e_1, e_2 connecting $v_1, \hat{v}$ and $\hat{v}, v_2$ respectively such that the total length of the graph is preserved, then the Kirchhoff condition simply reduces to a continuity statement of the derivatives. As usual we define $\widetilde{H^k}(\mathcal{G}) = \widetilde{W^{k,2}}(\mathcal{G})$ and $H^k(\mathcal{G}) = W^{k,2}(\mathcal{G})$. Thus, in particular, the spaces defined are isometrically isomorphic under isometric isomorphisms of the graph, such as the insertion or deletion of dummy vertices.

Remark 2.2.2. While the Sobolev spaces as defined here are domains of self-adjoint realizations of differential operators on $L^2(\mathcal{G})$, the definitions are not necessarily canonical. We refer to [GM17] for a discussion on self-adjoint extension of the Bilaplacian, and a discussion for $W^{2,p}$ spaces on graphs.

In this context, we are going to define some useful related spaces:

$$\begin{aligned} \widetilde{W_0^{k,p}}(\mathcal{G}) &:= \{u \in \widetilde{W^{k,p}}(\mathcal{G}) | u^{(l)}(\mathsf{v}) = 0, \quad \forall 1 \leq l \leq k-1, \quad \forall \mathsf{v} \in \mathcal{V}\} \\ \widetilde{W_c^{k,p}}(\mathcal{G}) &:= \left\{ u \in \widetilde{W_0^{k,p}}(\mathcal{G}) | \operatorname{supp}(u) \text{ compact} \right\}. \end{aligned}$$

Of special importantance will be the following test function spaces:

$$\widetilde{C^\infty(\mathcal{G})} := \bigcap_{k \in \mathbb{N}} \widetilde{W^{k,\infty}}(\mathcal{G}), \quad \widetilde{C_b^\infty(\mathcal{G})} := \bigcap_{k \in \mathbb{N}} \widetilde{W_0^{k,\infty}}(\mathcal{G}), \quad \widetilde{C_c^\infty(\mathcal{G})} := \bigcap_{k \in \mathbb{N}} \widetilde{W_c^{k,\infty}}(\mathcal{G}). \tag{2.7}$$

Consider the norm on $W^{k,p}$ defined as

$$|u|_{W^{k,p}} := \left(\int_{\mathcal{G}} |u^{(k)}|^2 + |u|^2 \, \mathrm{d}x \right)^{1/p}$$

and for $p = 2$ we define as usual $|\cdot|_{H^k} := |\cdot|_{W^{k,2}}$. Then due to the Gagliardo-Nirenberg interpolation inequality on intervals (see e.g. [Leo17, Theorem 7.41]) applied edgewise we have:

Proposition 2.2.3. *Let $\mathcal{G}$ be a locally finite graph, then the norms $\|\cdot\|_{W^{k,p}}$ are equivalent, i.e. for $u \in W^{k,p}(\mathcal{G})$ we have*

$$|u|^2_{W^{k,p}} \le \|u\|^2_{W^{k,p}} \le C|u|^2_{W^{k,p}}$$

for some $C > 0$.

2.2.3 On the density of Sobolev spaces

Proposition 2.2.4. *Let $\mathcal{G}$ be a finite, connected metric graph and $p \in [1,\infty)$, then $W^{m,p}(\mathcal{G})$ is dense in $W^{n,p}(\mathcal{G})$ for $m \ge n \ge 1$.*

In particular, when $n = 0$ this includes the statement that $W^{m,p}$ is dense in L^p for all $m \ge 1$.

Proof of Proposition 2.2.4. It suffices to prove that $W^{k+1,p}(\mathcal{G})$ is dense in $W^{k,p}(\mathcal{G})$. To this end, let $u \in W^k(\mathcal{G})$ arbitrary and u_n be an edgewise approximating sequence in $\oplus_{e\in\mathcal{E}} C^\infty(I_e) \cap W^{k+1,p}(I_e)$ such that

$$\sum_{e\in\mathcal{E}} \left\| u_n - u\big|_e \right\|_{W^{k,p}} \le \frac{1}{2^n} \tag{2.8}$$

for all $n \in \mathbb{N}$. The general idea is to construct sequences $v_n \in \oplus_{e\in\mathcal{E}} W^{k+1,p}(I_e)$ such that $u_n + v_n \in W^{k+1,p}(\mathcal{G})$ and

$$u_n + v_n \xrightarrow{W^{k,p}} u \qquad (n \to \infty).$$

For fixed $\mathsf{v} \in \mathcal{V}$ and for n satisfying

$$\frac{2}{n} \le \inf_{e\in\mathcal{E}} |I_e|$$

for all $e \succ \mathsf{v}$ and $\hat{k} \in \{0,\dots,k\}$ we define

$$v_{n,\hat{k},\mathsf{v}}(x)\big|_e = \begin{cases} \frac{c_{n,\hat{k},\mathsf{v}}}{\hat{k}!} x_{\mathsf{v}}^{\hat{k}} \left(1 - n x_{\mathsf{v}}\right)^{k+1}, & \text{for } x \in e \text{ with } x_{\mathsf{v}} := \operatorname{dist}(x,\mathsf{v}) \le \frac{1}{n} \\ 0, & \text{otherwise.} \end{cases}$$

where $c_{n,\hat{k},\mathsf{v}}$ is given by

$$\begin{aligned} \text{for } \hat{k} = 0: &\qquad c_{n,0,\mathsf{v}} = u - u_n\big|_e(0_{\mathsf{v}}) \\ \text{for } 1 \le \hat{k} \le k-1: &\qquad c_{n,\hat{k},\mathsf{v}} = u^{(\hat{k})} - u_n^{(\hat{k})}\big|_e(0_{\mathsf{v}}) - \sum_{\ell=0}^{\hat{k}-1} (k+1)_\ell (-n)^\ell c_{n,\ell,\mathsf{v}}. \end{aligned}$$

We can extend the functions $v_{n,\hat{k},\mathsf{v}}$ by zero on the rest of the graph. With the Leibniz rule for $1 \le \ell \le k+1$ we compute

$$v^{(\ell)}_{n,\hat{k},v}(x)\big|_e = \chi_{\{x_{\mathsf{v}} \le \frac{1}{n}\}} \sum_{m=0}^{\ell} \frac{1}{\hat{k}!} \binom{\ell}{m} c_{n,\hat{k},\mathsf{v}} (-n)^{\ell-m} (\hat{k})_m (k)_{\ell-m} x_{\mathsf{v}}^{\hat{k}-m} (1 - n x_{\mathsf{v}})^{k+m+1-\ell} \tag{2.9}$$

Then

$$\widetilde{v}_n := \sum_{\ell=0}^{k-1} \sum_{\mathsf{v}\in\mathcal{V}} v_{n,\ell,\mathsf{v}}$$

satisfies $\widetilde{v}_n \in \oplus_{e\in\mathcal{E}} W^{k+1,p}(I_e)$ and $u_n + \widetilde{v}_n \in W^{k,p}(\mathcal{G})$ since $u_n + \widetilde{v}_n$ coincides in all $k-1$ derivatives with u by construction. Indeed, the restrictions of the k^{th} derivatives at the vertices are of rank $\leq 2|\mathcal{E}|$. Then we can find $c_{n,k,\mathsf{v}}$ for all $\mathsf{v} \in \mathcal{V}$

$$v_{n,k,\mathsf{v}}\big|_e(x) = \begin{cases} \frac{c_{n,k,\mathsf{v}}}{k!} x_{\mathsf{v}}^k \left(1 - \max\{n, c_{n,k,\mathsf{v}}^2\} x_{\mathsf{v}}\right)^{k+1}, & \text{for } x \in e \text{ with} \\ & x_{\mathsf{v}} \leq \min\{n^{-1}, c_{n,k,\mathsf{v}}^{-2}\} \\ 0, & \text{otherwise.} \end{cases}$$

such that

$$u_n + \widetilde{v}_n + \sum_{\mathsf{v}\in\mathcal{V}} v_{n,k,\mathsf{v}} \in W^{k+1,p}(\mathcal{G}).$$

By assumption (2.8) we deduce by applying the Sobolev imbedding edgewise

$$\sum_{e\in\mathcal{E}} \left\| u_n - u\big|_e \right\|_{C^{k-1}} \leq \frac{C}{2^n}$$

for all $n \in \mathbb{N}$ and some $C > 0$ and satisfies by construction

$$(-n)^\ell c_{n,\hat{k},\mathsf{v}} \to 0 \qquad (n \to \infty) \tag{2.10}$$

for all $1 \leq \ell \leq k$ and $\mathsf{v} \in \mathcal{V}$. By a change of variables we then compute for $0 \leq m \leq \ell \leq k$

$$\begin{aligned} n^{\ell-m} \int_{I_e} x_{\mathsf{v}}^{\hat{k}-m} (1 - n x_{\mathsf{v}})^{k+m+1-\ell} \, \mathrm{d}x_{\mathsf{v}} &= n^{\ell-1-\hat{k}} \int_0^1 t^{\hat{k}-m} (1-t)^{k+m+1-\ell} \, \mathrm{d}t \\ c_{n,k,\mathsf{v}} \max\{n, c_{n,k,\mathsf{v}}^2\}^{\ell-m} \int_{I_e} x_{\mathsf{v}}^{k-m} (1 - \max\{n, c_{n,k,\mathsf{v}}^2\} x_{\mathsf{v}})^{k+m+1-\ell} \, \mathrm{d}x_{\mathsf{v}} & \\ = c_{n,k,\mathsf{v}} \min\{n^{-1}, c_{n,k,\mathsf{v}}^{-2}\}^{k+1-\ell} \int_0^1 t^{k-m} (1-t)^{k+m+1-\ell} \, \mathrm{d}t &\longrightarrow 0 \\ & (n \to \infty) \end{aligned}$$

and with (2.9) and (2.10) we conclude

$$\begin{aligned} &\left\| u - \left[u_n + \widetilde{v}_n + \sum_{\mathsf{v}\in\mathcal{V}} v_{n,k,\mathsf{v}} \right] \right\|_{W^{k,p}} \\ &\qquad \leq \|u - u_n\|_{W^{k,p}} + \left\| \widetilde{v}_n + \sum_{\mathsf{v}\in\mathcal{V}} v_{n,k,\mathsf{v}} \right\|_{W^{k,p}} \longrightarrow 0 \qquad (n \to \infty). \end{aligned}$$

$\square$

Lemma 2.2.5. *Let $\mathcal{G}$ be a locally finite, connected metric graph and $p \in [1,\infty)$. Then*

$$W_c^{1,p}(\mathcal{G}) = \{u \in W^{1,p}(\mathcal{G}) |\, \operatorname{supp} u \textit{ is bounded}\}$$

is dense in $W^{1,p}(\mathcal{G})$.

Proof. Let K be a bounded, connected subgraph of $\mathcal{G}$. For $R > 0$ set

$$K_R := \{x \in \mathcal{G} |\, \operatorname{dist}(x, K) < R\}.$$

We define the cut-off functions ψ_n via

$$\widetilde{\psi_n} := \frac{1}{n} \max\{n, \operatorname{dist}(x, K_n)\}, \quad \psi_n := 1 - \widetilde{\psi_n}$$

For all $u \in W^{1,p}(\mathcal{G})$ one then computes

$$\begin{aligned}\limsup_{n\to\infty} \|u - \psi_n u\|_{W^{1,p}}^p &= \limsup_{n\to\infty} \left[\int_{\mathcal{G}} \left|\frac{\mathrm{d}}{\mathrm{d}x}\widetilde{\psi_n} u\right|^p \mathrm{d}x + \int_{\mathcal{G}} \left|\widetilde{\psi_n} u\right|^p \mathrm{d}x\right] \\ &\le \limsup_{n\to\infty} \left[\frac{2^p}{n^p} \int_{\mathcal{G}\setminus K_n} |u|^p \,\mathrm{d}x + 2^p \int_{\mathcal{G}\setminus K_n} \left|\widetilde{\psi_n} u\right|^p \mathrm{d}x + \int_{\mathcal{G}\setminus K_n} \left|\widetilde{\psi_n} u\right|^p \mathrm{d}x\right] = 0,\end{aligned}$$

where in the equation we used

$$\int_{\mathcal{G}\setminus K_n} |\widetilde{\psi_n} u|^p \,\mathrm{d}x \le \int_{\mathcal{G}\setminus K_n} |u|^p \,\mathrm{d}x \to 0 \qquad (n \to \infty).$$

As such $\psi_n u \to u$ in $W^{1,p}(\mathcal{G})$ as $n \to \infty$. □

A simple consequence of Proposition 2.2.4 and Lemma 2.2.6 is then the following:

Proposition 2.2.6. *Let $\mathcal{G}$ be a locally finite, connected metric graph and $p \in [1,\infty)$. Then*

$$W_c^{2,p}(\mathcal{G}) = \{u \in W^{2,p}(\mathcal{G}) |\, \operatorname{supp} u \textit{ is bounded}\}$$

is dense in $W^{1,p}$.

Proof. Let $u \in W^{1,p}(\mathcal{G})$. By Lemma 2.2.5 we can find a sequence $u_n \in W_c^{1,p}(\mathcal{G})$ with $u_n \to u$ in $W^{1,p}$. Then by Proposition 2.2.4 for each n we find a sequence $u_{n,m} \in W^{2,p}(\mathcal{G})$, after extending by zero on the whole graph, converging towards u_n in $W^{1,p}(\mathcal{G})$ as $m \to \infty$. Then one can construct a sequence in $W_c^{2,p}(\mathcal{G})$ converging to u in $W^{1,p}$ by a diagonal argument. □

Remark 2.2.7. Proposition 2.2.6 does not depend on the particular choice of vertex conditions. For instance, if $M \in H^1 + W^{1,\infty}(\mathcal{G})$ then we may equally show

$$D_c(A^M) = \left\{u \in \widetilde{W^{2,p}}(\mathcal{G}) |\, \sum_{e \succ \mathsf{v}} \left(i\frac{\partial}{\partial\nu} - M\right) u_e(\mathsf{v}) = 0 \text{ and } \operatorname{supp} u \text{ is bounded}\right\}$$

is dense in $W^{1,p}(\mathcal{G})$. The vertex conditions are special cases of complex delta conditions and it can be similarly shown for all such conditions.

2.2.4 Characterization of $W^{1,\infty}$

We give a characterization of $W^{1,\infty}$ on locally finite, connected metric graphs in the following:

Proposition 2.2.8. *Let $\mathcal{G}$ be a locally finite, connected metric graph. Then $W^{1,\infty}(\mathcal{G}) = C_b^{0,1}(\mathcal{G})$ is the set of uniformly bounded, Lipschitz continuous functions.*

Proof. Assume $u \in W^{1,\infty}(\mathcal{G})$. Let $x, y \in \mathcal{G}$ and γ be a path of length $L(\gamma)$ connecting x, y, parametrized by arc length. In the first step let us assume $u \in C^1$ edgewise, then using the continuity of u we have

$$|u(x) - u(y)| \leq \int_0^{L(\gamma)} |u'(\gamma)| \,\mathrm{d}|\gamma| \leq \operatorname{ess\,sup}_t |u'(\gamma(t))| L(\gamma).$$

Due to density this holds also for $W^{1,\infty}(\mathcal{G})$. Taking the infimum over all paths connecting x, y we conclude

$$|u(x) - u(y)| \leq \|u'\|_\infty \operatorname{dist}(x, y)$$

and thus $u \in C_b^{0,1}(\mathcal{G})$. On the other hand, let $u \in C_b^{0,1}(\mathcal{G})$, then

$$\frac{|u(x) - u(y)|}{\operatorname{dist}(x, y)} \leq L$$

for some constant $L > 0$. Using the fact that the characterization holds for intervals on each edge $e \in \mathcal{E}$ then $u \in W^{1,\infty}(I_e)$ and u' exists a.e. and

$$\|u'\|_\infty \leq L.$$

We conclude $u \in W^{1,\infty}(\mathcal{G})$ since u is also uniformly bounded by assumption. □

2.3 Self-adjoint realizations of Schrödinger operators

2.3.1 On Higher-order Schrödinger operators

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a finite metric graph. We will discuss however some extensions to locally finite metric graphs in §2.3.2. Consider the quadratic form $a : H^k(\mathcal{G}) \cap H_c^1(\mathcal{G}) \times H^k(\mathcal{G}) \cap H_c^1(\mathcal{G}) \to \mathbb{R}$ defined via

$$a^m(\varphi, \psi) = \int_{\mathcal{G}} \varphi^{(k)} \psi^{(k)} + m\varphi\psi \,\mathrm{d}x \tag{2.11}$$

with $m \in L^1_{\mathrm{loc}}(\mathcal{G})$ real-valued satisfying $m_- \in L^1 + L^\infty(\mathcal{G})$, i.e. there exists $m_1 \in L^1(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ such that $m_- = m_1 + m_\infty$.

Theorem 2.3.1. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a finite metric graph. Then a^m defines a semibounded form, i.e. for every $0 < \varepsilon < 1$ there exists $C_\varepsilon > 0$ such that*

$$a^m(u,u) \geq (1-\varepsilon)|u|^2_{H^k} - C_\varepsilon \|u\|^2_{L^2}.$$

Proof. Let $\epsilon, \delta > 0$ arbitrary but fixed. Consider a decomposition of $m_- \in L^1 + L^\infty(\mathcal{G})$ such that

$$m_- = m_1 + m_\infty, \qquad \|m_1\|_1 \leq \epsilon.$$

Then there exists $C_\delta, C > 0$ such that

$$\begin{aligned} a^m(u,u) &\geq \|u^{(k)}\|_2^2 - \|m_1\|_1 \|u\|^2_\infty - \|m_\infty\|^2_\infty \|u\|^2_2 \\ &\geq (1-\delta - C\epsilon)|u|^2_{H^k} - (C_\delta \|m_\infty\|_\infty + 1 + \|m_1\|_1)\|u\|_2 \end{aligned}$$

and the statement follows since ϵ, δ were arbitrary. □

Let $A^m : D(A^m) \to L^2(\mathcal{G})$ be the Friedrichs extension of a^m. Let us further characterize the operator A^m under some additional assumptions.

Lemma 2.3.2. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a finite metric graph. Then*

$$\begin{aligned} A^0 &= (-\Delta)^k \\ D(A^0) &= H^{2k}(\mathcal{G}) \end{aligned} \tag{2.12}$$

is the Friedrichs extension of the form a^0, where $(-\Delta)^k$ is defined edgewise by $(-1)^{2k}\frac{\mathrm{d}^k u}{\mathrm{d}x^k}$.

Proof. $D(A^0)$ is densely defined in H^k by Proposition 2.2.4. Hence, there exists a unique self-adjoint extension of the operator, with form domain contained in $H^k(\mathcal{G})$ (see also [RS75, Theorem X.23]). It suffices therefore to show that A^0 is a self-adjoint operator.

For $\varphi, \psi \in D(A^0)$ with integration by parts one easily computes

$$\left\langle A^0\varphi, \psi \right\rangle_{L^2} = a^m(\varphi, \psi) = \left\langle \varphi, A^0\psi \right\rangle_{L^2}$$

and A^0 is symmetric, hence $A^0 \subset (A^0)^*$. Let $e \in \mathcal{E}$ be fixedbut arbitrary, then suppose $u \in D((A^0)^*)$ and $v \in D(A^0)$ to be supported on e and $v_e \in C_c^\infty(I_e)$, then

$$\left\langle \varphi_e, (A^0\psi)_e \right\rangle_{L^2} = \langle \varphi, A\psi \rangle_{L^2} = \left\langle (A^0)^*\varphi, \psi \right\rangle_{L^2} = \left\langle ((A^0)^*\varphi)_e, \psi_e \right\rangle_{L^2}$$

Since e and v were arbitrary we deduce

$$(-\Delta)^k \varphi_e \in L^2(I_e)$$

in the distributional sense. Thus, $\varphi_e \in H^{2k}(I_e)$ for each $e \in \mathcal{E}$. Now, suppose $\varphi \in D((A^0)^*)$

and $\psi \in D(A^0)$ arbitrary. Then by integration by parts we compute

$$\left\langle \varphi, A^0\psi \right\rangle_{L^2} = \left\langle A^0\varphi, \psi \right\rangle_{L^2} + \sum_{i=0}^{k-1} \sum_{\mathsf{v}\in\mathcal{V}} \sum_{e\succ \mathsf{v}} \left(\overline{\varphi_e^{(i)}} \psi_e^{(2k-1-i)} - \psi_e^{(i)} \overline{\varphi_e^{(2k-i-1)}} \right)(\mathsf{v})$$

Since the choice of φ, ψ is arbitrary we deduce $\varphi \in H^{2k}(\mathcal{G})$ and we compute

$$\begin{aligned}
\left\langle (A^0)^*\varphi, \psi \right\rangle &= \left\langle \varphi, A^0\psi \right\rangle_{L^2} \\
&= \left\langle A^0\varphi, \psi \right\rangle_{L^2} + \sum_{\substack{0\le i\le k-1 \\ i \text{ even}}} \sum_{\mathsf{v}\in\mathcal{V}} \overline{\varphi_e^{(i)}(\mathsf{v})} \sum_{e\succ\mathsf{v}} \psi_e^{(2k-1-i)}(\mathsf{v}) \\
&\quad - \sum_{\substack{0\le i\le k-1 \\ i \text{ even}}} \sum_{\mathsf{v}\in\mathcal{V}} \psi_e^{(i)}(\mathsf{v}) \sum_{e\succ\mathsf{v}} \varphi_e^{(2k-i-1)}(\mathsf{v}) \\
&\quad + \sum_{\substack{0\le i\le k-1 \\ i \text{ odd}}} \sum_{\mathsf{v}\in\mathcal{V}} \psi_e^{(2k-1-i)}(\mathsf{v}) \sum_{e\succ\mathsf{v}} \overline{\varphi_e^{(i)}}(\mathsf{v}) \\
&\quad - \sum_{\substack{0\le i\le k-1 \\ i \text{ odd}}} \overline{\varphi_e^{(2k-i-1)}}(\mathsf{v}) \sum_{e\succ\mathsf{v}} \psi_e^{(i)}(\mathsf{v}) \\
&= \left\langle A^0\varphi, \psi \right\rangle_{L^2}
\end{aligned}$$

Hence $D((A^0)^*) = D(A^0) = H^{2k}(\mathcal{G})$ and we infer $A^0 = (A^0)^*$. □

Proposition 2.3.3. *Let $\mathcal{G}$ be a finite metric graph. Suppose $m \in L^2 + L^\infty(\mathcal{G})$, then the multiplication operator associated to m, i.e. $u \mapsto mu$, is relatively bounded to A^0, such that for every $0 < \varepsilon < 1$ there exists $C_\varepsilon > 0$ such that*

$$\|mu\|_2^2 \le \varepsilon \|u\|_{a^0}^2 + C_\varepsilon \|u\|_2^2. \tag{2.13}$$

In particular A^m is self-adjoint.

Proof. Let $\epsilon > 0$ arbitrary but fixed. Consider a decomposition of $m \in L^2 + L^\infty(\mathcal{G})$ such that

$$m = m_2 + m_\infty, \qquad \|m\|_2^2 \le \epsilon.$$

Then there exists $C > 0$ such that

$$\|mu\|_2^2 \le \|m_2\|_2^2 \|u\|_\infty^2 + \|m_\infty\|^2 \|u\|_2^2 \quad \le C\epsilon \|u\|_{a^0}^2 + \|m_\infty\|^2 \|u\|_2^2$$

and since ϵ was fixed but arbitrary we deduce the statement. Since the multiplication operator associated to m is a symmetric operator the selfadjointness of A^m is an immediate consequence of the Kato–Rellich theorem (see e.g. [RS75, Theorem X.12]) since for every δ there exists

$C_\delta > 0$ such that

$$\|u\|_{a^0}^2 = \langle A^0 u, u\rangle \le \|A^0 u\|_2 \|u\|_2 \le \delta \|A^0 u\|_2^2 + C_\delta \|u\|_2^2.$$

and with (2.13) we infer for all $\varepsilon > 0$ that there exists $C_\varepsilon > 0$ such that

$$\|mu\|_2^2 \le \varepsilon \|A^0 u\|^2 + C_\varepsilon \|u\|_2^2.$$

□

In the following we will be interested in the spectrum of A^m. Of particular interest in our context is the decomposition of the spectrum in essential and discrete spectrum. In fact, there exists a decomposition of the spectrum $\sigma(A^m)$ in essential and discrete spectrum

$$\sigma(A^m) = \sigma_{\text{ess}}(A^m) \sqcup \sigma_{\text{disc}}(A^m)$$

where

$$\sigma_{\text{disc}}(A^m) = \{\lambda \in \mathbb{R} | \lambda \text{ is eigenvalue of } A^m \text{ with finite algebraic multiplicity}\}$$
$$\sigma_{\text{ess}} = \sigma(A^m) \setminus \sigma_{\text{disc}}(A^m).$$

The essential spectrum can then be characterized by Weyl's theorem [RS80, Theorem VII.12]

$$\lambda \in \sigma_{\text{ess}}(A^m) \iff \exists_{\substack{(u_n)_{n=1}^\infty \\ u_i \perp u_j,\, i \neq j}} \lim_{n\to\infty} \|(A^m - \lambda) u_n\|_{L^2} = 0.$$

An important set in the context of the spectrum is the numerical range of a self-adjoint operator:

Definition 2.3.4. Let A be a self-adjoint operator on a Hilbert space H with inner product $\langle \cdot, \cdot \rangle$, then the *numerical range* of the operator A is given as

$$\operatorname{num}(A) = \{\langle u, Au\rangle | u \in D(A) \text{ with } \|u\| = 1\}.$$

The spectrum of $(-\Delta)^k$ can then be related with the numerical range as the following shows:

Theorem 2.3.5. *Let $\mathcal{G}$ be a metric graph with at least one ray. Then $\sigma_{\text{disc}}((-\Delta)^k) = \emptyset$ and*

$$\sigma((-\Delta)^k) = \sigma_{ess}((-\Delta)^k) = [0, \infty).$$

Proof. By [RS75, Problem VIII.46] we have $\sigma((-\Delta)^k) \subset \overline{\operatorname{num}((-\Delta)^k)}$. In particular, since

$$\langle u, (-\Delta)^k u\rangle \ge 0$$

for all $u \in D((-\Delta)^k)$ we infer $\sigma((-\Delta)^k) \subset [0,\infty)$. Then the result is a consequence of the result on the real line, i.e.

$$\sigma_{\text{ess}}((-\Delta)^k) = \sigma((-\Delta)^k) = [0,\infty)$$

holds since the operator is equivalent to a multiplication operator with range $[0,\infty)$ under Fourier transformation. Indeed let $\lambda > 0$ and consider a Weyl sequence $\varphi_n \in C_c^\infty(\mathbb{R})$ such that $\|(((-\Delta)^k - \lambda)\varphi_n\|_2^2 \to 0$ as $n \to \infty$. Then w.l.o.g. by translation invariance we may assume φ_n to be supported in $(0,\infty)$ and since by assumption $\mathcal{G}$ contains a ray we can extend φ_n by zero on the whole graph and by construction this is a Weyl sequence on the respective graph. Hence,

$$\inf \sigma((-\Delta)^k) = \inf \sigma_{\text{ess}}((-\Delta)^k) = [0,\infty).$$

□

2.3.2 On Schrödinger operators with magnetic potentials

Let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be a metric graph. Consider the quadratic form $a : H_c^1(\mathcal{G}) \times H_c^1(\mathcal{G}) \to \mathbb{R}$ defined via

$$a^{M,m}(u,v) = \int_{\mathcal{G}} \overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u} \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) v + m\bar{u}v \,\mathrm{d}x + \sum_{\mathsf{v}\in V} \Lambda_{\mathsf{v}}\bar{u}v(\mathsf{v}). \tag{2.14}$$

with $m \in L^1_{\text{loc}}(\mathcal{G})$ and $M \in C(\mathcal{G}) \cap L^\infty(\mathcal{G})$ real-valued satisfying $m_- \in L^1 + L^\infty(\mathcal{G})$, i.e. there exists $m_1 \in L^1(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ such that $m_- = m_1 + m_\infty$ for all $\mathsf{v} \in \mathcal{V}$.

Theorem 2.3.6. *Let $\mathcal{G} = (\mathcal{V},\mathcal{E})$ be a metric graph. Then $a^{M,m}$ defines a semibounded form and for every $0 < \varepsilon < 1$ there exists $C_\varepsilon > 0$ such that the energy estimate*

$$a^{M,m}(u,u) \geq (1-\varepsilon)\|u\|_{H^1}^2 - C_\varepsilon \|u\|_{L^2}^2$$

is satisfied.

Proof. Let $\epsilon, \delta > 0$ arbitrary but fixed. Consider a decomposition of $m_- \in L^1 + L^\infty(\mathcal{G})$ such that

$$m_- = m_1 + m_\infty, \qquad \|m_1\|_1 \leq \epsilon.$$

Then there exists $C_\delta, C > 0$ such that

$$\begin{aligned} a^{M,m}(u,u) &\geq (\|u'\|_2 - \||M|^{1/2}u\|_2^2)^2 - \|m_1\|_1\|u\|_\infty^2 - \|m_\infty\|_\infty^2\|u\|_2^2 \\ &\geq (1-\delta-C\epsilon)\|u\|_{H^1}^2 - (C_\delta\|M\|_\infty + 1 + \|m_\infty\|_1)\|u\|_2 \end{aligned}$$

and the statement follows since ϵ, δ were arbitrary. □

Let $A^{M,m} : D(A^{M,m}) \to L^2(\mathcal{G})$ be the Friedrichs extension of the operator associated to the quadratic form $a^{M,m}$. Let us further characterize the operator $A^{M,m}$ under some additional assumptions:

Lemma 2.3.7. *Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a metric graph. Suppose $M \in H^1 + W^{1,\infty}(\mathcal{G})$, then*

$$\begin{aligned} A^{M,0} &= \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 \\ D(A^{M,0}) &= \Bigg\{u \in C(\mathcal{G}) | u_e \in H^2(e) \text{ for all } e \in \mathcal{E} \text{ and} \\ &\qquad \sum_{\mathsf{e} \succ \mathsf{v}} \left(i\frac{\mathrm{d}}{\mathrm{d}\nu} + M\right) u_e(\mathsf{v}) = \Lambda_{\mathsf{v}} u(\mathsf{v}) \text{ for all } \mathsf{v} \in V\Bigg\} \end{aligned}$$

is the Friedrichs extension of the form $a^{M,0}$.

Proof. $D(A^{M,0})$ is densely defined in $H^1(\mathcal{G})$, such that $a^{M,0}$ is the closure of the form associated to $A^{M,0}$. Hence, there exists a unique self-adjoint extension of the operator, with form domain contained in $H^1(\mathcal{G})$ (see also [RS75, Theorem X.23]). It suffices therefore to show that $A = A^{M,0}$ is a self-adjoint operator.

For $\varphi, \psi \in D(A)$ with integration by parts one easily computes

$$\langle A\varphi, \psi\rangle_{L^2} = a(\varphi, \psi) = \langle \varphi, A\psi\rangle_{L^2}$$

and A is symmetric, hence $A \subset A^*$. Let $e \in \mathcal{E}$ be fixed but arbitrary, then suppose $\varphi \in D(A^*)$ and $\psi \in D(A)$ to be supported on e and $\psi_e \in C_c^\infty(I_e)$, then

$$\langle \varphi_e, (A\psi)_e\rangle_{L^2} = \langle \varphi, A\psi\rangle_{L^2} = \langle A^*\varphi, \psi\rangle_{L^2} = \langle (A^*\varphi)_e, \psi_e\rangle_{L^2}$$

Since e and ψ were arbitrary we deduce

$$\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 \varphi_e \in L^2(I_e)$$

in the distributional sense. Thus, $\varphi_e \in H^2(I_e)$ for each $e \in \mathcal{E}$. Now, suppose $\varphi \in D(A^*)$ and $\psi \in D(A)$ arbitrary. Then by integration by parts we compute

$$\langle \varphi, A\psi\rangle_{L^2} = \langle A\varphi, \psi\rangle_{L^2} + \sum_{\mathsf{v} \in \mathcal{V}} \sum_{e \succ \mathsf{v}} \left(\overline{\varphi_e} \left(i\frac{\partial}{\partial\nu} + M\right) \psi_e - \psi_e \overline{\left(i\frac{\partial}{\partial\nu} + M\right)\varphi_e} \right)(\mathsf{v})$$

Since the choice of φ, ψ is arbitrary we deduce $\varphi \in C(\mathcal{G})$ and we compute

$$\begin{aligned}\langle A^*\varphi, \psi\rangle &= \langle \varphi, A\psi\rangle_{L^2} \\ &= \langle A\varphi, \psi\rangle_{L^2} + \sum_{\mathsf{v}\in\mathcal{V}} \left(\overline{\varphi(\mathsf{v})} \left(\sum_{e\succ\mathsf{v}} \left(i\frac{\partial}{\partial\nu} + M\right) \psi_e(\mathsf{v}) \right) \right. \\ &\qquad\qquad \left. -\psi(\mathsf{v}) \left(\sum_{e\succ\mathsf{v}} \overline{\left(i\frac{\partial}{\partial\nu} + M\right) \varphi_e(\mathsf{v})} \right) \right) \\ &= \langle A\varphi, v\rangle_{L^2} + \sum_{v\in\mathcal{V}} \psi(\mathsf{v}) \left(\overline{\sum_{e\succ\mathsf{v}} \left(i\frac{\partial}{\partial\nu} + M\right) \varphi_e(\mathsf{v})} \right).\end{aligned}$$

Hence $u \in D(A)$ and we infer $A = A^*$. □

Proposition 2.3.8. *Let $\mathcal{G}$ be a metric graph. Suppose $m \in L^2 + L^\infty(\mathcal{G})$ and $M \in H^1 + W^{1,\infty}(\mathcal{G})$, then the multiplication operator associated to m is relatively bounded with respect to $A^{M,0}$. More precisely, for every $0 < \varepsilon < 1$ there exists $C_\varepsilon > 0$ such that*

$$\|mu\|_2^2 \leq \varepsilon \|u\|^2_{a^{M,0}} + C_\varepsilon \|u\|_2^2. \tag{2.15}$$

In particular $A^{M,m}$ is self-adjoint.

Proof. Let $\epsilon > 0$ arbitrary but fixed. Consider a decomposition of $m \in L^2 + L^\infty(\mathcal{G})$ such that

$$m = m_2 + m_\infty, \qquad \|m\|_2^2 \leq \epsilon.$$

Then there exists $C > 0$ such that

$$\|mu\|_2^2 \leq \|m_2\|_2^2 \|u\|_\infty^2 + \|m_\infty\|^2 \|u\|_2^2 \quad \leq C\epsilon \|u\|^2_{a^{M,0}} + \|m_\infty\|^2 \|u\|_2^2$$

and since ϵ was fixed but arbitrary we deduce the statement. Since the multiplication operator associated to m is a symmetric operator the selfadjointness of A^m is an immediate consequence of the Kato–Rellich theorem since for every δ there exists $C_\delta > 0$ such that

$$\|u\|^2_{a^{M,0}} = \langle A^0 u, u\rangle \leq \|A^{M,0}u\|_2 \|u\|_2 \leq \delta \|A^{M,0}u\|_2^2 + C_\delta \|u\|_2^2.$$

and with (2.15) we infer for all $\varepsilon > 0$ that there exists $C_\varepsilon > 0$ such that

$$\|mu\|_2^2 \leq \varepsilon \|A^{M,0}\|^2 + C_\varepsilon \|u\|_2^2.$$

□

As in §2.3.1 we can characterize the spectrum if the graph contains at least one ray.

Theorem 2.3.9. *Let $\mathcal{G}$ be a metric graph with at least one ray. Then $\sigma_{\mathrm{disc}}(-\Delta) = \emptyset$ and*

$$\sigma(-\Delta) = \sigma_{ess}(-\Delta) = [0, \infty). \tag{2.16}$$

Proof. This is a direct consequence of Theorem 2.3.5 in the case $k = 1$. □

Example 2.3.10. For a metric graph without rays (2.16) does not necessarily hold. Consider the binary tree graph $\mathcal{T}$ which is an equilateral tree graph such that every vertex has degree 3 one can show the Poincaré inequality

$$\|u'\|_2^2 \geq \lambda_1 \|u\|_2^2 \tag{2.17}$$

with $\lambda_1 > 0$ (see e.g. [SS02]). For completeness let us give a short sketch of a proof for (2.17). Consider any fixed vertex $K = \{v\}$ and let us set

$$K_n := \{u \in \mathcal{T} | \operatorname{dist}(u, v) < n\}$$

By Lemma 2.2.5 it suffices to show the statement for $u \in H_c^1(\mathcal{G})$. Suppose n is large enough such that $\operatorname{supp} u \subset K_n$, then one can show

$$\frac{1}{4} \int_{K_n \backslash K_{n-1}} (u)^2 \, \mathrm{d}x \leq \frac{1}{2} \int_{K_n \backslash K_{n-1}} u'u \, \mathrm{d}x$$
$$\frac{1}{4} \int_{K_{n-1} \backslash K_{n-2}} (u)^2 \, \mathrm{d}x \leq \frac{1}{4} \int_{K_n < K_{n-1}} u'u \, \mathrm{d}x + \frac{1}{2} \int_{K_{n-1} \backslash K_{n-2}} u'u \, \mathrm{d}x$$

or more generally

$$\frac{1}{4} \int_{K_{n+1-i} \backslash K_{n-i}} (u)^2 \, \mathrm{d}x \leq \sum_{j=1}^{i} \frac{1}{2^{i+1-j}} \int_{K_{n+1-j} \backslash K_{n-j}} u'u$$

In particular follows

$$\frac{1}{4} \int_{\mathcal{G}} (u)^2 \, \mathrm{d}x \leq \sum_{i=1}^{n} \int_{K_{n+1-i} \backslash K_{n-i}} u^2 \, \mathrm{d}x \leq \sum_{i=1}^{n} \sum_{j=1}^{n+1-i} \frac{1}{2^j} \int_{K_{n+1-i} \backslash K_{n-i}} u'u \, \mathrm{d}x \leq \|u'\|_{L^2} \|u\|_{L^2}.$$

Hence,

$$\|u\|_2 \leq 4\|u'\|_2.$$

In particular, we have

$$\inf \sigma(-\Delta) = \inf_{u \in H^1(\mathcal{G}) \backslash \{0\}} \frac{\|u'\|_2^2}{\|u\|_2^2} > 0.$$

In [DST19] the Poincaré inequality (2.17) has been used in the context of nonexistence of minimizers to the stationary NLS energy functional for binary tree graphs.

2.3.3 Minimax principle for Schrödinger operators

Suppose $\mathcal{G}$ is a metric graph. In the following we will give a variational description of the eigenvalues of a Schrödinger operator. Let $A^{M,m}$ be the Schrödinger operator $M \in C(\mathcal{G}) \cap L^\infty(\mathcal{G})$ and $m \in L^1 + L^\infty(\mathcal{G})$, defined as in §2.3.2, then for $n \in \mathbb{N}$ denote

$$\mu_n(A^{M,m}) := \inf_{\substack{u_1,\dots,u_n \in H_c^1(\mathcal{G})\setminus\{0\} \\ u_i \perp u_j, \text{ for } i \neq j}} \sup_{\substack{u \in \operatorname{span}(u_1,\dots,u_n)\setminus\{0\} \\ \|u\|_2^2 = 1}} a^{M,m}(u,u). \tag{2.18}$$

By the minimax theorem for semi-bounded selfadjoint operators (see [Tes14, Theorem 4.14]; one can also find therein a max-min version [Tes14, Theorem 4.12]) (2.18) describes all eigenvalues below the essential spectrum. When $\mathcal{G}$ is compact $A^{M,m}$ has compact resolvent due to compact imbedding $H^1(\mathcal{G})$ in $L^2(\mathcal{G})$ and its spectrum is purely discrete in particular all eigenvalues can be characterized by (2.18) Note, that we may also treat Dirichlet conditions by replacing $H^1(\mathcal{G})$ by $H_0^1(\mathcal{G}, \mathcal{V}^D)$ for a set of vertices $\mathcal{V}^D \subset \mathcal{V}$, the so-called Dirichlet set. Similarly, the associated operators have purely discrete spectrum and we denote their eigenvalues by

$$\lambda_n(A^{M,m}, \mathcal{V}^D) := \inf_{u_1,\dots,u_n \in H_0^1(\mathcal{G},\mathcal{V}^D)\cap H_c^1(\mathcal{G})} \sup_{u \in \operatorname{span}(u_1,\dots,u_n), \|u\|_2^2 = 1} a^{M,m}(u,u). \tag{2.19}$$

If we suppose $\mathcal{V}^D = \mathcal{V}$, then the associated eigenfunctions satisfy Dirichlet vertex conditions at all vertices and we denote

$$\lambda_n^D(A^{M,m}) := \lambda_n(A^{M,m}, \mathcal{V}). \tag{2.20}$$

If it is clear what Schrödinger operators and Dirichlet sets we consider we also drop the arguments and write $\mu_n, \lambda_n, \lambda_n^D$.

2.4 Persson's Theorem for Schrödinger operators on Metric Graphs

In the following we want to establish a Persson theory, i.e. the development of decomposition type results which can be used to establish a characterization of the infimum of the essential spectrum for a general class of Schrödinger operators. A major tool is the choice of a sequence of partitions of unity to separate the supports of test functions. Let us briefly discuss the theory (see [HS96, §14.4]) for Schrödinger operators in $\mathbb{R}^N$. Schrödinger operators can be shown to satisfy the IMS formula (c.f. [HS96, (19.54)])

$$Au = \sum_{i=1}^{k} J_i A J_i u + |\nabla J_i|^2 u. \tag{2.21}$$

where $J_1, \dots, J_k \in C^\infty(\mathbb{R}^N)$ is a partition of unity that satisfy the normalization condition

$$\sum_{i=1}^{k} J_i^2 \equiv 1.$$

Then holds (c.f. [Sig82, §2]):

Theorem 2.4.1. *Suppose $A : D(A) \subset L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ is a self-adjoint operator that satisfies* (2.21)*, then*

$$\inf \sigma_{ess} = \sup_{K \Subset \mathbb{R}^n} \inf_{\substack{u \in D(A) \\ \|u\|_{L^2}^2 = 1,\ \operatorname{supp} u \subset \mathbb{R}^n \setminus K}} \langle u, Au \rangle_{L^2}.$$

2.4.1 Persson theory for Higher-order Schrödinger operators

2.4.1.1 Partitions of unity in $\widetilde{C_b^\infty}$

Let $\mathcal{G}$ be any locally finite, connected graph and $\mathcal{O}$ be a finite covering of $\mathcal{O}$. We construct a partition of unity in $\widetilde{C_b^\infty}(\mathcal{G})$ (c.f. (2.7)) by choosing appropriate partitions of unities subordinate to the covering. One rather different "normalization" of the usual partition of unity will be especially useful in applications in §3:

Lemma 2.4.2. *Let $\mathcal{G}$ be a metric graph. Consider any finite open covering $\mathcal{O}$ of $\mathcal{G}$. There exists a partition of unity subordinate to $\mathcal{O}$ in $\widetilde{C_b^\infty}$ satisfying*

$$\sum_{O \in \mathcal{O}} \Psi_O^2 \equiv 1. \tag{2.22}$$

Proof. Consider any smooth partition of unity $\{\psi_O\}_{O \in \mathcal{O}}$ on the graph subordinate to the open covering $\mathcal{O}$ satisfying

$$\sum_{O \in \mathcal{O}} \Psi_O \equiv 1.$$

Then we may define

$$\Psi_O := \frac{\psi_O}{\sqrt{\sum_{O \in \mathcal{O}} \psi_O^2}}$$

for all $O \in \mathcal{O}$, which is smooth restricted as functions on all edges since $\sum_{O \in \mathcal{O}} \psi_O^2(y) \neq 0$ for all $y \in \mathcal{G}$. Furthermore, it is constant in a neighborhood of any vertex and we infer $\Psi_O \in \widetilde{C_b^\infty}(\mathcal{G})$. By construction we conclude

$$\sum_{O \in \mathcal{O}} \Psi_O^2 \equiv 1.$$

□

Remark 2.4.3. The normalization in (2.22) replaces in this context the typical normalization, where one assumes

$$\sum_{O \in \mathcal{O}} \psi_O \equiv 1.$$

Mostly, we will work with partitions of unity that satisfy the normalization (2.22).

In the following we define for $R > 0$ the open and closed R-neighborhoods of a subset $K \subset \mathcal{G}$ by

$$\begin{aligned} K_R &:= \{x \in \mathcal{G} |\, \mathrm{dist}(x, K) < R\} \\ \overline{K_R} &:= \{x \in \mathcal{M} |\, \mathrm{dist}(x, K) \leq R\}. \end{aligned} \tag{2.23}$$

Example 2.4.4. Let $\mathcal{G}$ be a finite, connected metric graph with core $K = \mathcal{G} \setminus \mathcal{E}_\infty$. Consider on $\mathcal{G}$ the open covering $\mathcal{O}$ given by K_2 and $\mathcal{G} \setminus K_1$, where K_1 and K_2 are the neighborhoods of K given as in (2.23), such that $\mathcal{G} \setminus K_1$ only consists of disjoint rays. Consider the partition of unity subordinate to $\mathcal{O}$ from Lemma 2.4.2 given by $\psi_K, \{\psi_e\}_{e \in \mathcal{E}_\infty}$ respective to K_2 and $\mathcal{G} \setminus K_1$, then we define slight modifications

$$\psi_{K,R}(x) = \begin{cases} 1, & \text{on } K \\ \psi_K(x/R) & \text{on all rays } e \in \mathcal{E}_\infty; \end{cases}$$

$$\psi_{e,R}(x) = \begin{cases} 0, & \text{on } \mathcal{G} \setminus \{e\} \\ \psi_e(x/R) & \text{on } e \in \mathcal{E}_\infty. \end{cases}$$

By Lemma 2.4.2 there exists a sequence of partitions of unity

$$\Psi_n := \Psi_{K,n}, \qquad \widetilde{\Psi_n} := \sum_{e \in \mathcal{E}_\infty} \Psi_{e,n}$$

in $\widetilde{C_b^\infty}(\mathcal{G})$ satisfying

$$\Psi_n^2 + \widetilde{\Psi_n}^2 \equiv 1.$$

Then by definition, $\{\Psi_n \widetilde{\Psi}_n\}$ satisfies furthermore

- $\mathrm{supp}\, \Psi_n, \mathrm{supp}\, \widetilde{\Psi}_n$ define a covering of $\mathcal{G}$
- $\mathrm{supp}\, \Psi_n = K_{2n}$
- $\mathrm{supp}\, \widetilde{\Psi}_n = \mathcal{G} \setminus K_n$.

These properties make the choice for the sequence of partitions of unity useful in applications, among others in §3 this sequence will be an example for a *vanishing-compatible sequence of partitions of unity* subordinate to the open coverings given by K_{2n} and $\mathcal{G} \setminus K_n$ (c.f. §3).

2.4.1.2 A decomposition formula

In the following we identify a given function $f \in \widetilde{C_b^\infty}(\mathcal{G})$ with its corresponding multiplication operator $\mathcal{M}_f \varphi := f\varphi$. Let A be an operator such that $fD(A) \subset D(A)$, then we can define the commutator $[A, f] = Af - fA$ and

$$fAf = f^2A + f[A, f]$$
$$fAf = Af^2 + [A, f]f.$$

Averaging the two preceding equations we conclude

$$fAf = \frac{1}{2}(f^2A + Af^2) + \frac{1}{2}(f[A, f] - [A, f]f). \tag{2.24}$$

Lemma 2.4.5. *Let $\mathcal{G}$ be a locally finite metric graph. Assume $\{\psi_k\}_{k=1}^N$ is a family of function in $\widetilde{C_b^\infty}(\mathcal{G})$ with $0 \le \psi_k \le 1$ for all $k \in \{1, \dots, k\}$ and*

$$\sum_{k=1}^N \psi_k^2 \equiv 1.$$

Assume $D(A)$ is invariant under multiplication by elements in $\widetilde{C_b^\infty}(\mathcal{G})$, then

$$A = \sum_{k=1}^N \psi_k A \psi_k - \frac{1}{2}(\psi_k[A, \psi_k] - [A, \psi_k]\psi_k). \tag{2.25}$$

Proof. Follows immediately with (2.24). □

We refer to (2.25) as a decomposition formula for A. In the following, we develop a decomposition formula for the Polylaplacian $A = (-\Delta)^k$.

Lemma 2.4.6. *Let $\mathcal{G}$ be a locally finite connected graph. Let $A = (-\Delta)^k$ with $D(A) = H^{2k}$, then*

(i) $fD(A) \subset D(A)$ for all $f \in \widetilde{C_b^\infty}(\mathcal{G})$.

(ii) Let $f \in \widetilde{C_b^\infty}(\mathcal{G})$, then the operator fAf is given by

$$\begin{aligned}(fAf)\,\varphi = {} & \frac{1}{2}(f^2A + Af^2)\varphi \\ & + \frac{(-1)^{k+1}}{2} \sum_{m=1}^{2k-1} \sum_{n=1}^{2k-m} \frac{(2k)_{m+n}}{m!n!} f^{(m)} f^{(n)} \varphi^{(2k-m-n)}\end{aligned} \tag{2.26}$$

for all $\varphi \in D(A)$.

Proof. We apply Leibniz' formula and compute

$$\begin{aligned}[A, f]\varphi &= (-\Delta)^k f\varphi - f(-\Delta)^k\varphi \\ &= (-1)^k \sum_{m=1}^{2k} \binom{2k}{l} f^{(m)} \varphi^{(2k-m)}.\end{aligned}$$

Then we apply Leibniz' formula again and compute

$$\begin{aligned}([A,f]f)\,\varphi &= (-1)^k \sum_{m=1}^{2k}\sum_{n=0}^{2k-m}\binom{2k}{m}\binom{2k-m}{n} f^{(m)} f^{(n)} \varphi^{2k-m-n} \\ &= (-1)^k \sum_{m=1}^{2k}\sum_{n=0}^{2k-m} \frac{(2k)_{m+n}}{m!n!} f^{(m)} f^{(n)} \varphi^{(2k-m-n)}\end{aligned}$$

and we conclude

$$\frac{1}{2}(f[A,f]-[A,f]f)\varphi = \frac{(-1)^{k+1}}{2}\sum_{m=1}^{2k-1}\sum_{n=1}^{2k-m}\frac{(2k)_{m+n}}{m!n!} f^{(m)} f^{(n)} \varphi^{(2k-m-n)}.$$

The statement follows upon combining this with (2.25). □

2.4.1.3 A Persson type theory for Higher-order Schrödinger operators on metric graphs

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a connected finite metric graph in this first part of the section. In particular $\mathcal{G}$ consists of a compact subset $K \subset \mathcal{G}$, which we call the *core graph* of $\mathcal{G}$, upon removal of the rays $\mathcal{E}_\infty \subset \mathcal{E}$ of $\mathcal{G}$. Consider the Schrödinger operator with $m \in L^2 + L^\infty(\mathcal{G})$ as defined in §2.3.1. Combining Lemma 2.4.5 and the abstract decomposition formula in Lemma 2.4.6 we have the decomposition formula for the Polylaplacian:

Lemma 2.4.7. *Let $\mathcal{G} = (V, \mathcal{E})$ be a connected finite metric graph and assume $\{\Psi_1, \ldots, \Psi_N\}$ to be a partition of unity subordinate to an open covering $\mathcal{O} = \{O_1, \ldots, O_n\}$ satisfying*

$$\sum_{k=1}^{N} \Psi_k^2 \equiv 1.$$

Then

$$A^m\varphi = \sum_{j=1}^{k} \Psi_j A^m \Psi_j \varphi + \frac{(-1)^k}{2}\sum_{m=1}^{2k}\sum_{n=1}^{2k-m}\frac{(2k)_{m+n}}{m!n!}\Psi_j^{(m)}\Psi_j^{(n)}\varphi^{(2k-m-n)} \tag{2.27}$$

for all $\varphi \in D(A)$.

Given the core graph

$$K = \mathcal{G} \setminus \mathcal{E}_\infty \tag{2.28}$$

we define for $R > 0$

$$\begin{aligned}D_R &= \{\varphi \in D(A^m) |\, \mathrm{supp}(\varphi) \subset \mathcal{G} \setminus K_R\} \\ \Sigma_R^m &= \inf\{\langle \varphi, A\varphi\rangle | \varphi \in D_R, \|\varphi\|_2^2 = 1\}.\end{aligned}$$

Since $D(A^m)$ is nontrivial and invariant under multiplication by test functions in $\widetilde{C_c^\infty}$ the set D_R is nonempty.

For $R = 0$ we set

$$\begin{aligned} D_0 &= D(A^m) \\ \Sigma_0^m &= \inf\{\langle \varphi, A\varphi\rangle | \varphi \in D(A), \|\varphi\|_2^2 = 1\} \end{aligned} \tag{2.29}$$

and recall that

$$\Sigma^m = \lim_{R\to\infty} \Sigma_R^m = \sup_{R>0} \Sigma_R^m. \tag{2.30}$$

In the following we characterize the quantities that were central to the existence theorems in the existence results before. Since A is self-adjoint one can show (see also Remark 2.4.17)

$$\Sigma_0^m = \inf \sigma(A^m).$$

By the following theorem also holds

$$\Sigma^m = \inf \sigma_{\text{ess}}(A^m);$$

with Σ_0, Σ analogously as in (2.29) and (2.30) defined for a general self-adjoint operator A we get:

Theorem 2.4.8. *Assume $\mathcal{G}$ is a connected finite metric graph. Let A be a self-adjoint, nonnegative operator on $L^2(\mathcal{G})$ that satisfies the decomposition formula* (2.27)*. Additionally let $f(A+i)^{-1}$ be compact for all $f \in \widetilde{C_c^\infty}(\mathcal{G})$. Then*

$$\Sigma = \inf \sigma_{ess}(A).$$

Proof. $\inf \sigma_{ess}(A) \geq \Sigma$. Let $\lambda \in \sigma_{\text{ess}}(A)$ and let (φ_n) be an associated Weyl sequence satisfying $\|\varphi_n\|_2^2 = 1$. Consider the sequence of partitions of unity $\Psi_n, \widetilde{\Psi_n}$ from Example 2.4.4.

Since $\Psi_R^2(A+i)^{-1}$ is compact for all $R > 0$, and since $(A+i)\varphi_n \rightharpoonup 0$ as $n \to \infty$ we deduce that

$$\|\Psi_R \varphi_n\|_2 = \|\Psi_R(A+i)^{-1}(A+i)\varphi_n\|_2 \to 0 \qquad (n \to \infty)$$

and passing to a subsequence, still denoted by φ_n, we may assume

$$\|\Psi_n \varphi_n\|_2 = \|\Psi_n(A+i)^{-1}(A+i)\varphi_n\|_2 \to 0.$$

Furthermore, with (2.39) we deduce that

$$\|\varphi_n\|_{H^{2k}} \leq C|\varphi_n|_{H^{2k}} = C\left(\|A\varphi_n\|_2^2 + \|\varphi_n\|_2^2\right)^{1/2}$$

is uniformly bounded. Since φ_n is a Weyl sequence for $\lambda \in \sigma_{\text{ess}}(A)$ with the decomposition formula in Lemma 2.4.7 we then compute

$$\begin{aligned}
\lambda &= \lim_{n\to\infty} \langle \varphi_n, A\varphi_n\rangle_{L^2} \\
&= \lim_{n\to\infty} \langle \Psi_n\varphi_n, A\Psi_n\varphi_n\rangle_{L^2} + \langle \widetilde{\Psi_n}\varphi_n, A\widetilde{\Psi_n}\varphi_n\rangle_{L^2} + O\left(\frac{1}{n^2}\right) \\
&\geq \lim_{n\to\infty} \sum_{e\in\mathcal{E}_\infty} \langle \widetilde{\Psi_n}\varphi_n, A\widetilde{\Psi_n}\varphi_n\rangle_{L^2} \geq \lim_{n\to\infty} \Sigma_n = \Sigma.
\end{aligned}$$

Since $\lambda \in \sigma_{\text{ess}}(A)$ was arbitrary, we conclude $\inf \sigma_{\text{ess}}(A) \geq \Sigma$.

$\inf \sigma_{ess}(A) \leq \Sigma$. Assume for a contradiction that $\inf \sigma_{\text{ess}}(A) \geq \Sigma + 3\varepsilon$ with $\varepsilon > 0$. Then $\sigma(A) \cap (-\infty, \Sigma + 2\varepsilon]$ is discrete and since A is bounded from below, the spectral projector $P_\Sigma := P_{(-\infty,\Sigma+2\varepsilon]}$ is of finite rank. Assume $\varphi_n \in D_n(A)$ is a sequence such that

$$\langle \varphi_n, A\varphi_n\rangle \leq \Sigma + \varepsilon$$

and $\varphi_n \rightharpoonup 0$ in L^2. Then since $(A + \Sigma + 2\varepsilon)\, P_\Sigma$ is a compact operator and

$$(A + \Sigma + 2\varepsilon)\, P_\Sigma\varphi_n \to 0 \qquad (n \to \infty).$$

Hence

$$\begin{aligned}
\langle \varphi_n, A\varphi_n\rangle_{L^2} &= \langle \varphi_n, A(1 - P_\Sigma)\varphi_n\rangle + \langle \varphi_n, AP_\Sigma\varphi_n\rangle_{L^2} \\
&\geq (\Sigma + 2\varepsilon)\langle \varphi_n, (1 - P_\Sigma)\varphi_n\rangle_{L^2} + \langle \varphi_n, AP_\Sigma\varphi_n\rangle_{L^2} \\
&\geq \Sigma + 2\varepsilon + \langle \varphi_n, (A + \Sigma + 2\varepsilon)\, P_\Sigma\varphi_n\rangle_{L^2}\,.
\end{aligned}$$

Passing to the limit we conclude

$$\liminf_{n\to\infty} \langle \varphi_n, A\varphi_n\rangle_{L^2} \geq \Sigma + 2\varepsilon$$

and we infer the statement by contradiction. □

2.4.2 Schrödinger operators with magnetic potentials on general metric graphs

2.4.2.1 Partitions of unity in $W^{1,\infty}(\mathcal{G})$

Here we give an important example for a partition of unity in $W^{1,\infty}(\mathcal{G}) = C_b^{0,1}(\mathcal{G})$. Given any partition of unity in $W^{1,\infty}(\mathcal{G})$ one can always find a renormalization as in Lemma 2.4.2:

Lemma 2.4.9. *Let $\mathcal{G}$ be a connected, locally finite metric graph. Consider any finite open covering $\mathcal{O}$ of $\mathcal{G}$. Then there exists a partition of unity in $W^{1,\infty}(\mathcal{G})$ subordinate to $\mathcal{O}$ satisfying*

$$\sum_{O\in\mathcal{O}} \Psi_O^2 \equiv 1.$$

Proof. Consider a partition of unity $\{\psi_O\}_{O\in\mathcal{O}}$ on the graph subordinate to the open covering $\mathcal{O}$. Then we define

$$\Psi_O := \frac{\psi_O}{\sqrt{\sum_{O\in\mathcal{O}}\psi_O^2}}$$

for all $O \in \mathcal{O}$. As a product of uniformly bounded Lipschitz continuous functions, Ψ_O is also one; and by Proposition 2.2.8 we conclude $\psi_O \in W^{1,\infty}(\mathcal{G})$. Moreover, $\sum_{O\in\mathcal{O}}\psi_O^2 \equiv 1$ by construction. $\square$

Example 2.4.10. Let $\mathcal{G}$ be a locally finite metric graph and let K be some bounded, connected subgraph. Consider the partition of unity in $W^{1,\infty}(\mathcal{G})$

$$\psi(x) = \max\{\operatorname{dist}(\mathcal{G}\setminus K_2, x), 1\}, \qquad \widetilde{\psi}(x) = 1 - \psi(x).$$

We construct a sequence of partitions of unity via

$$\psi_n(x) = \frac{1}{n}\max\{\operatorname{dist}(\mathcal{G}\setminus K_{2n}, x), n\}, \qquad \widetilde{\psi_n}(x) = 1 - \psi_n(x).$$

By Lemma 2.4.9 we can rescale them in such a way that

$$\Psi_n^2 + \widetilde{\Psi_n}^2 \equiv 1.$$

Then as in Example 2.4.4 the sequence $\Psi_n, \widetilde{\Psi}_n$ satisfies

$$\operatorname{supp}\Psi_n = K_{2n}, \qquad \operatorname{supp}\widetilde{\Psi}_n = \mathcal{G}\setminus K_n.$$

This sequence will be used in applications in §3 and is also an example for a vanishing-compatible sequence in $W^{1,\infty}(\mathcal{G})$ (c.f. Definition 3.2.16 for details).

Definition 2.4.11. Let $f \in C^{0,1}(\mathcal{G})$. We call a point $x \in \mathcal{G}$ a Kirchhoff point of f if one of the following holds:

(1) $x \in \mathcal{V}$ is a vertex of degree $d_x \neq 2$, the derivatives $f_e'(x)$ exist for all $e \succ x$, and f satisfies the Kirchhoff condition

$$\sum_{e\succ x}\tfrac{\partial}{\partial\nu}f_e(x) = 0,$$

(2) $x \in \mathcal{G}$ is an interior point of an edge (equivalently, a dummy vertex of degree 2), and f is differentiable at x.

We call the set

$$\mathcal{N}_f = \mathcal{G}\setminus\{x \in \mathcal{G} : x \text{ is a Kirchhoff point of } f\}$$

the non-Kirchoff set of f.

Remark 2.4.12. The approach to construct sequences of partitions of unities in $\widetilde{C}_b^\infty(\mathcal{G})$ in Example 2.4.4 is not applicable due to the absence of a core graph here. Instead, We are going to consider the sequence of partitions of unity in Example 2.4.10. This concrete sequence has some interesting properties, such that for all $n \in \mathbb{N}$

$$\|\psi_n'\|_{L^\infty} = \frac{1}{n} \qquad \|\widetilde{\psi_n}'\|_{L^\infty} = \frac{1}{n}$$

and in particular

$$\|\Psi_n'\|_{L^\infty} \leq \frac{C}{n} \qquad \|\widetilde{\Psi_n}'\|_{L^\infty} \leq \frac{C}{n}$$

for a $C = C(\mathcal{G})$ only dependent on the graph.

2.4.2.2 A decomposition formula

For the Schrödinger operator with magnetic potential

$$\widetilde{A} = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2$$
$$D(\widetilde{A}) = \widetilde{H^2}(\mathcal{G})$$

one can show as in §2.4.1.2, see Lemma 2.4.6:

Lemma 2.4.13. *Let $\mathcal{G}$ be a locally finite connected metric graph. Let*

$$\widetilde{A} := \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2$$
$$D(\widetilde{A}) := \widetilde{H^2}(\mathcal{G})$$

edgewise defined, i.e.

$$\left(\widetilde{A}\varphi\right)_e = \widetilde{A}\varphi_e.$$

Then $\widetilde{A}$ defines a closed operator on $L^2(\mathcal{G})$ and satisfies

(i) $fD(\widetilde{A}) \subset D(\widetilde{A})$ for all $f \in \widetilde{C^\infty}(\mathcal{G})$.

(ii) Let $f \in \widetilde{C^\infty}(\mathcal{G})$, then the operator $f\widetilde{A}f$ is given by

$$f\widetilde{A}f = \frac{1}{2}\left(f^2\widetilde{A} + \widetilde{A}f^2\right) + |f'|^2 \tag{2.31}$$

Proof. The proof is analogous to the one in Lemma 2.4.6. □

Remark 2.4.14. (2.31) does not uniquely determine an operator. Indeed (2.31) is the special case of (2.26) when $k = 1$. In particular, formula (2.26) in the case $k = 1$ holds for all self-adjoint realizations of the magnetic Schrödinger operators and independent of the choice of $M \in H^1 + W^{1,\infty}(\mathcal{G})$ as we will see in the following Lemma 2.4.15.

We will be interested in a decomposition lemma for the form associated to A as given in (2.11).

Lemma 2.4.15. *Let $\mathcal{G}$ be a locally finite, connected metric graph and $a(\cdot,\cdot)$ be the symmetric sesquilinear form given by*

$$a(u,v) := \int_{\mathcal{G}} \overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u} \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) v \,\mathrm{d}x$$

for $u, v \in H^1(\mathcal{G})$ Then for $f \in W^{1,\infty}(\mathcal{G}) \cap \widetilde{C^\infty}(\mathcal{G})$ we have

$$a(fu, fv) = \frac{1}{2}\left(a_{\mathcal{G}}(u, f^2 v) + a(f^2 u, v)\right) + \langle |f'|^2 u, v\rangle_{L^2(\mathcal{G})}.$$

Proof. By Proposition 2.2.6 we may assume $u, v \in D_c(A^{M,0})$ and $fu, fv \in \widetilde{H^2}(\mathcal{G}) \cap H^1_c(\mathcal{G})$. Integrating by parts on an arbitrary bounded subgraph K containing $\operatorname{supp} u$ and $\operatorname{supp} v$ we compute

$$\begin{aligned} a(fu, fv) &= \int_K \overline{(fAf)\, u} v \,\mathrm{d}x + \sum_{\mathsf{v}\in\mathcal{N}_f\cap K} \sum_{e\succ\mathsf{v}} \left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) fu}\right]_e fv(\mathsf{v}) \\ &= \int_K \overline{\left(\frac{1}{2}\left(f^2\widetilde{A} + \widetilde{A}f^2\right) u + |f'|^2 u\right)} v \,\mathrm{d}x \\ &\qquad + \sum_{\mathsf{v}\in\mathcal{N}_f\cap K} \sum_{e\succ\mathsf{v}} \left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) fu}\right]_e fv(\mathsf{v}) \end{aligned}$$

Similarly we compute

$$\begin{aligned} &\frac{1}{2}\left(a(u, f^2 v) + a(f^2 u, v)\right) + \int_{\mathcal{G}} |f'|^2 \overline{u} v \,\mathrm{d}x \\ &\quad = \int_K \overline{\left(\frac{1}{2}\left(f^2\widetilde{A} + \widetilde{A}f^2\right) u + |f'|^2 u\right)} v \,\mathrm{d}x \\ &\qquad + \sum_{\mathsf{v}\in\mathcal{N}_f\cap K} \sum_{e\succ\mathsf{v}} \frac{1}{2}\left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) f^2 u}\right]_e v(\mathsf{v}) + \frac{1}{2}\left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u}\right]_e f^2 v(\mathsf{v}) \end{aligned}$$

Moreover, we have

$$\left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) fu}\right]_e fv(\mathsf{v}) = \frac{1}{2}\left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) f^2 u}\right]_e v(\mathsf{v}) + \frac{1}{2}\left[\overline{\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u}\right]_e f^2 v(\mathsf{v})$$

for all $\mathsf{v} \in \mathcal{N}_f$ and we deduce

$$a(fu, fv) = \frac{1}{2}\left(a(u, f^2 v) + a(f^2 u, v)\right) + \int_{\mathcal{G}} |f'|^2 \overline{u} v \,\mathrm{d}x$$

for all $u, v \in D_c(A^M)$ and the statement follows by density of $D_c(A^M)$ in $D(A^M)$. $\square$

2.4.2.3 Persson's Theorem

In this section we discuss quantities related to the spectrum and essential spectrum to treat the general case. In fact, by [RS80, §6 Problem 44] for a self-adjoint operator A we have $\sigma(A) \subset \overline{\operatorname{num}(A)}$ and furthermore we can even characterize the bottom of its spectrum and essential spectrum via the numerical range of the operator and show a form version of Theorem 2.4.8 for Schrödinger operators:

Theorem 2.4.16. *Suppose $A^{M,m}$ is the self-adjoint operator associated to $a^{M,m}$, then*

$$\inf \sigma(A^{M,m}) = \inf \left\{ a^{M,m}(\varphi,\varphi) | \varphi \in H^1(\mathcal{G}) \textit{ with } \|\varphi\| = 1 \right\} =: \Sigma_0^{M,m}$$
$$\inf \sigma_{ess}(A^{M,m}) = \sup_{K \Subset \mathcal{G}} \inf \left\{ a^{M,m}(\varphi,\varphi) | \varphi \in H^1(\mathcal{G}) \textit{ with } \|\varphi\| = 1 \textit{ and } \operatorname{supp}(\varphi) \subset \mathcal{G} \setminus K \right\} =: \Sigma^{M,m}.$$

Remark 2.4.17. In fact, by the arguments below

$$\inf \sigma(A) = \inf \left\{ a(\varphi,\varphi) | \varphi \in H^1(\mathcal{G}) \text{ with } \|\varphi\| = 1 \right\}$$

holds for any self-adjoint operator with associated form given by the Friedrichs extension $a(\cdot,\cdot)$.

Proof of Theorem 2.4.16. Let us define

$$\begin{aligned} \Sigma_0^{M,m} &:= \inf \left\{ a^{M,m}(\varphi,\varphi) | \varphi \in H^1(\mathcal{G}) \text{ with } \|\varphi\| = 1 \right\} \\ \Sigma^{M,m} &:= \sup_{K \Subset \mathcal{G}} \inf \left\{ a^{M,m}(\varphi,\varphi) | \varphi \in H^1(\mathcal{G}) \text{ with } \|\varphi\| = 1 \text{ and } \operatorname{supp}(\varphi) \subset \mathcal{G} \setminus K \right\}. \end{aligned} \tag{2.32}$$

Let $\lambda_0 := \inf \sigma(A^{M,m})$. From Weyl's theorem we infer the existence of a sequence $\{u_n\}$ with $\|u_n\|_2 = 1$ such that

$$\|(A^{M,m} - \lambda)u_n\|_2 \to 0 \qquad (n \to \infty)$$

and we infer

$$\left|\langle (A^{M,m} - \lambda_0)u_n, u_n\rangle\right| \le \|(H - \lambda)u_n\|_2 \to 0 \qquad (n \to \infty).$$

Hence,

$$\inf \sigma(A^{M,m}) = \lambda_0 = \lim_{n\to\infty} \langle A^{M,m} u_n, u_n\rangle \ge \Sigma_0^{M,m}.$$

The reverse inequality is an immediate consequence of the fact that $\sigma(A^{M,m}) \subset \overline{\operatorname{num}(A^{M,m})}$

(see also [RS75, Problem VIII.46]) and we infer

$$\inf \sigma(A^{M,0}) = \Sigma_0^{M,m}.$$

Consider the sequence of partitions of unity $\Psi_n, \widetilde{\Psi_n}$ from Example 2.4.10 and the proof of the statement follows verbatim as in Theorem 2.4.8 using the decomposition formula in Lemma 2.4.15. □

If we have

$$\Sigma_0^{M,m} < \Sigma^{M,m},$$

then by Theorem 2.4.16 in particular there exists discrete spectrum below the essential spectrum and there exists a spectral minimizer of

$$\inf\{a(\varphi,\varphi)|\varphi \in H^1(\mathcal{G}) \text{ with } \|\varphi\|_{L^2}^2 = 1\}.$$

In the following we will refer to such minimizer as *ground states* of $A^{M,m}$:

Definition 2.4.18. Suppose H is a Hilbert space and A is a self-adjoint operator on H. We say $\varphi \in D(A)$ with $\|\varphi\| = 1$ is a *ground state* if and only if

$$\inf \sigma(A) = \langle A\varphi, \varphi\rangle.$$

By Theorem 2.4.20 there exists a minimizer of

$$\Sigma_0^{M,m} = \inf\left\{a^{M,m}(\varphi,\varphi)|\varphi \in H^1(\mathcal{G}) \text{ with } \|\varphi\| = 1\right\}.$$

An important class of potential we refer to are potentials that have certain decaying properties:

Definition 2.4.19. Let $\mathcal{G}$ be a metric graph. Then we say $m \in L^1 + L^\infty(\mathcal{G})$ is *a falling potential* if

$$\inf_{K \Subset \mathcal{G}} \sup_{x \in \mathcal{G}\setminus K} |m_\infty(x)| = 0.$$

As a consequence of Theorem 2.4.16 we get in particular:

Theorem 2.4.20. *Let $\mathcal{G}$ be a metric graph. Suppose $m \in L^1 + L^\infty(\mathcal{G})$ is a falling potential, then*

$$\Sigma^{M,m} = \inf \sigma_{ess}(A^{M,m}) \geq 0.$$

In particular, if

$$\Sigma_0^{M,m} = \inf \sigma(A^{M,m}) < 0,$$

then $\Sigma_0^{M,m} \in \sigma_{disc}(A^{M,m})$.

Theorem 2.4.16 can be generalized to a wider class of operators, namely those satisfying the so called IMS formula (see [Sig82]):

Definition 2.4.21 (IMS formula on locally finite metric graphs)**.** Let $\mathcal{G}$ be a locally finite, connected metric graph. Let $A : D(A) \subset L^2(\mathcal{G}) \to L^2(\mathcal{G})$ be a densely defined, self-adjoint operator and assume $a(\cdot, \cdot)$ is the associated symmetric, sesquilinear form, defined on $H^1(\mathcal{G})$. We say A satisfies the IMS formula if for all $f \in W^{1,\infty}(\mathcal{G}) \cap \widetilde{C^\infty}(\mathcal{G})$

$$a(fu, fv) \quad = \quad \frac{1}{2}\big(a(u, f^2 v) + a(f^2 u, v)\big) \; + \; \langle |f'|^2 u, v\rangle_{L^2}, \qquad \forall u, v \quad \in \quad D(A). \quad (2.33)$$

From Lemma 2.4.15 one easily sees that the magnetic Schrödinger operator $A^{M,m}$ associated to the form $a^{M,m}$ as considered in §2.3.2 satisfies the IMS formula (2.33); and in particular the Persson theory can be generalized to a broad class of operators:

Theorem 2.4.22. *Assume $\mathcal{G}$ is a locally finite, connected metric graph. Let A be a self-adjoint, nonnegative operator on $L^2(\mathcal{G})$ that satisfies the IMS formula* (2.33)*. Additionally let $f(A+i)^{-1}$ be compact for all $f \in C_c^{0,1} \cap \widetilde{C^\infty}$ then*

$$\Sigma = \inf \sigma_{ess}(A).$$

2.5 Rearrangement techniques and Sobolev inequalities on graphs

2.5.1 Decreasing and symmetric rearrangement

Let $\mathcal{G}$ be a locally finite metric graph. In this section we introduce rearrangement techniques on metric graphs. For intervals our main references are [Kaw85] and [Duf67].

Definition 2.5.1. Given $u \in H^1(\mathcal{G})$ with $u \geq 0$ we define the distribution function

$$\rho(t) = |\{x \in \mathcal{G} | u(x) > t\}|$$

for $t \geq 0$. Furthermore, we define

- the decreasing rearrangement $u^* : H^1(\mathcal{G}) \to H^1(I^*)$ with $I^* = (0, |\mathcal{G}|)$ via

$$u^*(x) = \inf\{t \geq 0 | \rho(t) \leq x\}, \quad x \in I^*;$$

- the symmetric rearrangement $\widehat{u} : H^1(\mathcal{G}) \to H^1(\widehat{I})$ with $\widehat{I} = (-\frac{|\mathcal{G}|}{2}, \frac{|\mathcal{G}|}{2})$ via

$$\widehat{u}(x) = \inf\{t \geq 0 | \rho(t) \leq 2|x|\}, \quad x \in \widehat{I}.$$

Let us briefly in heuristic terms explain what these rearrangement do – u^* is a monotonically decreasing function each of whose sublevel sets has the same total length as the corresponding sublevel set of u and $\widehat{u}(x) = u^*(\frac{|x|}{2})$ be definition.

Definition 2.5.2. Given a function $u \in H^1(\mathcal{G}) \cap C(\mathcal{G})$ we define the number of preimages

$$N(t) = \#\{x \in \mathcal{G} | u(x) = t\}$$

for $t \in \mathrm{im}(u)$.

The following results are well known for intervals, and the statements in fact transfer to graphs with no major complications:

Lemma 2.5.3. *Let $\mathcal{G}$ be a locally finite metric graph and $\alpha \in (0, 1]$. Let $u \in C^{0,\alpha}(\mathcal{G})$, then $u^*, \widehat{u} \in C^{0,\alpha}(\mathcal{G})$ and monotone.*

Proof. Monotonicity is easy to see and can be inferred by definition. Let $u_1, u_2 \geq 0$ such that $\mathrm{im}(u) = [u_1, u_2]$. To show the Hölder continuity suppose $c_1, c_2 \in \mathrm{im}(u)$ and w.l.o.g. $c_1 > c_2$, then we have

$$|c_1 - c_2| = \inf_{x \in u^{-1}(c_1), y \in u^{-1}(c_2)} |u(x) - u(y)| \leq L \inf_{x \in u^{-1}(c_1), y \in u^{-1}(c_2)} \mathrm{dist}(x, y)^\alpha$$

Then

$$\begin{aligned} |\rho(c_2) - \rho(c_1)| &= |\{x \in \mathcal{G} | c_1 \leq u(x) < c_2\}| \\ &= \int_{\{x \in \mathcal{G} | c_1 \leq u(t) < c_2\}} 1 \, \mathrm{d}t \\ &\geq \inf_{x \in u^{-1}(c_1), y \in u^{-1}(c_2)} \mathrm{dist}(x, y) \geq \frac{1}{L^{1/\alpha}} |c_1 - c_2|^{1/\alpha}. \end{aligned} \tag{2.34}$$

ρ is monotone decreasing, hence ρ^{-1} exists and

$$|y - x| \geq \frac{1}{L} |\rho^{-1}(y) - \rho^{-1}(x)|$$

By definition $u^*(x) = \rho^{-1}(x)$ for $x \in \mathrm{im}(\rho)$ and is locally constant otherwise and with (2.34) we infer $u^* \in C^{0,\alpha}(\mathcal{G})$.

Similarly $\widehat{u}(\frac{x}{2}) = \rho^{-1}(|x|)$ for $|x| \in \mathrm{im}(\rho)$ and is locally constant otherwise and we easily infer $\widehat{u} \in C^{0,\alpha}(\mathcal{G})$ as before. ☐

Proposition 2.5.4. *Let $\mathcal{G}$ be a metric graph and $p \in [1, \infty)$. Suppose $u \in L^p(\mathcal{G})$, then $u^* \in L^p(I^*), \widehat{u} \in L^p(\widehat{I})$ and*

$$\int_{I^*} |u^*(x)|^p \, \mathrm{d}x = \int_{\widehat{I}} |\widehat{u}|^p \, \mathrm{d}x = \int_{\mathcal{G}} |u|^p \, \mathrm{d}x.$$

Proof. By equimeasurability, i.e.

$$|\{x \in I^* : u^*(x) > t\}| = |\{x \in \mathcal{G} : u(x) > t\}| = |\{x \in \widehat{I} : \widehat{u}(x) > t\}| \tag{2.35}$$

for all $t \geq 0$ we have

$$|u(x)|^p = \int_0^\infty \mathbb{1}_{\{y:|u|^p>t\}}(x)\,\mathrm{d}t$$
$$|u^*(x)|^p = \int_0^\infty \mathbb{1}_{\{y:|u^*|^p>t\}}(x)\,\mathrm{d}t$$
$$|\widehat{u}(x)|^p = \int_0^\infty \mathbb{1}_{\{y:|u^*|^p>t\}}(x)\,\mathrm{d}t$$

With Cavalieri's principle and (2.35) we therefore infer

$$\int_{I^*} |u^*|^p\,\mathrm{d}x = \int_{\widehat{I}} |\widehat{u}|^p\,\mathrm{d}x = \int_{\mathcal{G}} |u|^p\,\mathrm{d}x.$$

□

Theorem 2.5.5 (Pólya–Szegő)**.** *Let $\mathcal{G}$ be a metric graph and let $1 < p < \infty$. Let $u \in W^{1,p}(\mathcal{G})$, then $u^*, \widehat{u} \in W^{1,p}(\mathcal{G})$ and the following properties hold:*

- *the decreasing rearrangement satisfies*

$$\int_0^{|\mathcal{G}|} |(u^*)'|^p\,\mathrm{d}x \leq \int_{\mathcal{G}} |u'|^p\,\mathrm{d}x$$

with strictness in the inequality if and only if there exists $N(t) \geq 2$ for some $t > 0$

- *then suppose $N(t) \geq 2$ for all $t > 0$, then*

$$\int_{-|\mathcal{G}|/2}^{|\mathcal{G}|/2} |(\widehat{u})'|^p\,\mathrm{d}x \leq \int_{\mathcal{G}} |u'|^p\,\mathrm{d}x$$

with equality if and only if $N(t) = 2$ for all $t \in \mathrm{im}(u)$.

Proof. By density it suffices to show the statement for simple functions $u \in C(\mathcal{G})$, i.e. u_e is piecewise linear for all $e \in \mathcal{E}$. Consider a partition of $\mathrm{im}(u)$ in

$$[a_1, a_2], [a_2, a_3], \ldots, [a_{M-1}, a_M]$$

with

$$a_1 < a_2 < a_3 < \cdots < a_M$$

such that for each a_i there exists $x_i \in \mathcal{G}$ such that $u(x_i) = a_i$, but the function is not extended on the particular edge by a linear function smoothly. If we define

$$D_i = \{x \in \mathcal{G} | a_i < u(x) < a_{i+1}\}, \qquad i = 1, \ldots, M-1$$

then each D_i decomposes in intervals $(Y_{i,j})$ possibly supported on different edges such that u restricted to $Y_{i,j} = [b_{i,j}, b_{i,j+1}]$ is linear and $u(Y_i) = [a_i, a_{i+1}]$. Then if $\rho_j(\lambda)$ is the unique value for which $u(\rho_j) = \lambda$ for $\lambda \in [a_i, a_{i+1}]$. Then

$$\rho^{-1}(x) = \sum_j (-\operatorname{sign} u'\big|_{Y_{i,j}})\rho_j(x) + \text{const.} \tag{2.36}$$

With Jensen's inequality we infer

$$\begin{aligned}\sum_j \int_{Y_{i,j}} |u'|^p \, \mathrm{d}x &= (a_{i+1} - a_i) \sum_j \frac{|\rho_j'|}{\sum_k |\rho_k'|} \left(|\rho_j|^{-1}\right)^p \left(\sum_k |\rho_k'|\right) \\ &\geq (a_{i+1} - a_i) \left| \left(\sum_k |\rho_k'|\right)^{-1} \right|^p \left(\sum_k |\rho_k'|\right)\end{aligned}$$

Using (2.36) and $u^* = \rho^{-1}$ on D_i we compute

$$\begin{aligned}\int_{D_i} |(u^*)'|^p \, \mathrm{d}x, &= (a_{i+1} - a_i) \left| \left(\sum_k (-\operatorname{sign} u'\big|_{Y_{i,k}})\rho_k'\right)^{-1} \right|^p \left(\sum_k (-\operatorname{sign} u'\big|_{Y_{i,k}})\rho_k'\right) \\ &= (a_{i+1} - a_i) \left| \left(\sum_k |\rho_k'|\right)^{-1} \right|^p \left(\sum_k |\rho_k'|\right)\end{aligned}$$

and we deduce

$$\sum_j \int_{Y_{i,j}} |u'|^p \, \mathrm{d}x \leq \int_{D_i} |(u^*)'|^p \, \mathrm{d}x.$$

Summing over all i leads to

$$\int_{I^*} |(u^*)'|^p \, \mathrm{d}x = \sum_i \int_{D_i} |(u^*)'|^p \, \mathrm{d}x \leq \sum_{i,j} \int_{Y_{i,j}} |u'|^p \, \mathrm{d}x \leq \int_{\mathcal{G}} |u'|^p \, \mathrm{d}x$$

since u' and (u^*) are piecewise constant. The inequality is strict if and only if there exists $N(t) \geq 2$ for some $t > 0$ due to strictness in Jensen's inequality. Similarly, strictness in the inequality can be shown for $u \in W^{1,p}(\mathcal{G})$. In fact, following [Duf70, Theorem 1] supposing $N(t) \geq N$ for almost all $t \in \operatorname{im} u$ the inequality can be strengthened to

$$\int_{I^*} |(u^*)'|^p \, \mathrm{d}x \leq \int_{\mathcal{G}} \left| \frac{u'}{N} \right|^p \, \mathrm{d}x$$

and similarly we get

$$\int_{\widehat{I}} |(\widehat{u})'|^p \, \mathrm{d}x = 2^p \int_{I^*} |(u^*)'|^p \, \mathrm{d}x \leq \int_{\mathcal{G}} \frac{2}{N} \left|u'\right|^p \, \mathrm{d}x \leq \int_{\mathcal{G}} \left|u'\right|^p \, \mathrm{d}x$$

and the inequality is strict if $N(t) > 2$ for any $t > 0$.

□

2.5.2 Gagliardo–Nirenberg and Sobolev inequalities

Gagliardo–Nirenberg inequalities on metric graphs were discussed also in [AST15] for finite metric graphs, we will need an adapted version here:

Proposition 2.5.6 (Gagliardo–Nirenberg inequality)**.** *Let $\mathcal{G}$ be a locally finite, connected metric graph and $M \in C(\mathcal{G})$. For $p \in [2, \infty)$ there exists a constant $C > 0$ independent of M such that*

$$\|u\|_p^p \leq C \left\| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right\|_2^{\frac{p-2}{2}} \|u\|_2^{\frac{p+2}{2}}, \tag{2.37}$$

for all $u \in H^1(\mathcal{G})$.

Proof. Suppose $\mathcal{G}$ is a tree graph at first. Then using the unitary gauge transform $G : H^1(\mathcal{G}) \to H^1(\mathcal{G})$ (see also §3.4.4 for details) we deduce that (2.37) is equivalent to

$$\|u\|_p^p \leq C \|u'\|_2^{\frac{p-2}{2}} \|u\|_2^{\frac{p+2}{2}},$$

which can be shown via symmetrization methods as considered in [AST15]; although this was shown there for finite metric graphs, the proof can be simply adapted to locally finite ones. In particular, the constant $C > 0$ can be chosen independent of M. Cutting the graph at a discrete set of points on the metric graph, i.e. we can find a tree graph $\widetilde{\mathcal{G}}$ such that identifying a discrete set of points on the graph results in a graph isometrically isomorph to $\mathcal{G}$. Hence, there exists lifts of the norms on $H^1(\mathcal{G})$ to $H^1(\widetilde{\mathcal{G}})$ preserving the norms and (2.37) also holds for $H^1(\widetilde{\mathcal{G}})$ and the constant $C > 0$ can be chosen independent of $M \in C(\mathcal{G})$. □

Proposition 2.5.7 (Sobolev inequality)**.** *Let $\mathcal{G}$ be a locally finite, connected metric graph and $M \in C(\mathcal{G})$. Let $p \in [2, \infty]$ then there exists a constant $C > 0$ independent of M such that*

$$\|u\|_p \leq C \left(\int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 \mathrm{d}x + \int_{\mathcal{G}} |u|^2 \, \mathrm{d}x \right)^{1/2}, \tag{2.38}$$

for all $u \in H^1(\mathcal{G})$.

Proof. The aproach is similar as before, indeeed we can use the known result in absence of M and use a gauge transform to show that (2.38) holds with a constant $C > 0$ independent of the potential $M \in C(\mathcal{G})$. □

Proposition 2.5.8 (Gagliardo–Nirenberg interpolation inequalities)**.** *Let $k \in \mathbb{N}$ and $\mathcal{G}$ be a finite metric graph. Then*

$$\|u\|_p^p \leq C \|u\|_2^{\frac{(2k-1)p+2}{2k}} |u|_{H^k}^{\frac{p-2}{2k}}$$

for all $u \in H^k(\mathcal{G})$.

Proof. From the Gagliardo–Nirenberg inequality on metric graphs and Gagliardo–Nirenberg interpolation inequality on intervals we compute

$$\|u\|_p^p \le C_1 \|u\|_2^{\frac{p}{2}+1} \|u'\|_2^{\frac{p}{2}-1} \le \cdots \le C_k \, \|u\|_2^{\frac{(2k-1)p+2}{2k}} \, |u|_{H^k}^{\frac{p-2}{2k}}.$$

□

Consider the norm on $H^k(\mathcal{G})$ defined as

$$|u|_{H^k} := \left(\int_{\mathcal{G}} |u^{(k)}|^2 + |u|^2 \,\mathrm{d}x \right)^{1/2}.$$

Then due to the Gagliardo–Nirenberg interpolation inequality on intervals (see e.g. [Leo17, Theorem 7.41]) applied edgewise

$$|u|_{H^k}^2 \le \|u\|_{H^k}^2 \le C |u|_{H^k}^2 \tag{2.39}$$

and we conclude that $\|\cdot\|_{H^k}$ and $|\cdot|_{H^k}$ are equivalent norms in $H^k(\mathcal{G})$.

Proposition 2.5.9. *Let* $k \in \mathbb{N}$ *and* $\mathcal{G}$ *be a finite metric graph. Then*

$$\|u\|_p^p \le C \|u\|_2^{\frac{(2k-1)p+2}{2k}} |u|_{H^k}^{\frac{p-2}{2k}}$$

for all $u \in H^k(\mathcal{G})$.

Proof. From the Gagliardo–Nirenberg inequality on metric graphs and Gagliardo–Nirenberg interpolation inequality on intervals we compute

$$\begin{aligned} \|u\|_p^p &\le C_1 \|u\|_2^{\frac{p}{2}+1} \|u'\|_2^{\frac{p}{2}-1} \\ &\le C_k \, \|u\|_2^{\frac{(2k-1)p+2}{2k}} \, |u|_{H^k}^{\frac{p-2}{2k}}. \end{aligned}$$

□

2.6 Analytic dependence of eigenvalues

The proof of the analytic dependence of the length parameter of the Laplacian on a given metric graph $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ is due to Kato's perturbation theory. For accessibility we would like to summarize the result with the following theorem. Note that the statement and proof of the following theorem is loosely based on [BKL19, Theorem 4.1], in which a similar study on analyticity of the Robin Laplacian on a domain in the real space was made.

Given a metric graph $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ we consider a rescaled operator which is isospectral to the Laplacian. Namely, $\lambda \in \mathbb{R}$ is an eigenvalue with eigenfunction $u \in H^1(\mathcal{G}(G, \mathbf{1}))$ if and only if

$$\sum_{\mathrm{e}\in E} \int_0^1 \frac{1}{\ell_e^2} u'v' - \lambda uv \,\mathrm{d}x = 0$$

for all $v \in H^1(\mathcal{G}(G, \mathbf{1}))$ and we apply the Kato theory to the operator associated to the corresponding closed form

$$a_{\mathcal{G}(G,\boldsymbol{\ell})}(u, v) := \sum_{e\in E} \int_0^1 \frac{1}{\ell_e^2} \overline{u_e'} v_e' \,\mathrm{d}x$$
$$\mathfrak{D}(a_{\mathcal{G}(G,\boldsymbol{\ell})}) := H^1(\mathcal{G}(G, \mathbf{1})).$$

Hence, the form domain is independent of length parameter and we may apply Kato's theory [Kat13, Chapter VII, §4] as we shall lay out below.

Since $a_{\mathcal{G}(G,\boldsymbol{\ell})} : H^1(\mathcal{G}(G, \boldsymbol{\ell})) \times H^1(\mathcal{G}(G, \boldsymbol{\ell})) \to \mathbb{R}$ is a bounded symmetric form. Consider the weak formulation of the eigenvalue problem associated to the (1.15), i.e. λ is an eigenvalue if and only if

$$a_{\mathcal{G}(G,\boldsymbol{\ell})}(u, v) = \lambda \langle u, v \rangle_{L^2(\mathcal{G})}$$

for all $u, v \in H^1(\mathcal{G})$. Then the operator $-\Delta$ associated to $a_{\mathcal{G}(G,\boldsymbol{\ell}}$ has compact resolvent and the spectrum is purely discrete and there exists a sequence of eigenvalues

$$0 = \lambda_1(\mathcal{G}) < \lambda_2(\mathcal{G}) \le \cdots$$

such that $\lambda_n(\mathcal{G}) \to \infty$.

In this context, suppose $\gamma(t) : [0, 1] \to \mathbb{R}^{|E|}_{>0}$ is a locally analytic curve, then in an abuse of notation we define

$$-\Delta(t) := -\Delta_{\mathcal{G}(G,\gamma(t))}, \quad a_{G,t} := a_{\mathcal{G}(G,\gamma(t))} \tag{2.40}$$

Theorem 2.6.1. *Let $\mathcal{G}$ be a metric graph. Consider the family of sesquilinear bounded forms $a_{G,\boldsymbol{\ell}(t)}$ as defined in* (2.40). *Then*

(i) $a_{G,t}$ is a self-adjoint holomorphic family of Kato type (a), i.e. for all $u \in H^1(\mathcal{G})$

$$\overline{a_{G,t}(u, u)} = a_{G,t}(u, u).$$

(ii) Each eigenvalue $\lambda_k(t)$ can be extended to a real locally analytic function for $t \in \mathbb{R}$, and their eigenfunctions $u_k(t)$ can be chosen to form an orthonormal basis of $L^2(\mathcal{G})$.

(iii) The algebraic multiplicity of each eigenvalue is constant up to a finite number of points and at most finitely many eigenvalue branches can meet in these algebraic singularities.

Proof. We follow closely the arguments in [Kat13, Chapter VII §4]. By definition, it is immediate that $a_{G,t}(u, u)$ is locally analytic for all $t \in \mathbb{R}$. By analyticity, there exists a holmorphic extension of the associated form operator $T(\cdot) : H^1(\mathcal{G}) \to H^1(\mathcal{G})$ on a domain $[0,1] \subset D \subset \mathbb{C}$ and by construction $T(t)^* = T(\bar{t})$ for all $t \in D$. Then $T(t)$ defines a selfadjoint family of operators in the sense of Kato. In particular, by [Kat13, Chapter VII §3.1] each eigenvalue can be extended locally analytically to a function $\lambda_i(t)$ and the eigenprojectors also depend locally analytical on the parameter. As discussed in [Kat13, Chapter VII §3.1] one can then find an orthonormal basis of eigenfunctions $u_i(t)$ associated to $\lambda_i(t)$ each dependending locally analytic on t.

For the last part of the statement we give a slightly different proof. In fact, by [GS06] each eigenvalue $\lambda = k^2 > 0$ is characterized by the secular equation

$$\zeta_h(\boldsymbol{\ell}, k) := \det\left(I - S_V(\boldsymbol{\ell}, k)\right) = 0$$

such that $S_V(\boldsymbol{\ell}, k) \in \mathbb{C}^{|V|\times|V|}$ is unitary and all the entries are analytic functions. Suppose $0 \in I_0$ is a finite interval,

$$\gamma : I_0 \mapsto \mathbb{R}^{|E|}_{>0}$$

and $\lambda_i(t) > 0$ is an analytic curve such that

$$\zeta_h(\gamma(t), \sqrt{\lambda_i(t)}) = 0.$$

In particular, there exists a orthonormal basis of eigenfunctions $\widetilde{u}_i(t)$ associated to eigenvalue $\mu_i(t)$ of $S_V(\gamma(t), \sqrt{\lambda_i(t)})$ by [Kat13, Theorem 1.10] and the algebraic multiplicity of the eigenvalue of any eigenvalue of 1 for any $t \in I_0$ coincides with the algebraic multiplicity of the eigenvalue $\lambda_i(t) > 0$.

Then for any $j \in \mathbb{N}$ either

$$\frac{\partial^j}{\partial k^j}\zeta_h(\gamma(t), \sqrt{\lambda_i(t)}) \equiv 0 \tag{2.41}$$

or the set of zeroes is finite. In other words, there are at most finitely many points such that the algebraic multiplicity is unequal to j, where $j \in \mathbb{N}$ is the smallest integer such that (2.41) is not satisfied. Since the algebraic multiplicity of any eigenvalue by the spectral theory is at most finite, at most finitely many eigenvalue can meet at any such point. In particular, the number of such intersections is locally finite. □

Chapter 3

Stationary NLS ground states on metric measure spaces

In this chapter we discuss the existence of ground states for energy functionals via a general existence theory for functionals on metric measure spaces. In particular, we show existence principles for NLS type functionals, which we previously introduced in §1.3.1. In §3.2 we introduce the theory and give first examples for domains. In §3.3 we show an existence theory for ground states of general NLS type functionals with application to the stationary higher-order NLS functional on finite (noncompact) graphs. In §3.4 we conclude this chapter with some discussion on the stationary NLS functional on locally finite graphs with application on infinite tree graphs. This chapter is based on [Hof19]; however with some additions, most notably the discussion of the general existence theory applied on general NLS type functionals in §3.2. We note that one can find more discussions on the higher-order NLS energy type functional, that was considered in §3.3.2, therein.

3.1 Overview and definitions

In general, one cannot expect existence of ground states of functionals in the noncompact case via the direct method of the calculus of variations due to the lack of strongly convergent subsequences. In this context, [Lio84] invented a very effective principle based on concentration compactness for functionals defined on $\mathbb{R}^N$, where in principle strongly convergent subsequences could be reached in the compact setting. In general, the dichotomy result obtained here, but also for instance in [AST17] or [CFN17] are in the flavor of Lion's original result. Namely, due to the subadditivity of the functional for a minimizing sequence either the so called *concentration function* goes to zero or one has in fact existence of minimizers. In principal there are two strategies to retrieve strongly convergent minimizing sequences. Either to exclude the case where the concentration function goes to zero or to retrieve non-vanishing minimizing sequences by construction due to translation invariance, which in principal on general metric measure spaces might not be possible due to the lack of concept of translation invariance. In our context, we strengthen the structural setting based on spectral theoretical results that we develop to exclude that minimizing sequences vanish and infer therefore existence of minimizers to the ground state problems considered.

Let us be now more precise about the abstract setting we will consider. Let $(\mathcal{M}, d, \mu)$ be a nonempty metric measure space (see also Definition 3.2.1). Assume $p \in [1, \infty]$ and let $X(\mathcal{M}) \subset L^p(\mathcal{M})$ be a Banach space continuously and locally compactly imbedded in $L^p(\mathcal{M})$, i.e. for any precompact, connected subset K, the restriction $X(K)$ is compactly imbedded in $L^p(K)$. In the case of a metric graph $\mathcal{G}$ a prototype would be $H^1(\mathcal{G})$, but we will also apply this to higher-order Sobolev spaces $H^k(\mathcal{G})$ with $k \in \mathbb{N}$ and $H^1(\Omega)$ for an open subset $\Omega \subset \mathbb{R}^N$ with $N \in \mathbb{N}$.

In §3.2 we establish a general existence theory for constrained minimization problems for functionals of the form

$$E := \inf_{\substack{u \in X(\mathcal{M}) \\ \|u\|_{L^p}^p = 1}} E(u) \tag{3.1}$$

with $E \in C(X(\mathcal{M}), \mathbb{R})$, and $E(0) = 0$, such that the mapping

$$t \mapsto E_t := \inf_{\substack{u \in X(\mathcal{M}) \\ \|u\|_{L^p}^p = t}} E(u)$$

is continuous for $t \geq 0$. To motivate our approach, let us briefly revisit a classical method in $\mathbb{R}^N$ that has served as inspiration to obtain results on metric graphs in previous works. In general, one cannot expect existence of minimizers when $X(\mathcal{M})$ is only locally compactly imbedded into L^p due to the lack of globally strongly convergent subsequences. P.L. Lions introduced in [Lio84] a very effective dichotomy principle based on concentration compactness for functionals defined on $\mathbb{R}^N$ to tackle this major difficulty. We will make some technical assumptions (see Definition 3.2.7, and Definition 3.2.17) that guarantee a dichotomy result (Theorem 3.2.8) for the constrained minimization problem (3.1) in the flavor of Lion's original result, as has also appeared in adapted form in [AST17] and [CFN17] in specific applications. Namely, due to the subadditivity of the functional either the so called *concentration function* for a minimizing sequence tends to zero or one has in fact existence of minimizers.

In principle there are two strategies to recover strongly convergent minimizing sequences. Traditionally, one uses translation invariance to recover non-vanishing minimizing sequences from vanishing ones; however, on general metric measure spaces this is not possible. The second possibility is to exclude the case of vanishing minimizing sequences altogether by other means. Under the correct assumptions, including the structural assumption that roughly speaking $E \in C(X(\mathcal{M}), \mathbb{R})$ is of the form

$$E(u) = \frac{1}{2} a(u, u) + \text{ nonlinear perturbation },$$

where $a(\cdot,\cdot)$ is a suitable sesquilinear form, more specifically under the assumptions in §3.3, associated to some self-adjoint operator A, we draw connections to spectral theoretical quantities of A to exclude the case when minimizing sequences of (3.1) vanish. In particular, this covers the problems considered in [AST17] and [CFN17].

More specifically, we show as a consequence of Theorem 3.2.19 (see Corollary 3.2.20) that existence holds for ground state energies that satisfy the additional relation

$$E < \widetilde{E} := \lim_{n\to\infty} \inf_{\substack{u\in X(\mathcal{M}) \\ \operatorname{supp} u \subset \mathcal{M}\setminus K_n,\ \|u\|_{L^p}^p = 1}} E(u), \tag{3.2}$$

where $K_n := \{x \in \mathcal{M} \,|\, d(x, K) < n\}$ is the expanding ball around some precompact set K; this will turn out to be a generalization of (1.9). But (3.2) has a natural spectral theoretical interpretation. In fact, given a Schrödinger operator $A = -\Delta + m$ on $\mathbb{R}^N$ there exists an analogous result for the linear ground state problem. As a consequence of Persson's Theorem (see for instance [HS96, §14.4]) ground states of A exist if

$$\inf_{\substack{u\in D(A) \\ \|u\|_2^2=1}} \langle Au, u\rangle < \lim_{n\to\infty} \inf_{\substack{u\in D(A) \\ \operatorname{supp} u\subset \mathbb{R}^N\setminus K_n(0),\ \|u\|_{L^2}^2=1}} \langle Au, u\rangle, \tag{3.3}$$

which is equivalent to (1.11) (cf. §2.4.1.3). In our applications, we will use (3.3) and a perturbation argument to show (3.2) for small nonlinearities, although in some cases we can remove or specify this restriction. In this context, the IMS localization formula (see [Sig82]) and analogues for similar problems which we will develop will be useful tools (see §2.4.2.2 and §2.4.1.2). We note that unlike [AST16] the general existence principle does not rely on symmetrization techniques.

As alluded to, the functionals (1.7) and (1.10) as considered in [AST16] and [CFN17] satisfy the prerequisites of this theory (see Example 3.4.13 and Example 3.3.13). In fact, one application of the existence theory constructed in §3.2 will be to a natural generalization of (1.10), namely the higher-order stationary NLS energy functional in §3.3.2. We will also generalize existence results on the stationary NLS energy functional with magnetic potential for general locally finite graphs, using the abstract structural assumptions of the spaces considered, which main results we present in §1.3.1.

Let us now be more precise about the operators we investigate in this context. Given a metric graph $\mathcal{G}$ we define the higher-order stationary NLS energy functional

$$E^{(k)}(u) = \frac{1}{2}\int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \qquad \begin{array}{r} \mu > 0, \quad 2 < q < 4k+2, \\ m \in L^2 + L^\infty(\mathcal{G}) \end{array} \tag{3.4}$$

and consider the ground state problem

$$E^{(k)} = \inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \tag{3.5}$$

with $H^k(\mathcal{G})$ being a higher-order Sobolev space as defined in §2. When $k = 1$ the energy functional (3.4) reduces to the stationary NLS energy functional and we derive conditions for which the theory is applicable. Minimizers of (3.5) satisfy the stationary higher-order nonlinear Schrödinger equation

$$\begin{cases} (-1)^k u_e^{(2k)} + (m + \lambda)\, u_e = \mu |u_e|^{q-1} u_e, \qquad \forall e \in \mathcal{E} \\ u^{(i)} \in C(\mathcal{G}) \quad \text{for all } i \leq 2k-1 \text{ even} \qquad \textit{(Continuity)} \\ \qquad \wedge \quad \displaystyle\sum_{e : e \succ \mathsf{v}} u_e^{(k)}(\mathsf{v}) = 0 \quad \forall i \leq 2k-1 \text{ odd } \forall \mathsf{v} \in V \\ \qquad\qquad\qquad\qquad\qquad \textit{(Kirchhoff condition).} \end{cases}$$

for some Lagrange multiplier $\lambda \in \mathbb{R}$. While to the best of our knowledge this functional has not yet been considered on metric graphs, the stationary higher-order nonlinear Schrödinger equation on the real line of 4^{th} order is for instance related to traveling wave solutions of the nonlinear higher-order Schrödinger equation for the pulse envelope with higher-order dispersion as shown in [Kru19, §II]. For combinatorial locally finite metric graphs a discussion on the existence of solutions of the nonlinear higher-order Schrödinger equation of 4^{th} order was for instance considered recently in [HSZ19].

A minor difficulty in defining (3.5) is that one needs to define higher-order Sobolev spaces $H^k(\mathcal{G})$, as to date no standard way to define these spaces has emerged. We will define them in such a way that the formal Polylaplacian

$$A = (-\Delta)^k + m$$
$$D(A) = H^{2k}(\mathcal{G})$$

is a self-adjoint operator on $L^2(\mathcal{G})$ as shown in §2.3.1. We remark that the choice is not necessarily unique. A discussion of self-adjoint realizations for the Bilaplacian on metric graphs can be for instance found in [GM17].

The results in Theorem 1.3.1 and Theorem 1.3.2 are shown for metric graphs with finitely many edges, which we refer to as finite metric graphs throughout the thesis. Such graphs consist of a finite number (possibly zero) of edges of infinite length, i.e. half-lines, which we call rays, and a complement, which is compact, and which we will call the core of the graph. In [CFN17], [Cac18] such graphs are called starlike (see also Figure 3.1-left).

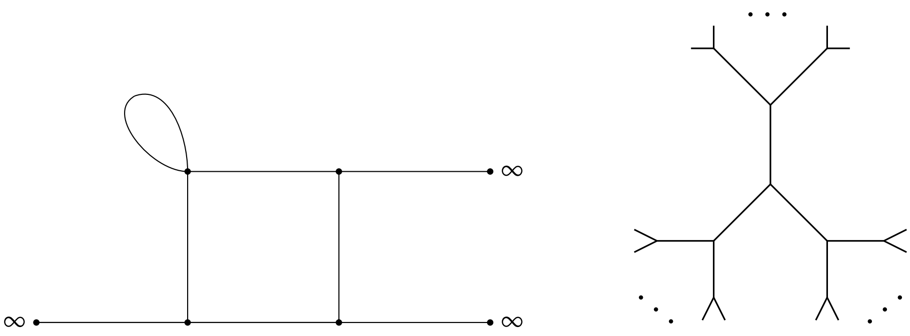


Figure 3.1: Finite vs locally finite graphs. An illustration for the classes of graphs that are considered. To the left a finite metric graph, sometimes referred to as starlike, consisting of a core graph K and attached rays and to the right an infinite tree graph as considered in Theorem 1.3.4 as an example for a locally finite metric graph, i.e. finite on any precompact set.

Our theory also allows us to handle more general graphs, however, in the case $k = 1$ (c.f. Theorem 1.3.3 in §1.3.1). It remains an open question if for the stationary higher order NLS ground state problem on locally finite graphs one can show similar existence results. If $k = 1$ the minimization problem (3.5) reduces to the existence of ground states of the stationary NLS energy functional. In fact we will consider a class of graphs with countable edge set, which is finite when restricted to any precompact subset. We will refer to such graphs as locally finite metric graphs in the following as introduced in §2.1. Moreover, to illustrate the scope of our techniques, we will consider (without much extra effort) the more general situation of a magnetic Schrödinger operator. On locally finite metric graphs we consider the following variant of the NLS energy functional

$$E_{\text{NLS}}^{(\mathcal{K})}(u) = \frac{1}{2}\int_{\mathcal{G}} \left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)u\right|^2 + m|u|^2\,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{K}} |u|^q\,\mathrm{d}x, \qquad \mu > 0, \quad 2 < q < 4k+2, \quad m \in L^2 + L^\infty(\mathcal{G}) \tag{3.6}$$

where $\mathcal{K} \subseteq \mathcal{G}$ is a subgraph of $\mathcal{G}$ and consider the ground state problem

$$E_{\text{NLS}}^{(\mathcal{K})} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = 1}} E_{\text{NLS}}^{(\mathcal{K})}(u). \tag{3.7}$$

Here we focus on the subcritical case $2 < q < 4k + 2$, but we remark that the general existence theory developed in this chapter can be also applied in the critical case $q = 4k + 2$ if (3.7) is bounded from below.

In this context, we study properties of the magnetic Schrödinger operator with potential

$$A^M = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m$$

for $M \in H^1 + W^{1,\infty}(\mathcal{G})$ and $m \in L^2 + L^\infty(\mathcal{G})$ with its natural domain of definition, which we described in detail in §2.3.

Let us finish this section by mentioning a few other recent results on related topics and that the corresponding research can be also found in [Hof19]. For a broad overview of spectral theory of operators we refer to [RS80]. We refer to [EKMN18] for a recent article on spectral theory for metric graphs with infinitely many edges. The stationary energy functional

$$\begin{aligned} E_{\mathrm{NLS}}(u,\mathcal{G}) &= \frac{1}{2}\int_{\mathcal{G}} |u'|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_{\mathcal{G}} |u|^q \,\mathrm{d}x, \qquad \|u\|_{L^2}^2 = 1, \\ E_{\mathrm{NLS}}^{(\mathcal{K})}(u,\mathcal{G}) &= \frac{1}{2}\int_{\mathcal{G}} |u'|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_{\mathcal{K}} |u|^q \,\mathrm{d}x, \qquad \|u\|_{L^2}^2 = 1, \end{aligned} \tag{3.8}$$

and the corresponding ground state problems

$$E_{\mathrm{NLS}}(\mathcal{G}) = \inf_{\substack{u\in H^1(\mathcal{G})\\ \|u\|_2^2=1}} E_{\mathrm{NLS}}(u,\mathcal{G}), \qquad E_{\mathrm{NLS}}^{(\mathcal{K})}(\mathcal{G}) = \inf_{\substack{u\in H^1(\mathcal{G})\\ \|u\|_2^2=1}} E_{\mathrm{NLS}}^{(\mathcal{K})}(u,\mathcal{G}) \tag{3.9}$$

with $\mathcal{K} = \mathcal{G}$ was considered in [ACFN12], [AST15], [AST16], [AST17] among others. A variant of the problem with localized nonlinearities in the L^2-subcritical case was considered in [Ten16] and for the L^2-critical case extended in [DT18b] and [DT18a], where the area of integration in the nonlinearity is taken to be a bounded subgraph $\mathcal{K}$. A very recent survey on results on the stationary NLS energy functional with localized nonlinearity can be found in [BCT19]. Recently, classes of graphs that do not necessarily consist of finitely many edges have also been considered. For instance, [DST19] deals with a certain class of infinite tree graphs, which fall into the category of the locally finite metric graphs that we consider here. We would also like to mention the results obtained by [AP19] for the NLS energy functional with growing potentials for a class of general metric graphs satisfying certain volume growth assumptions using a generalized Nehari approach.

3.2 A general existence theory

In this section we derive an existence theory for ground states of functionals as in (3.4) and (3.6). To do so, we derive a more general existence principle for functionals on function spaces defined on metric measure spaces, which we will apply later to the functionals introduced before to discuss the existence of minimizers. We prove a dichotomy result for minimizing sequences and discuss in this context the existence principle based on threshold energies for the stationary higher-order NLS functional.

3.2.1 Preliminaries: Metric measure spaces and Brézis–Lieb Lemma

Metric measure spaces are general objects that contain a large class of spaces such as oriented Riemannian manifolds, but are not limited to manifolds and in fact metric graphs or combinatorial graphs are not manifolds due to ramifications but are still metric measure spaces by definition:

Definition 3.2.1. A metric measure space $(\mathcal{M}, d, \mu)$ is a metric space $(\mathcal{M}, d)$ with Borel measure μ.

Then any oriented Riemannian manifold becomes a metric measure space with an intrinsic metric and induced volume form. In particular, open domains $\Omega \subset \mathbb{R}^N$ with Euclidean distance and Lebesgue measure are metric measure spaces. Metric graphs as discussed in §2.1 have a notion a distance and inherent a measure from the Lebesgue measure on the edges. In the following, we will statea useful result we will need a few times throughout this chapter:

Theorem 3.2.2 (Brézis–Lieb Lemma, [BL83])**.** *Let (Ω, Σ, μ) be a measure space and let $\{f_n\}_{n=1}^{\infty}$ be a sequence of complex values measurable functions which are uniformly bounded in $L^p = L^p(\Omega, \Sigma, \mu)$ for some $0 < p < \infty$. Suppose that $f_n \to f$ pointwise almost everywhere, then*

$$\lim_{n\to\infty} \|f_n\|_p^p - \|f_n - f\|_p^p = \|f\|_p^p$$

In the following we work with functions defined on an abstract space $X(\mathcal{M})$, namely a function space on a metric measure space $(\mathcal{M}, d, \mu)$ with the following properties:

Assumption 3.2.3. *Let $p \in [1, \infty)$. Let $(\mathcal{M}, d, \mu)$ be a metric space with a locally finite Borel measure μ on $\mathcal{M}$. Assume $X = X(\mathcal{M}) \subset L^p(\mathcal{M})$ is a nontrivial Banach function space continuously and locally compactly imbedded in $L^p(\mathcal{M})$, i.e. $\mathcal{M}$ restricted to*

$$K_R(y) := \{x \in \mathcal{M} |\, \mathrm{dist}(x, y) \leq R\}$$

is compactly imbedded in $L^p(K_R(y))$ for all $R > 0$ and $y \in \mathcal{M}$.

Remark 3.2.4. Our prototype to satisfy Assumption 3.2.3 is $X(\mathcal{G}) = H^1(\mathcal{G})$ where $\mathcal{G}$ is a connected, locally finite metric graph. However, it is for instance also satisfied by $X(\Omega) = H^1(\Omega)$ for a bounded domain $\Omega \subset \mathbb{R}^N$ with $N \in \mathbb{N}$.

If the underlying function space of our functional satisfies Assumption 3.2.3 the following is a known consequence:

Corollary 3.2.5. *Suppose $(\mathcal{M}, d, \mu)$ be a metric measure space and $X(\mathcal{M})$ be a function space satisfying Assumption 3.2.3. Suppose f_n is a bounded sequence in $X(\mathcal{M})$, then there exists $f \in L^p(\mathcal{M})$, such that up to a subsequence $f_n \to f$ a.e. and*

$$\lim_{n\to\infty} \|f_n\|_p^p - \|f_n - f\|_p^p = \|f\|_p^p$$

Proof. By continuous imbedding f_n is a bounded sequence $L^p(\mathcal{M})$ and by locally compact imbedding there exists a subsequence $f_n \to f$ in $L^p_{\mathrm{loc}}(\mathcal{M})$ and in particular we can find a subsequence such that $f_n \to f$ almost everywhere. The statement is then a consequence of Theorem 3.2.2. $\square$

Let us conclude the prelimary section with a similar result for Hilbert spaces H.

Proposition 3.2.6. *Let H be a Hilbert space with scalar product $\langle\cdot,\cdot,\rangle$ and norm $\|\cdot\| = \sqrt{\langle\cdot,\cdot\rangle}$. Suppose $f_n \rightharpoonup f$ weakly in H, then*

$$\lim_{n\to\infty} \|f_n\|^2 - \|f_n - f\|^2 = \|f\|^2$$

Proof. By weak convergence $\langle f_n, f\rangle \to \|f\|^2$ as $n \to \infty$ and by definition

$$\|f_n\|^2 - \|f_n - f\|^2 = 2\Re\langle f_n, f\rangle - \|f\|^2 \to \|f\|^2 \qquad (n \to \infty).$$

□

3.2.2 A dichotomy result

We consider the constrained minimization problem

$$E := \inf_{\substack{u\in X(\mathcal{M})\\ \|u\|_p^p=1}} E(u)$$

for a functional $E \in C(X(\mathcal{M}), \mathbb{R})$ satisfying the following technical properties:

Definition 3.2.7. Let $p \geq 2$ and let $\mathcal{M}$ and $X = X(\mathcal{M})$ be as in Assumption 3.2.3. Let $E \in C(X(\mathcal{M}), \mathbb{R})$ such that $E(0) = 0$ and

$$E_t := \inf_{\substack{u\in X(\mathcal{M})\\ \|u\|_p^p=t}} E(u) > -\infty$$

for any $t \geq 0$ and $E(0) = 0$. We say:

(1) $t \mapsto E_t$ is *strictly subadditive* if

$$E_1 < E_t + E_{1-t}, \qquad \forall t \in (0, 1).$$

(2) E is *weak limit superadditive* in X if for all $c > 0$ any weakly convergent minimizing sequence $u_n \rightharpoonup u$ in $X(\mathcal{M})$ of E_c satisfies

$$\limsup_{n\to\infty} E(u_n) \geq E(u) + \limsup_{n\to\infty} E(u_n - u).$$

up to a subsequence.

Theorem 3.2.8. *Let $p \in [2, \infty)$, and let $\mathcal{M}$, $X = X(\mathcal{M})$ be as in Assumption 3.2.3. Let*

$E \in C(X(\mathcal{M}), \mathbb{R})$ *be a weak limit superadditive functional in* X. *Let*

$$t \mapsto E_t = \inf_{\substack{u \in X(\mathcal{M}) \\ \|u\|_p^p = t}} E(u)$$

be a strictly subadditive, continuous function of $t \in [0,1]$. *Let* u_n *be a minimizing sequence of* E, *and assume there exists* $u \in X$ *such that up to a subsequence* $u_n \rightharpoonup u$ *weakly in* X. *Then either* $u \equiv 0$, *or* $u_n \to u$ *strongly in* $L^p(\mathcal{M})$ *and* $u \not\equiv 0$ *is a minimizer.*

Remark 3.2.9. Theorem 3.2.8 gives rise to a dichotomy. If the requirements of Theorem 3.2.8 are satisfied, then a minimizing sequence satisfies either $u_n \rightharpoonup 0$ in X or there exists a strongly L^p convergent subsequence converging to a minimizer of E. In case a minimizing sequence does not strongly converge towards a minimizer of E from $u_n \rightharpoonup 0$ in $X(\mathcal{M})$ we infer $\|u_n\|_{L^p(K)} \to 0$ on any bounded subset K of $\mathcal{M}$. In particular, since $\|u_n\|_p^p = 1$ for all $n \in \mathbb{N}$ the mass needs to move outside any compact set.

Definition 3.2.10. In virtue of Theorem 3.2.8 we say a minimizing sequence of E is *vanishing* if $u_n \rightharpoonup 0$ in X and *non-vanishing* otherwise.

Proof of Theorem 3.2.8. Suppose $u_n \in X(\mathcal{M})$ be a minimizing sequence of E. Let $u \in X(\mathcal{M})$, such that $u_n \rightharpoonup u$ weakly in X with $u \neq 0$. Then since $u_n \to u$ in L^p_{loc} we deduce $u \neq 0$ and

$$1 \geq \|u\|_p^p > 0.$$

Up to a subsequence $u_n \to u$ pointwise almost everywhere, and from Theorem 3.2.2,the Brézis–Lieb Lemma, we conclude

$$\|u\|_p^p + \limsup_{n\to\infty} \|u_n - u\|_p^p = 1.$$

By weak limit superadditivity, strict subadditivity, and continuity of $t \mapsto E_t$ we deduce that up to a subsequence

$$\begin{aligned} E_c &\geq E(u) + \limsup_{n\to\infty} E(u - u_n) \\ &\geq E_{\|u\|_p^p} + \limsup_{n\to\infty} E_{\|u-u_n\|_p^p} \\ &\geq E_{\|u\|_p^p} + E_{\limsup_{n\to\infty} \|u_n - u\|_p^p} \geq E_1. \end{aligned}$$

where equality is only attained when $\|u\|_p^p = 1$ and $\limsup_{n\to\infty} \|u_n - u\|_p^p = 0$. Thus $\|u\|_p^p = c$ and we conclude

$$E_c = E(u)$$

and u is a minimizer of E. $\square$

Example 3.2.11 (Subcritical NLS ground states). Let $N \in \mathbb{N}$. Suppose $\Omega \subset \mathbb{R}^N$ is a connected, unbounded, open set, then with the Euclidean metric d and Lebesgue measure $\mathrm{d}x$ the triple

$(\Omega, d, \mathrm{d}x)$ defines a metric measure space. For every precompact open set $K \subset \Omega$ the Rellich–Kondrachov theorem asserts that $H^1(K)$ compactly imbeds in $L^p(K)$ for $1 \le p < p^*$ with

$$p^* := \frac{np}{n-p}.$$

If $N = 1, 2$ we have $p^* = \infty$ and $H^1(K)$ compactly imbeds to $L^p(K)$ for all $1 \le p < \infty$. In particular, Assumption 3.2.3 is satisfied for $1 \le p < p^*$.

Consider the NLS energy functional

$$E_{\text{NLS}}(u) := \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_\Omega |u|^q \,\mathrm{d}x$$
$$D(E_{\text{NLS}}) := \{u \in H_0^1(\Omega) | \|u\|_2^2 = 1\}$$

for $\mu > 0$ and $2 < q < 2 + \frac{4}{N}$. We are going to demonstrate in the following that this functional satisfies continuity, subadditivity and weak superadditivity and that Theorem 3.2.8 is in fact applicable.

With the Gagliardo–Nirenberg inequality we have

$$\|u\|_q^q \le \|u\|_2^\alpha \|u\|_{H^1}^{1-\alpha}$$

for $\alpha = \frac{N(q-2)}{2q}$. Hence for sufficiently small $\varepsilon > 0$ there exists $C_\varepsilon > 0$ such that

$$E_{\text{NLS}}(u) \ge \left(\frac{1}{2} - \varepsilon\right)\int_\Omega |u'|^2 \,\mathrm{d}x - C_\varepsilon \ge -C_\varepsilon$$

and E_{NLS} is bounded below.

Define

$$t \mapsto E_t := \inf_{\substack{u \in H_0^1(\Omega) \\ \|u\|_2^2 = t}} E_{\text{NLS}}(u),$$

then since $t \mapsto E(t^{1/2}u)$ is concave for each fixed $u \in D(E_{\text{NLS}})$ and $t \in (0,1)$, we deduce

$$E_{\text{NLS}}(t^{1/2}u) \le tE_{\text{NLS}}(u)$$

and hence $E_t \le tE_1$. For a contradiction, suppose $E_t = tE_1$ for some $t \in (0,1)$, then we have

$$E_t = t \inf_{u \in D(E_{\text{NLS}})} \frac{1}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x - t^{\frac{q-2}{2}} \frac{\mu}{q}\int_\Omega |u|^q \,\mathrm{d}x. \tag{3.10}$$

Let $u_n \in D(E_{\text{NLS}})$ be such that $E_{\text{NLS}}(u_n) \to E_1$. With (3.10) we deduce

$$\int_\Omega |u_n|^q \,\mathrm{d}x \to 0$$

since otherwise

$$E_t \leq \lim_{n\to\infty} E_{\text{NLS}}(t^{1/2}u_n) < \lim_{n\to\infty} tE_{\text{NLS}}(u_n) = tE_1.$$

In particular, we infer $E_1 \geq 0$. Then E_t is strictly subadditive if the ground state energy is negative, i.e.

$$E_1 = \min_{u\in D(E_{NLS})} E_{\text{NLS}}(u) < 0,$$

since $E_t < tE_1$ and we have

$$E_t + E_{1-t} < E_1.$$

In fact, for sufficiently large $\mu > 0$ this condition is always satisfied by a test function argument. In fact, suppose $\varphi \in C_c^\infty(\Omega)$ with $\|\varphi\|_2^2 = 1$, then for sufficiently big $\mu > 0$ we have

$$E_1 \leq \frac{1}{2}\int_\Omega |\nabla\varphi|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_\Omega |\varphi|^q \,\mathrm{d}x < 0.$$

We remark, that in fact $t \mapsto E_t$ is concave as the infimum of concave functions and therefore in particular continuous. The weak superadditivity is then an immediate consequence of Corollary 3.2.5 and Proposition 3.2.6. In fact, there exists then a subsequence such that

$$\begin{aligned}\lim_{n\to\infty} \|u_n\|_{H^1}^2 &= \|u\|^2 + \lim_{n\to\infty} \|u-u_n\|_{H^1}^2\\ \lim_{n\to\infty} \|u_n\|_q^q &= \|u\|_q^q + \lim_{n\to\infty} \|u-u_n\|_q^q\end{aligned}$$

and we have

$$\lim_{n\to\infty} E(u_n) = E(u) + \lim_{n\to\infty} E(u-u_n)$$

for a subsequence of u_n.

Example 3.2.12 (NLS with potential)**.** Suppose $m \in L^{\frac{2^*}{2^*-2}} + L^\infty(\Omega)$, then the NLS energy functional with potential is defined via

$$\begin{aligned}E_{\text{NLS}}^m(u) &:= \frac{1}{2}\int_\Omega |\nabla u|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_\Omega |u|^q \,\mathrm{d}x\\ D(E_{\text{NLS}}^m) &:= \{u \in H_0^1(\Omega) | \|u\|_2^2 = 1\}\end{aligned}$$

for $\mu > 0$ and $2 < q < 2 + \frac{4}{N}$. Suppose $m = m_1 + m_2$ with $m_1 \in L^{\frac{2^*}{2^*-2}}(\Omega)$ and $m_2 \in L^\infty(\Omega)$ such that $\|m_1\|_{\frac{2^*}{2^*-2}} < \varepsilon$ with $\varepsilon > 0$ sufficiently small. With the Hölder inequality we compute

$$\begin{aligned}\left|\int_\Omega m|u|^2 \,\mathrm{d}x\right| &\leq \|m_1\|_{L^{\frac{2^*}{2^*-2}}} \|u\|_{L^{2^*}}^2 + \|m_2\|_{L^\infty}\|u\|_{L^2}^2\\ &\leq C(\Omega)\varepsilon\|u\|_{H^1}^2 + \|m_2\|_{L^\infty}\|u\|_{L^2}^2.\end{aligned}$$

Then as in Example 3.2.11 we infer that E_{NLS}^m is bounded below and as in Example 3.2.11 we infer that

$$t \mapsto E_t^m := \inf_{\substack{u \in H_0^1(\Omega) \\ \|u\|_2^2 = t}} E_{\mathrm{NLS}}(u)$$

is strictly subadditive, if

$$E_1^m < \inf_{u \in D(E_{\mathrm{NLS}})} \frac{1}{2} \int_\Omega |\nabla u|^2 + m|u|^2 \, \mathrm{d}x,$$

which is satisfied for sufficiently large $\mu > 0$. In fact, by the same arguments as in Example 3.2.11 we also can infer continuity and weak limit superadditivity and Theorem 3.2.8 is applicable.

3.2.3 Vanishing sequences and threshold energies

As in the previous subsection we consider $\mathcal{M}$ to be a metric measure space and $X(\mathcal{M}) \subset L^p(\mathcal{M})$ to be a function space which is locally compactly imbedded in $L^p(\mathcal{M})$. In the following we want to introduce partitions of unity and therefore assume the following:

Assumption 3.2.13. *Let $(\mathcal{M}, d)$ be a metric space with locally finite Borel measure μ on $\mathcal{M}$ and $X(\mathcal{M})$ as in Assumption 3.2.3. Then we assume $Y(\mathcal{M})$ to be a set of μ measurable functions on $\mathcal{M}$ such that $X(\mathcal{M})$ is invariant with respect to multiplication of elements in $Y(\mathcal{M})$.*

Remark 3.2.14. For our prototype $X(\mathcal{M}) = H^1(\mathcal{G})$, then $Y(\mathcal{M}) = W^{1,\infty}(\mathcal{G})$ would be an example to satisfy Assumption 3.2.13 and we refer to the more detailed example in Example 3.2.18.

In this section we show that the existence of vanishing sequences gives a bound from below on the ground state energy E_c, which allows us, under stronger assumptions, to deduce an existence result from Theorem 3.2.8.

Definition 3.2.15. Let $Y(\mathcal{M})$ be as in Assumption 3.2.13. Assume $\cup_{O \in \mathcal{O}} O = \mathcal{G}$ is a locally finite open covering $\mathcal{O}$ of $\mathcal{M}$. Then we say a family of nonnegative functions $\psi_O \in Y(\mathcal{G})$ is a partition of unity subordinate to $\mathcal{O}$ if

$$\operatorname{supp} \psi_O \subset O, \quad \forall O \in \mathcal{O} \quad \wedge \quad \bigcup_{O \in \mathcal{O}} \operatorname{supp} \psi_O = \mathcal{G} \quad \wedge \quad 0 \le \psi_O \le 1$$

and $\sum_{O \in \mathcal{O}} \psi_O(x) \neq 0$ for all $x \in \mathcal{M}$ and

$$\Psi_O(x) = 1, \qquad \forall x \in \operatorname{supp} \Psi_O \setminus \bigcup_{\widehat{O} \in \mathcal{O} \setminus \{O\}} \operatorname{supp} \Psi_{\widehat{O}}.$$

Given a vanishing sequence, the following property of a functional characterizes decomposability with regards to sequences of partition of unity with increasing core, namely given an arbitrary precompact subset K of $\mathcal{M}$, which we refer to as the core, we define the expanding set

K_R for $R > 0$ analogously to (2.23) via

$$K_R := \{x \in \mathcal{G} | \operatorname{dist}(x, K) < R\}. \tag{3.11}$$

Definition 3.2.16. Let $k \in \mathbb{N}$ and let $\mathcal{M}$ be a metric space. Let K be a bounded subset of $\mathcal{M}$ and K_n be defined by (3.11) for $n \in \mathbb{N}$. We say a sequence of open coverings $\mathcal{O}_n = \{O_n^{(1)}, \dots, O_n^{(k)}\}$ consisting of k open subsets (not necessarily connected) is *vanishing-compatible*, if

$$K_n \cap O_n^{(i)} = \emptyset, \qquad \forall i \in \{2, \dots, k\}$$

and $O_n^{(1)}$ is bounded for all n.

In particular, $K_n \subset O_n^{(1)}$. That is, for a sequence of open coverings $\mathcal{O}_n = \{O_n^{(1)}, \dots, O_n^{(k)}\}$ all its members except $O_n^{(1)}$ move away from K. Furthermore, this notion does not depend on the choice of K, i.e. up to a subsequence any sequence of open coverings is vanishing-compatible for any other K, since $\{K_n\}_{n\in\mathbb{N}}$ defines an open covering of $\mathcal{M}$.

Definition 3.2.17. Let $k \in \mathbb{N}$ and $\mathcal{O}_n = \{O_n^{(1)}, \dots, O_n^{(k)}\}$ be a vanishing-compatible sequence of open coverings. Then we say $E \in C(X(\mathcal{M}), \mathbb{R})$ is k-superadditive with respect to a fixed sequence of partitions of unity

$$\{\psi_O\}_{O\in\mathcal{O}_n} = \left\{\psi_{O_n^{(1)}}, \dots, \psi_{O_n^{(k)}}\right\}$$

if for any vanishing sequence (v_n), there exists a subsequence (keeping the indices by abuse of notation), such that

$$\limsup_{n\to\infty} E(v_n) \geq \sum_{i=1}^{k} \limsup_{n\to\infty} E(\psi_{O_n^{(i)}} v_n).$$

Given a fixed sequence of vanishing-compatible partitions of unity a functional may or may not satisfy this property. In other words, we need to construct a suitable sequence based on the problem. Let us consider the case on domains:

Example 3.2.18. Let $n \in \mathbb{N}$ and $N \in \mathbb{N}$. Suppose $\Omega \subset \mathbb{R}^N$ is a connected, unbounded, open set, then with the Euclidean metric d and Lebesgue measure $\mathrm{d}x$ the triple $(\Omega, d, \mathrm{d}x)$ defines a metric measure space. If $X(\Omega) = H_0^k(\Omega)$ and $Y(\Omega) = W^{k,\infty}(\Omega)$, then $X(\Omega)$ is invariant by multiplication of elements in $Y(\Omega)$. In fact, for $f \in H^1(\Omega)$ and $g \in W^{1,\infty}(\Omega)$ by the product rule we have $fg \in H^1(\Omega)$ and

$$\nabla(fg) = (\nabla f)g + (\nabla g)f.$$

Let $\Psi \in C^\infty(\mathbb{R})$ with $\operatorname{supp} \Psi \subset [-2, 2]$, such that $0 \leq \Psi \leq 1$ and $\Psi \equiv 1$ on $[-1, 1]$. Consider the open covering $\mathcal{O}$ defined by $K_{2n}(0), \Omega \setminus K_n(0)$, then we can define a partition of unity subordinate to $\mathcal{O}$ given by

$$\Psi_n(x) := \Psi\left(\frac{\|x\|}{n}\right), \qquad \widehat{\Psi}_n := 1 - \Psi_n$$

and by construction $\Psi_n + \widehat{\Psi}_n \equiv 1$.

Recall the stationary NLS energy functional in Example 3.2.12

$$\begin{aligned} E^m_{\mathrm{NLS}}(u) &:= \frac{1}{2}\int_\Omega |\nabla u|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{q}\int_\Omega |u|^q \,\mathrm{d}x \\ D(E^m_{\mathrm{NLS}}) &:= \{u \in H^1_0(\Omega) | \|u\|_2^2 = 1\} \end{aligned}$$

with $m \in L^{\frac{2^*}{2^*-2}} + L^\infty(\Omega)$ and $2 < q < 4 + \frac{2}{N}$ as in Example 3.2.12. We consider the ground state problem

$$E^m_{\mathrm{NLS}} = \inf_{u \in D(E^m_{\mathrm{NLS}}} E^m_{\mathrm{NLS}}(u).$$

Let us show that E^m_{NLS} satisfies superadditivity with respect to a vanishing-compatible sequence of partitions of unity.

Suppose $u_n \in C_c^\infty(\Omega)$ is a vanishing sequence, then there exists a subsequence, still denoted by u_n with abuse of notation, such that

$$\int_{K_{2n}} |u_n|^q \to 0 \qquad (n \to \infty). \tag{3.12}$$

Then the IMS formula (c.f. (2.33)) states that

$$\begin{aligned} (-\Delta + m)\, u = {} & \frac{\Psi_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} (-\Delta + m) \frac{\Psi_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} u \\ & + \frac{\overline{\Psi}_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} (-\Delta + m) \frac{\overline{\Psi}_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} \\ & + \left| \frac{\mathrm{d}}{\mathrm{d}x} \frac{\Psi_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} \right|^2 u + \left| \frac{\mathrm{d}}{\mathrm{d}x} \frac{\overline{\Psi}_k}{\sqrt{\Psi_k^2 + \widehat{\Psi}_k^2}} \right|^2 u \end{aligned}$$

For all $u \in C_c^\infty(\Omega)$ we compute with integration by parts

$$E^m_{\mathrm{NLS}}(u) = \frac{1}{2}\langle(-\Delta + m)\, u, u\rangle_{L^2} - \frac{\mu}{q}\|u\|_q^q. \tag{3.13}$$

In particular, with (3.12) and (3.13) we have

$$\lim_{n\to\infty} E^m_{\mathrm{NLS}}(u_n) = \lim_{n\to\infty} E^m_{\mathrm{NLS}}\left(\frac{\Psi_n}{\sqrt{\Psi_n^2 + \overline{\Psi}_n^2}} u_n\right) + \lim_{n\to\infty} E^m_{\mathrm{NLS}}\left(\frac{\overline{\Psi}_n}{\sqrt{\Psi_n^2 + \overline{\Psi}_n^2}} u_n\right)$$

and the functional E^m_{NLS} is superadditive with respect to a vanishing compatible sequence of partitions of unity.

This gives rise to our second main result:

Theorem 3.2.19. *Let $p \in [2,\infty)$, and let $(\mathcal{M},\mu)$, $X(\mathcal{M})$ and $Y(\mathcal{M})$ satisfy Assumption 3.2.3 and Assumption 3.2.13. Let K be a bounded, connected, nonempty set in $\mathcal{M}$. Let $E \in C(X(\mathcal{M}),\mathbb{R})$, such that*

$$t \mapsto E_t = \inf_{\substack{u\in X(\mathcal{M})\\ \|u\|_p^p=t}} E(u)$$

is continuous and assume E to be 2-superadditive with respect to a sequence of partitions of unity $\{\psi_O\}_{O\in\mathcal{O}_n}$ in $Y(\mathcal{M})$ subordinate to a vanishing-compatible sequence of open coverings $\mathcal{O}_n = (O_1^{(n)}, O_2^{(n)})$. If there exists a minimizing sequence which is vanishing, then

$$E = \lim_{R\to\infty} \inf_{\substack{u\in X(\mathcal{M}),\|u\|_p^p=1\\ \operatorname{supp} u\subset\mathcal{M}\setminus K_R}} E(u) =: \widetilde{E}.$$

Proof. Let u_n be a vanishing sequence. Assume $(O_n^{(1)}, O_n^{(2)})$ to be such that

$$K \subset O_n^{(1)}$$

and $O_n^{(1)}$ is bounded.

For each fixed $m \in \mathbb{N}$ we have

$$\int_{O_m^{(1)}} |u_n|^p \,\mathrm{d}\mu \to 0 \qquad (n\to\infty).$$

Then for any $m \in \mathbb{N}$ we find an n_m, such that for $n > n_m$

$$\int_{O_m^{(1)}} |u_n|^p \,\mathrm{d}\mu \le \frac{1}{m}.$$

Using a diagonal argument we deduce the existence of a subsequence of u_n, still denoted by u_n, such that

$$\int_{O_n^{(1)}} |u_n|^p \,\mathrm{d}\mu \to 0 \qquad (n\to\infty).$$

In particular,

$$0 \le \int_{O_n^{(1)}} |\psi_{O_n^{(1)}} u_n|^p \,\mathrm{d}\mu \le \int_{O_n^{(1)}} |u_n|^p \,\mathrm{d}\mu$$

$$c - \int_{O_n^{(1)}} |u_n|^p \,\mathrm{d}\mu \le \int_{O_n^{(2)}} |\psi_{O_n^{(2)}} u_n|^p \,\mathrm{d}\mu \le \int_{\mathcal{M}} |u_n|^p \,\mathrm{d}\mu = 1$$

and we obtain

$$\int_{O_n^{(1)}} |\psi_{O_n^{(1)}} u_n|^p \, \mathrm{d}\mu \to 0 \qquad (n \to \infty)$$
$$\int_{O_n^{(2)}} |\psi_{O_n^{(2)}} u_n|^p \, \mathrm{d}\mu \to 1 \qquad (n \to \infty).$$

Then by superadditivity we have

$$\begin{aligned} E_c &= \lim_{n\to\infty} E(u_n) \\ &\geq \limsup_{n\to\infty} E\left(\psi_{O_n^{(2)}} u_n\right) \geq \widetilde{E}. \end{aligned}$$

This concludes the inequality $E \geq \widetilde{E}$. The reverse inequality is trivial since

$$E \leq \inf_{\substack{u \in X(\mathcal{M}), \|u\|_p^p = 1 \\ \operatorname{supp} u \subset \mathcal{M} \setminus K_R}} E(u)$$

for all $R > 0$. □

Corollary 3.2.20. *Suppose the assumptions in Theorem 3.2.8 and Theorem 3.2.19 are satisfied and*

$$E < \widetilde{E},$$

then a minimizer of E exists, and any minimizing sequence for E admits a subsequence converging in L^p towards a minimizer of E.

Given a functional $E \in C(X(\mathcal{M}), \mathbb{R})$ defined on a function space on a metric measure space $(\mathcal{M}, d, \mu)$, we define the corresponding threshold energy

$$\widetilde{E} := \lim_{R\to\infty} \inf_{\substack{u \in X(\mathcal{M}),\, \|u\|_p^p = 1 \\ \operatorname{supp} u \subset \mathcal{M} \setminus K_R}} E(u). \tag{3.14}$$

Remark 3.2.21. In the case of many-body quantum particle systems, a quantity similar to (3.14) refers to the ionization energy (see [Gri04] and [Sim83]), namely the quantity that characterizes the bottom of the essential spectrum of Schrödinger operators associated to many-body quantum particles in the Persson theory (c.f. §2.4). Similarly, existence of bounded ground states can be inferred for measured energies below these theoretical thresholds.

Example 3.2.22. Let $N \in \mathbb{N}$. Suppose $\Omega \subset \mathbb{R}^N$ is an open, unbounded domain. Recall the stationary NLS energy functional in Example 3.2.12

$$\begin{aligned} E^m_{\mathrm{NLS}}(u) &:= \frac{1}{2} \int_\Omega |\nabla u|^2 + m|u|^2 \, \mathrm{d}x - \frac{\mu}{q} \int_\Omega |u|^q \, \mathrm{d}x \\ D(E^m_{\mathrm{NLS}}) &:= \{u \in H^1_0(\Omega) | \|u\|_2^2 = 1\} \end{aligned}$$

with $m \in L^{\frac{2^*}{2^*-2}} + L^\infty(\Omega)$ and $2 < q < 4 + \frac{2}{N}$ as in Example 3.2.12. We consider the ground state problem

$$E^m_{\text{NLS}} = \inf_{u \in D(E^m_{\text{NLS}}} E^m_{\text{NLS}}(u).$$

We already showed that E^m_{NLS} satisfies the preqrequisites of Theorem 3.2.8 in Example 3.2.12 and by Example 3.2.18 also the prerequisites of Theorem 3.2.19 are satisfied.Suppose $m \in L^{2^*} + L^\infty(\Omega)$ is a decaying potential, i.e. $\sup_{|x|\geq R} |m_\infty| \to 0$ as $R \to \infty$, then

$$\widetilde{E^m_{\text{NLS}}} = \widetilde{E^0_{\text{NLS}}} \geq E_{\text{NLS}}$$

and with Corollary 3.2.20 we deduce existence of minimizers if

$$E^m_{\text{NLS}} < E_{\text{NLS}}.$$

Suppose $\Omega = \mathbb{R}^N$. Then, by a translation argument, we can further characterize the threshold energy. In fact, using the Polya-Szego Theorem (c.f. Theorem 2.5.5) we can show

$$\widetilde{E^0_{\text{NLS}}} \geq E_{\text{NLS}}(\mathbb{R}^N),$$

where

$$E_{\text{NLS}}(\mathbb{R}^N) = \inf_{\substack{u \in H^1(\mathbb{R}^N) \\ \|u\|_{L^2}}} \frac{1}{2} \int_{\mathbb{R}^N} |\nabla u|^2 \,\mathrm{d}x - \frac{\mu}{q} \int_{\mathbb{R}^N} |u|^q \,\mathrm{d}x. \tag{3.15}$$

3.2.4 An existence result for translation invariant functionals on strip type spaces

In this section we are going to study general translation invariant functionals defined on function spaces $X(\mathcal{M})$ satisfying Assumption 3.2.3 on strip type spaces, that in principle could be extended to other types of translation invariances (c.f. Remark 3.2.26), which we define as follows

Definition 3.2.23. We say $(\mathcal{M}, d, \mu)$ is a strip type metric measure space, if there exists a measure space $(\mathcal{M}', \mathrm{d}y)$ such that

$$\mathcal{M} = \mathbb{R} \times \mathcal{M}'$$
$$\mu = \mathrm{d}x \otimes \mathrm{d}y$$

where $I \times \mathcal{M}' \subset \mathcal{M}$ is precompact for each finite interval $I \subset \mathbb{R}$ and $\mathrm{d}x$ is the Lebesgue measure.

Theorem 3.2.24. *Let $p \in [2, \infty)$, $c > 0$, and $\mathcal{M} = \mathbb{R} \times \mathcal{M}'$ be a strip type metric measure space and satisfy Assumption 3.2.3 and Assumption 3.2.13. Suppose $E \in C(X(\mathcal{M}), \mathbb{R})$ is translation invariant, i.e. if $T_\lambda u(x, y) = u(x - \lambda, y)$ then*

$$E(u) = E(T_\lambda u)$$

for all $\lambda \in \mathbb{R}$. *Let*

$$t \mapsto E_t = \inf_{\substack{u \in X(\mathcal{M}) \\ \|u\|_p^p = t}} E(u)$$

be a strictly subadditive functional in $X(\mathcal{M})$. *Assume* E *to be superadditive with respect to a sequence of partitions of unity in three parts* $\{\psi_O\}_{O \in \mathcal{O}_n}$ *subordinate to the vanishing-compatible sequence of open coverings*

$$\mathcal{O}_n = \{(-2n, 2n) \times \mathcal{M}', (n, \infty) \times \mathcal{M}', (-\infty, -n) \times \mathcal{M}'\},$$

then

$$E = \inf_{\substack{u \in X(\mathcal{M}) \\ \|u\|_p^p = 1}} E(u)$$

admits a minimizer.

Proof. By Theorem 3.2.19 we only need to construct non-vanishing minimizing sequences. Assume u_n to be a minimizing sequence of the functional E_c. Then we may construct such a sequence by using the translation invariance of the functional. Indeed, we may assume by translation invariance

$$\int_{\mathcal{M}'} \int_0^\infty |u_n|^p \,\mathrm{d}x \,\mathrm{d}y = \frac{1}{2}$$
$$\int_{\mathcal{M}'} \int_{-\infty}^0 |u_n|^p \,\mathrm{d}x \,\mathrm{d}y = \frac{1}{2}.$$

For a contradiction, assume u_n is vanishing. Then since $u_n \to 0$ in L^∞_{loc} (up to a subsequence) due to a diagonal argument, we have that

$$\int_{\mathcal{M}'} \int_{\mathbb{R}} |\psi_{(-2n,2n)} u_n|^p \,\mathrm{d}x \,\mathrm{d}y \to 0 \qquad (n \to \infty)$$
$$\int_{\mathcal{M}'} \int_{\mathbb{R}} |\psi_{(n,\infty)} u_n|^p \,\mathrm{d}x \,\mathrm{d}y \to \frac{1}{2} \qquad (n \to \infty)$$
$$\int_{\mathcal{M}'} \int_{\mathbb{R}} |\psi_{(-n,-\infty)} u_n|^p \,\mathrm{d}x \,\mathrm{d}y \to \frac{1}{2} \qquad (n \to \infty)$$

Then using the subadditivity of the functional and the strict subadditivity of $t \mapsto E_t$ we conclude

$$\begin{aligned} E &= \lim_{n\to\infty} E(u_n) \\ &\geq \limsup_{n\to\infty} E\left(\psi_{(-\infty,-n)} u_n\right) + \limsup_{n\to\infty} E\left(\psi_{(n,\infty)} u_n\right) \\ &\geq E_{1/2} + E_{1/2} > E. \end{aligned}$$

By contradiction after translating the u_n if necessary we can find a non-vanishing subsequence. Passing to a further subsequence there exists a weakly convergent subsequence in $H^1(\mathcal{G})$ that converges up to a further subsequence to a minimizer by Theorem 3.2.8. $\square$

Example 3.2.25. Suppose $\Omega = \mathbb{R} \times [0,1]^N$ and $m(\cdot, y) \equiv m(y)$. By Example 3.2.12 and Example 3.2.22 the NLS energy functional

$$\begin{aligned} E^m_{\mathrm{NLS}}(u) &:= \frac{1}{2}\int_\Omega |\nabla u|^2 + m|u|^2 \,\mathrm{d}x\,\mathrm{d}y - \frac{\mu}{q}\int_\Omega |u|^q \,\mathrm{d}x\,\mathrm{d}y \\ D(E^m_{\mathrm{NLS}}) &:= \{u \in H^1_0(\Omega) | \|u\|_2^2 = 1\}, \end{aligned} \tag{3.16}$$

with $m \in L^{\frac{2^*}{2^*-2}} + L^\infty(\mathcal{G})$ and $2 < q < 2 + \frac{4}{N}$, satisfies the prerequisites of Theorem 3.2.24 and we have existence of ground states of (3.16) for all $\mu > 0$.

To see this, suppose $\varphi \in C_c^\infty(\Omega)$ such that $\|\varphi\|_2^2 = 1$, then we rescale to obtain test functions

$$\varphi_\lambda(x, y) := \lambda^{1/2}\varphi(\lambda x, y)$$

and we compute

$$\begin{aligned} E^m_{NLS}(\varphi_\lambda) = \frac{1}{2}&\int_\Omega |\nabla_y \varphi|^2 + m|\varphi|^2 \,\mathrm{d}x\,\mathrm{d}y \\ &+ \lambda^2 \int_\Omega |\nabla_x \varphi|^2 \,\mathrm{d}x dy - \lambda^{\frac{q-2}{2}} \int_\Omega |\varphi|^q \,\mathrm{d}x\,\mathrm{d}y. \end{aligned} \tag{3.17}$$

Suppose u_2 is the minimizer of

$$\lambda([0,1]^N) := \min_{\substack{u \in H^1([0,1]^N) \\ \|u\|_2^2 = 1}} \int_{[0,1]^N} |\nabla u|^2 + m|u|^2 \,\mathrm{d}y$$

whose existence can be shown for instance by the direct method in the calculus of variations, then suppose $\varphi(x, y) := u_1(x)u_2(y)$ with $x \in \mathbb{R}$ and $y \in [0,1]^N$, then with (3.17) we compute

$$\begin{aligned} E^m_{NLS}(\varphi_\lambda) &= \frac{1}{2}\int_{[0,1]^N} |\nabla u_2|^2 + m|u_2|^2 \,\mathrm{d}y \\ &\quad + \lambda^2 \int_{\mathbb{R}} |\nabla u_1|^2 \,\mathrm{d}x - \lambda^{\frac{q-2}{2}} \int_\Omega |\varphi|^q \,\mathrm{d}x\,\mathrm{d}y \\ &< \frac{\lambda([0,1]^N)}{2} = \frac{1}{2} \inf_{u \in H^1([0,1]^N)\setminus\{0\}} \frac{\int_{[0,1]^N} |\nabla u|^2 + m|u|^2 \,\mathrm{d}y}{\int_{[0,1]^N} |u|^2 \,\mathrm{d}y} \\ &\le \frac{1}{2} \inf_{\substack{u \in H^1(\Omega) \\ \|u\|_2^2 = 1}} \int_{\mathbb{R}} \int_{[0,1]^N} |\nabla u|^2 + m|u|^2 \,\mathrm{d}x\,\mathrm{d}y. \end{aligned}$$

for sufficiently small $\lambda > 0$. In particular, E^m_{NLS} is strictly subadditive for all $\mu > 0$ due to the arguments in Example 3.2.11.

Remark 3.2.26. Strip-type spaces are only one example of translation invariance that can help to apply the theory in absence of energy thresholds in the setting of Corollary 3.2.20. In [DST19] for binary tree graphs it was shown that when strict subadditivity of the NLS energy functional can be guaranteed (for instance when $\mu > 0$ sufficiently large as in the case of domains (c.f. Example 3.2.12)) that one has existence of minimizers due to the fact that sequences can in a similar fashion moved to a central vertex to prevent them from vanishing.

3.3 A broad existence theory for ground states of a general stationary NLS functional

3.3.1 A generalized problem

Consider a metric space $(\mathcal{M}, d)$ with its corresponding Borel algebra, suppose μ_1, μ_2 are two locally finite measures on $(\mathcal{M}, d)$, and let $a : D(a) \times D(a) \to \mathbb{R}$ be a semibounded, closed quadratic form and suppose $D(a) \subset L^2(\mathcal{M}, \mu_1) \cap L^q(\mathcal{M}, \mu_2)$ for some $q \in (2, \infty)$. Let $C > 0$ such that

$$a(u, u) \geq -C\|u\|_2^2.$$

Then we define the scalar product

$$\langle u, v\rangle_a = a(u, v) + (C + 1)\langle u, v\rangle_2$$

and $D(a)$ becomes a Hilbert space. For the purpose of the application suppose the function space $D(a)$ satisfies Assumption 3.2.3 and Assumption 3.2.13. In particular, we assume $D(a)$ continuously imbeds to $L^2(\mathcal{M})$ and $L^q(\mathcal{M})$ and in fact imbeds compactly to $L^2_{\text{loc}}(\mathcal{M}, \mu_1)$, $L^q_{\text{loc}}(\mathcal{M}, \mu_2)$.

Let $\mathcal{K} \subset \mathcal{M}$. Suppose there exists $C(\|u\|_2^2) > 0$ such that

$$\int_{\mathcal{K}} |u|^q \, \mathrm{d}\mu_2 \leq C(\|u\|_2^2)\|u\|_a^2.$$

Suppose now the functional of the form

$$E(u) = \frac{1}{2}a(u, u) - \frac{\mu}{q}\int_{\mathcal{K}} |u|^q \, \mathrm{d}\mu_2,$$

satisfies

$$E(u) \geq -C(\|u\|_2^2)$$

for some $C \in \mathbb{R}$ only depending on the L^2-constraint (we do not track the constant C) and also suppose it is coercive, i.e.

$$E(u_n) \overset{n\to\infty}{\to} \infty \implies \|u_n\|_a \overset{n\to\infty}{\to} \infty.$$

In the following we consider the minimization problem

$$E := \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1}} E(u). \tag{3.18}$$

It turns out that for problems like this the problem reduces to respective form properties as we already demonstrated for the NLS problem on domains in Example 3.2.12, Example 3.2.18 and Example 3.2.22. More specifically we can show the following:

Theorem 3.3.1. *Suppose $D(a) \supset u \mapsto a(u,u)$ is superadditive with respect to a vanishing-compatible sequence of partitions of unity and satisfies*

$$\Sigma_0 := \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1}} a(u,u) < \sup_{K \Subset \mathcal{M}} \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1,\, \operatorname{supp}(u) \subset \mathcal{M} \setminus K}} a(u,u) =: \Sigma, \tag{3.19}$$

then there exists $\mu^* > 0$ such that (3.18) *admits a minimizer for $\mu \in (0, \mu^*)$. Furthermore, if $\mathcal{K} \Subset \mathcal{M}$ then we can choose $\mu^* = \infty$.*

Remark 3.3.2. In particular due to the decomposition formulas developed in §2.4 the forms associated to the Schrödinger operator and higher-order Schrödinger operators as defined in §2.3 satisfy this property. The quantities in (3.19) already appeared in this context and describe the infimum of the spectrum and essential spectrum respectively (see §2.4).

Proof of Theorem 3.3.1. E is strictly subadditive. In fact, one easily checks $t \mapsto E(t^{1/2}u)$ is concave for all $u \in D(a) \setminus \{0\}$ and $t \in (0,1)$. Hence,

$$E(tu) \le tE(u) + (1-t)E(0) = tE(u)$$

and we infer

$$E(tu) + E((1-t)u) \le E(u).$$

In particular

$$t \mapsto E_t = \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = t}} E(u)$$

is subadditive, i.e.

$$E_{t_1} + E_{t_2} \le \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = t_1 + t_2}} E(u) = E_1.$$

It suffices to show that

$$E_t < tE_1$$

for all $t \in (0,1)$. For a contradiction suppose

$$E_t = tE_1$$

for some $t \in (0,1)$. Then suppose (u_n) is a minimizing sequence for E_1 with

$$\|u_n\|_2^2 = 1.$$

Then by scaling we infer

$$\begin{aligned}\liminf_{n\to\infty} ta(u_n,u_n) - t^{q/2}\|u_n\|_q^q \geq E_t = tE_1 \\ = \lim_{n\to\infty} ta(u_n,u_n) - t\|u_n\|_q^q\end{aligned}$$

and we infer

$$\lim_{n\to\infty} \|u_n\|_q^q = 0.$$

Hence, $u_n \rightharpoonup 0$ weakly and there exists a sequence of functions Ψ_n with $\operatorname{supp}(\Psi_n) \subset \mathcal{M} \setminus K_n$ such that passing to a subsequence

$$\lim_{n\to\infty} \int_{\mathcal{M}} |\Psi_n u_n|^2 \,\mathrm{d}x = 1$$

and with superadditivity we infer

$$\begin{aligned}\inf_{\substack{u\in D(a)\\ \|u\|_2^2=1}} \frac{1}{2}a(u,u) &\geq \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1}} E(u) \\ &\lim_{n\to\infty} \frac{1}{2}a(u_n,u_n) - \frac{\mu}{q}\|u_n\|_q^q \\ &\geq \liminf_{n\to\infty} \frac{1}{2}a(\Psi_n u_n, \Psi_n u_n) \\ &\geq \sup_{K\Subset\mathcal{M}} \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1,\, \operatorname{supp} u\subset\mathcal{M}\setminus K}} \frac{1}{2}a(u,u),\end{aligned}$$

which is a contradiction to (3.19).

E is weak limit superadditive. Suppose $u_n \rightharpoonup u$ weakly in $D(a)$, then by the continuous imbedding of $D(a)$ in $L^2(\mathcal{M})$ we have $u_n \rightharpoonup u$ weakly in L^2 and we infer with Proposition 3.2.6

$$\|u_n - u\|_2^2 + \|u\|_2^2 \to 1 \qquad (n\to\infty)$$

Similarly we have

$$\lim_{n\to\infty} a(u_n,u_n) - a(u_n-u,u_n-u) = a(u,u)$$

and passing to a subsequence by Corollary 3.2.5 we have

$$\lim_{n\to\infty} \|u_n\|_q^q - \|u_n-u\|_q^q = \|u\|_q^q$$

Hence we have

$$\limsup_{n\to\infty} E(u-u_n) + E(u) \geq \liminf_{n\to\infty} E(u_n).$$

E is superadditive with respect to a vanishing compatible sequence of partitions of unity. Suppose u_n is a vanishing sequence, and suppose Ψ_n is a sequence of functions with $\mathcal{M} \setminus \mathrm{K_n}$ such that

$$\limsup_{n\to\infty} a(u_n) \geq \liminf_{n\to\infty} a(\Psi_n u_n)$$

then passing to a subsequence using a diagonal argument we can show that there exists N_n such that for $m > N_n$ we have

$$\lim_{n\to\infty} \|\Psi_m u_n\|_q^q = 0 \lim_{n\to\infty} \|u_n\|_q^q - \|\widetilde{\Psi}_n u_n\|_q^q \quad = 0$$

and passing to a subsequence we may assume $m = n$ and we have

$$\lim_{n\to\infty} \|\Psi_n u_n\|_q^q = 0 \lim_{n\to\infty} \|u_n\|_q^q - \|\widetilde{\Psi}_n u_n\|_q^q \quad = 0$$

and superadditivity with respect to a vanishing compatible sequence of partitions of unity is inherited by the form property.

Existence of minimizers. Let $u_n \in D(a)$ be a minimizing sequence. By coercivity any minimizing sequence is bounded and there exists a weakly convergent subsequence in $D(a)$. Then the prerequisites of Theorem 3.2.8 are satisfied, and either $u_n \rightharpoonup 0$ as $n \to \infty$ or there exists $u \not\equiv 0$ such that $u_n \to u$ strongly in $L^2(\mathcal{M}, \mu_1)$ and u is a minimizer of (3.18) admits a minimizer. In fact, if we choose

$$\mu^* = \frac{\frac{q}{2}(\Sigma - \Sigma_0)}{\Sigma + C(\|u\|_2^2) + 1} \sup_{K \Subset \mathcal{M}} \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1,\, \operatorname{supp} u \subset \mathcal{M}\setminus K}} \frac{\|u\|_a^2}{\|u\|_q^q}$$

then for all $\mu \in (0, \mu^*)$ there exists $K \Subset \mathcal{M}$ such that for all $u \in D(a)$ with $\|u\|_2^2 = 1$ and $\operatorname{supp} u \subset \mathcal{M} \setminus K$ we have

$$a(u,u) - \frac{\mu}{q} \int_{\mathcal{K}} |u|^q \,\mathrm{d} > \Sigma_0$$

and we infer

$$\sup_{K \Subset \mathcal{M}} \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1,\, \operatorname{supp}(u) \subset \mathcal{M}\setminus K}} E(u) > \Sigma_0 \geq \inf_{\substack{u \in D(a) \\ \|u\|_2^2 = 1}} E(u)$$

and since the prerequisites of Theorem 3.2.19 are satisfied as well we infer with Corollary 3.2.20 that for $\mu \in (0, \infty)$ the existence of minimizers of (3.18) is guaranteed. In fact, if $\mathcal{K} \Subset \mathcal{M}$ we have

$$\begin{aligned}\sup_{K\Subset\mathcal{M}} \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1,\ \mathrm{supp}(u)\subset\mathcal{M}\setminus K}} E(u) &\geq \sup_{K\Subset\mathcal{M}:\mathcal{K}\subset K} \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1,\ \mathrm{supp}(u)\subset\mathcal{M}\setminus K}} a(u,u)\\ &= \sup_{K\Subset\mathcal{M}:\mathcal{K}\subset K} \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1,\ \mathrm{supp}(u)\subset\mathcal{M}\setminus K}} a(u,u)\\ &> \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1}} a(u,u) \geq \inf_{\substack{u\in D(a)\\ \|u\|_2^2=1}} E(u).\end{aligned}$$

and the prerequisites of Corollary 3.2.20 are satisfied for $\mu \in (0,\infty)$ and we infer existence of minimizers for (3.18). □

3.3.2 NLS equation with Schrödinger operators with higher-order potentials on metric graphs

In this section, we give a first application of the results derived in on finite metric graphs.

3.3.2.1 Formulation of the problem

Let $\mathcal{G}$ be a connected, finite metric graph and let K be a connected subgraph of $\mathcal{G}$. For $k \in \mathbb{N}$ consider the energy functional

$$\begin{aligned}E^{(k)}(u) &= \frac{1}{2}\int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \,\mathrm{d}x\\ &= \frac{1}{2}a^m(u,u) - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \,\mathrm{d}x,\end{aligned} \tag{3.20}$$

with $2 < p < 4k+2$ and a^m is the form as defined in §2.3.1. Suppose $m \in L^1_{\mathrm{loc}}$ is a real-valued potential such that

$$m_- \in L^1 + L^\infty(\mathcal{G}).$$

Consider the minimization problem

$$E^{(k)} := \inf_{\substack{u\in H^k(\mathcal{G})\\ \|u\|_2^2=1}} E^{(k)}(u) \tag{3.21}$$

and the corresponding threshold energy

$$\widetilde{E}^{(k)} = \sup_{K\Subset\mathcal{M}} \inf_{\substack{u\in H^k(\mathcal{G})\\ \mathrm{supp}\, u\subset\mathcal{G}\setminus K, \|u\|_2^2=1}} E^{(k)}(u). \tag{3.22}$$

In the following we will present existence principles for (3.21) via Theorem 3.3.1. But first we will see that the associated energy functional is semi-bounded:

Lemma 3.3.3. *Let $\mathcal{G}$ be a finite connected metric graph. The functional $E^{(k)}$ under the L^2-constraint $\|\cdot\|_2^2 = 1$ is bounded below for $2 < p < 4k+2$. Moreover, for each $0 < \varepsilon < 1$ there exists a $C_\varepsilon > 0$, such that*

$$E^{(k)}(u) \geq \frac{1-\varepsilon}{2} \int_{\mathcal{G}} |u^{(k)}|^2 \,\mathrm{d}x - C_\varepsilon.$$

Proof. Let $\varepsilon_1, \varepsilon_2 > 0$ fixed but arbitrary. As in Theorem 2.3.1 we infer

$$\frac{1}{2} \int_{\mathcal{G}} |u^{(k)}|^2 + m|u|^2 \,\mathrm{d}x \geq \frac{1-\varepsilon_1}{2} \int_{\mathcal{G}} |u^{(k)}|^2 \,\mathrm{d}x - C_{\varepsilon_1}.$$

From Proposition 2.5.8 (Gagliardo–Nirenberg inequality) we have

$$\|u\|_{L^p}^p \leq C \,\|u\|_{L^2(\mathcal{G})}^{\frac{(2k-1)p+2}{2k}} \,\|u\|_{H^k}^{\frac{p-2}{2k}}$$

for some $C > 0$. Then with Young's inequality we infer for all $u \in H^k(\mathcal{G})$ with $\|u\|_2^2 = 1$

$$\frac{\mu}{p} \|u\|_{L^p}^p \leq \frac{\varepsilon_2}{2} \|u\|_{H^k}^2 + C_{\varepsilon_2}$$

for some $C_{\varepsilon_2} > 0$ and since $\varepsilon_1, \varepsilon_2$ are arbitrary in particularly we obtain

$$E^{(k)}(u) \geq \frac{1-\varepsilon}{2} \int_{\mathcal{G}} |u^{(k)}|^2 \,\mathrm{d}x - C_\varepsilon$$

for $2 < p < 4k+2$ for some $C_\varepsilon > 0$. □

Proposition 3.3.4. *Let $\mathcal{G}$ be a finite, connected metric graph. Suppose $m \in L^2 + L^\infty(\mathcal{G})$ and $u \in H^k(\mathcal{G})$ is a minimizer of $E^{(k)}$, then $u \in H^{2k}(\mathcal{G})$ and there exists $\lambda \in \mathbb{R}$ such that*

$$(-1)^k u_e^{(2k)} + (m+\lambda)\, u_e = \mu |u_e|^{p-1} u_e \tag{3.23}$$

for all $e \in \mathcal{E}$.

Proof. Since $E^{(k)} \in C^1(H^k(\mathcal{G}), \mathbb{R})$ and the L^2-constraint is also C^1, and u is a constrained critical point we can compute the Gâteaux derivative of the first variation

$$\int_{\mathcal{G}} \left(u^{(k)} \eta^{(k)} - u|u|^{p-2}\eta\right) \,\mathrm{d}x + \int_{\mathcal{G}} (m+\lambda)\, u\eta \,\mathrm{d}x = 0, \qquad \forall \eta \in H^k(\mathcal{G})$$

where λ is a Lagrange multiplier. Fixing an edge e, then with $\eta \in C_c^\infty(I_e)$ and integration by parts we deduce (3.23) for each $e \in \mathcal{E}$ and by elliptic regularity $u \in \widetilde{H^{2k}}(\mathcal{G})$. Fixing now $\mathsf{v} \in V$ and taking $\eta \in H^k(\mathcal{G})$ to be locally supported near v and not supported at any other vertex, then by integration by parts and (3.23) edgewise we deduce

$$\sum_{j=1}^{k}(-1)^j \sum_{e\succ \mathsf{v}} \tfrac{\partial^{(k+j-1)}}{\partial^{(k+j-1)}\nu} u_e \tfrac{\partial^{(k-j)}}{\partial^{(k-j)}\nu}\eta_e(\mathsf{v}) = \int_{\mathcal{G}} \left(u^{(k)}\eta^{(k)} - u|u|^{p-2}\eta\right)\,\mathrm{d}x + \int_{\mathcal{G}} (m+\lambda)\,u\eta\,\mathrm{d}x = 0.$$

Since the choice $\eta \in H^k$ is arbitrary we deduce

$$\begin{cases} \sum_{e\succ \mathsf{v}} \frac{\partial^\ell}{\partial \nu^\ell} u_e(\mathsf{v}) = 0, & \forall k \le \ell \le 2k-1 \text{ odd}, \\ u_{e_1}^{(\ell)}(\mathsf{v}) = u_{e_2}^{(\ell)}(\mathsf{v}), & \forall k \le \ell \le 2k-1 \text{ even and } \forall e_1, e_2 \text{ adjacent at } \mathsf{v} \end{cases}$$

for all $\mathsf{v} \in \mathcal{V}$. □

Let $A^m = (-\Delta)^k + m$ be the self-adjoint operator associated to the form a^m as defined in §2.3.1. Given the core $K = \mathcal{G} \setminus \mathcal{E}_\infty$ of $\mathcal{G}$ and $R > 0$ recall

$$\begin{aligned} D_R &:= \{\varphi \in D(A^m) \,|\, \operatorname{supp}(\varphi) \subset \mathcal{G} \setminus K_R\} \\ \Sigma_R^m &:= \inf\{\langle \varphi, A^m\varphi\rangle \,|\, \varphi \in D_R, \|\varphi\|_2^2 = 1\}, \end{aligned} \tag{3.24}$$

where K_R was defined in (2.23).

For $R = 0$ we set

$$\begin{aligned} D_0 &:= D(A) \\ \Sigma_0^m &:= \inf\{\langle \varphi, A^m\varphi\rangle \,|\, \varphi \in D(A), \|\varphi\|_2^2 = 1\}. \end{aligned} \tag{3.25}$$

The last relevant quantity we recall is

$$\Sigma^m = \lim_{R\to\infty} \Sigma_R = \sup_{R>0} \Sigma_R. \tag{3.26}$$

By §2.4 due to the Persson theory there exists a relation to the spectrum via

$$\Sigma_0^{=} \inf \sigma(A^m), \qquad \Sigma^{=} \inf \sigma_{\text{ess}}(A^m).$$

Theorem 3.3.5. *Let $\mathcal{G}$ be a finite, connected graph and let $c > 0$. Assume*

$$\Sigma_0^m < \Sigma^m$$

as defined in (3.25) *and* (3.26)*, then there exists $\mu^* > 0$ such that $E_c^{(k)}(\mathcal{G})$ admits a minimizer for $\mu \in (0, \mu^*)$.*

Proof. Let $\{\Psi_n, \widetilde{\Psi}_n\}$ be the vanishing compatible sequence of partitions of unity in Example 2.4.4. Suppose $\varphi_n \rightharpoonup 0$ is a vanishing sequence, then there exists a subsequence such that

$$\int_{\mathcal{G}} |\Psi_n \varphi_n|\,\mathrm{d}x \to 0 \qquad (n \to \infty).$$

By Lemma 2.4.7 we infer

$$a^m(\varphi_n, \varphi_n) = a^m(\Psi_n\varphi_n, \Psi_n\varphi_n) + a^m(\widetilde{\Psi}_n\varphi_n, \widetilde{\Psi}_n\varphi_n) + O\left(\frac{1}{n^2}\right) \qquad (n \to \infty)$$

and the statement follows from Theorem 3.3.1. □

Remark 3.3.6. Similarly, if we consider the minimization problem under the prerequisites of Theorem 3.3.5 we can derive existence of minimizers of the minimization problem with localized nonlinearity $\mathcal{K} \Subset \mathcal{G}$

$$\inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_2^2 = 1}} \frac{1}{2} a^m(u,u) - \frac{\mu}{p} \int_{\mathcal{K}} |u|^p \,\mathrm{d}x$$

for all $\mu > 0$ using Theorem 3.3.1. For more discussions on ground state problems with NLS type functional associated to higher-order Schrödinger operators we refer to [Hof19, §4].

3.3.2.2 Sufficient conditions for the threshold condition for the Polylaplacian

Recall the self-adjoint Polylaplace operator $A^m = (-\Delta)^k + m$ with $m \in L^2 + L^\infty(\mathcal{G})$ as considered in §2.3.1. Let us give in the following some sufficient conditions for existence of spectrum below the essential spectrum using the characterization of the bottom of the spectrum and essential spectrum in the context of the Persson theory in §2.4.

Proposition 3.3.7. *Let $\mathcal{G}$ be a finite, connected metric graph and $k \geq 1$. Assume $\sigma_{ess}((-\Delta)^k + m) \subset [0, \infty)$ and assume additionally either*

(i) $m \in L^1(\mathcal{G})$ *and*

$$\int_{\mathcal{G}} m \,\mathrm{d}x < 0$$

(ii) or $m < 0$ on $\mathcal{G}$.

Then $\Sigma_0 < \Sigma$ (as defined in (3.38) *and* (3.39)*) and there exists $\hat{\mu} > 0$, such that the minimization problem*

$$E^{(k)} = \inf_{\substack{u \in H^k(\mathcal{G}) \\ \|u\|_2^2 = 1}} E^{(k)}(u) \tag{3.27}$$

admits a minimizer for $\mu \in (0, \hat{\mu})$.

Proof. Consider as test functions Ψ_n as defined as in Example 2.4.4, then we only need to show that for n sufficiently large, the Rayleigh quotient

$$\mathcal{R}[\Psi_n] := \frac{\int_{\mathcal{G}} |\Psi_n^{(k)}|^2 + m|\Psi_n|^2 \,\mathrm{d}x}{\int_{\mathcal{G}} |\Psi_n|^2 \,\mathrm{d}x} < 0.$$

Since $\|\Psi_n^{(k)}\|_\infty^2 \leq \frac{C}{n^{2k}}$ for some $C > 0$ we have

$$\|\Psi_n^{(k)}\|_2^2 \leq \frac{C}{n^{2k}} \to 0 \qquad (n \to \infty).$$

If $m < 0$ then let $K = \mathcal{G} \setminus \mathcal{E}_\infty$ be any core graph of $\mathcal{G}$, then for sufficiently large n and $\varepsilon > 0$ sufficiently small

$$\int_{\mathcal{G}} m|\Psi_n|^2 \,\mathrm{d}x \leq -|\{x \in K_n : m(x) \leq -\varepsilon\}|\varepsilon < 0.$$

If $\int_{\mathcal{G}} m \,\mathrm{d}x < 0$, using also that m is intergrable then by dominated convergence

$$\liminf_{n\to\infty} \int_{\mathcal{G}} m|\Psi_n|^2 \,\mathrm{d}x = \int_{\mathcal{G}} m \,\mathrm{d}x < 0$$

We deduce $\mathcal{R}[\Psi_n] < 0$ for sufficiently large n and thus $\inf \sigma((-\Delta)^k + m) < 0$. Then $\Sigma_0 < \Sigma$ and we conclude the existence of a minimizer of (3.27) by Theorem 3.3.5. □

Remark 3.3.8. If $m \in L^2 + L^\infty(\mathcal{G})$ is a relativly compact perturbation of $(-\Delta)^k$, i.e.

$$m\left((-\Delta)^k + i\right)^{-1}$$

is compact, then $\inf \sigma_{\text{ess}}\left((-\Delta)^k + m\right) = 0$ and we deduce

$$\sigma_{\text{ess}}\left((-\Delta)^k + m\right) \subset [0, \infty).$$

Note that one can actually show using Weyl sequences on the real line that $\sigma_{\text{ess}}\left((-\Delta)^k + m\right)$. If $\mathcal{G}$ contains at least one ray by Theorem 2.3.5 we can infer then

$$\sigma_{\text{ess}}((-\Delta)^k + m) = \sigma_{\text{ess}}((-\Delta)^k) = 0.$$

We finish the section by giving a criterion for the potential m such that

$$\Sigma = \lim_{n\to\infty} \inf_{\substack{u \in D(A^m) \\ \|u\|_2^2 = 1,\, \operatorname{supp} u \subset \mathcal{G}\setminus K_n}} \langle u, A^m u\rangle \geq 0.$$

which in particular due to Theorem 2.4.8 implies

$$\sigma_{\text{ess}}((-\Delta)^k + m) \subset [0, \infty)$$

by Remark 3.3.8. Consider in the following decaying potentials $m = m_2 + m_\infty$ with $m_2 \in L^2(\mathcal{G})$

and $m_\infty \in L^\infty(\mathcal{G})$ such that

$$\sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)| \to 0 \qquad (n\to\infty). \tag{3.28}$$

Proposition 3.3.9. *Let $\mathcal{G}$ be a finite metric graph. Assume $m \in L^2 + L^\infty(\mathcal{G})$ satisfies* (3.28). *Let $A^m = (-\Delta)^k + m$, then*

$$\Sigma = \lim_{n\to\infty} \inf_{\substack{u\in H^{2k}(\mathcal{G})\\ \|u\|_2^2=1,\, \operatorname{supp} u\subset\mathcal{G}\setminus K_n}} \langle u, A^m u\rangle_{L^2} = 0.$$

Proof. Assume u_n is a minimizing sequence, such that $\|u_n\|_{L^2}^2$, $\operatorname{supp} u \subset \mathcal{G}\setminus K_n$ and

$$\langle u_n, A^m u_n\rangle_{L^2} \to \Sigma.$$

With (2.39) we deduce that

$$\|u_n\|_{H^k} \le C\left(\langle u_n, A^m u_n\rangle_{L^2}^2 + \|u_n\|_2^2\right) \tag{3.29}$$

is uniformly bounded. Integrating by parts and using (3.29) we infer

$$\int_{\mathcal{G}} \left|u_n^{(k)}\right|^2 + m|u_n|^2\,\mathrm{d}x \ge \int_{\mathcal{G}} \left|u_n^{(k)}\right|^2\,\mathrm{d}x - \widetilde{C}\left(\left(\int_{\mathcal{G}\setminus K_n} |m|^2\,\mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right).$$

We have

$$\left(\left(\int_{\mathcal{G}\setminus K_n} |m|^2\,\mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right) \to 0 \qquad (n\to\infty).$$

Thus,

$$\Sigma = \lim_{n\to\infty} \langle u_n, A^m u_n\rangle_{L^2} \ge 0.$$

In fact, suppose $\varphi \in C_c^\infty(\mathbb{R})$, then we can define

$$\varphi_n := \frac{1}{\sqrt{n}}\varphi\left(\frac{x}{n}\right).$$

We imbed φ_n to a function $\varphi \in \widetilde{C_b^\infty}(\mathcal{G})$ on the graph by defining it on one ray and then extending it to the rest of the graph by zero and w.l.o.g. we may assume $\operatorname{supp}\varphi_n \subset \mathcal{G}\setminus K_n$, then we have

$$\begin{aligned}\Sigma &\le \lim_{n\to\infty} \int_{\mathcal{G}} |\varphi_n^{(k)}|^k +, |\varphi_n|^2\,\mathrm{d}x\\ &\le \int_{\mathcal{G}} \frac{1}{n^k}|\varphi^{(k}|\,\mathrm{d}x - \widehat{C}\left(\left(\int_{\mathcal{G}\setminus K_n} |m|^2\,\mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right) = 0.\end{aligned}$$

$\square$

3.3.3 Decaying potentials

In the following we study the minimization problem on finite metric graphs $\mathcal{G}$ under the assumption as considered in Proposition 3.3.9 that $m = m_2 + m_\infty$ with $m_2 \in L^2(\mathcal{G}), m_\infty \in L^\infty(\mathcal{G})$ such that

$$m_\infty(x) \to 0 \qquad (x \to \infty) \tag{3.30}$$

on all of the rays. Consider the quantitities

$$E^{(k)} = \inf_{\substack{\varphi \in D(A) \\ \|\varphi\|_{L^2}^2 = 1}} E^{(k)}(u) \qquad \widetilde{E}^{(k)} = \lim_{R\to\infty} \inf_{\substack{\varphi \in D_R(A) \\ \|\varphi\|_{L^2}^2 = 1}} E^{(k)}(u)$$

$$E^{(k)}(\mathbb{R}) = \inf_{\substack{u \in H^1(\mathbb{R}) \\ \|u\|_{L^2(\mathbb{R})}^2 = 1}} \frac{1}{2}\int_{\mathbb{R}} |u^{(k)}|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathbb{R}} |u|^p \,\mathrm{d}x.$$

Lemma 3.3.10. *Let $\mathcal{G}$ be a finite metric graph and assume that $m \in L^2 + L^\infty(\mathcal{G})$ satisfies* (3.30)*. Then*

$$\widetilde{E}^{(k)} = E^{(k)}(\mathbb{R}).$$

Proof. Due to density of $C_c^\infty(\mathbb{R})$ in $H^k(\mathbb{R})$, we can consider a minimizing sequence u_n for $E^{(k)}(\mathbb{R})$ in $C_c^\infty(\mathbb{R})$ satisfying $\|u_n\|_2^2 = 1$, such that $u_n \to \varphi$ strongly in H^k as $n \to \infty$. Now by translation invariance we may assume that u_n is supported in $[n, \infty)$ for $n \in \mathbb{N}$. identifying the half-line with one of the rays of $\mathcal{G}$, we may consider u_n as a function in $H^k(\mathcal{G})$. Then

$$\begin{aligned} \left|\int_{\mathcal{G}} m|u_n|^2 \,\mathrm{d}x\right| &= \left|\int_{\mathcal{G}\setminus K_n} m|u_n|^2 \,\mathrm{d}x\right| \\ &\le C\left(\sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|^2 + \int_{\mathcal{G}\setminus K_n} |m_2|^2 \,\mathrm{d}x\right) \to 0 \qquad (n\to\infty) \end{aligned}$$

and we compute

$$\begin{aligned} E^{(k)}(\mathbb{R}) &= \lim_{n\to\infty} E^{(k)}(u_n) \\ &= \lim_{n\to\infty} \frac{1}{2}\int_{\mathcal{G}} |u_n^{(k)}|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \,\mathrm{d}x \\ &= \lim_{n\to\infty} E^{(k)}(u_n) \ge \widetilde{E}^{(k)}. \end{aligned}$$

On the other hand given a minimizing sequence u_n for $\widetilde{E}^{(k)}$, such that $\operatorname{supp} u_n \subset \mathcal{G} \setminus K_n$ then the functions in the sequence are supported on each of the rays and

$$\begin{aligned} \left|\int_{\mathcal{G}} m|u_n|^2 \,\mathrm{d}x\right| &= \left|\int_{\mathcal{G}\setminus K_n} m|u_n|^2 \,\mathrm{d}x\right| \\ &\le C\left(\sup_{x\in\mathcal{G}\setminus K_n} |V_\infty(x)| + \left(\int_{\mathcal{G}\setminus K_n} |m_2|^2 \,\mathrm{d}x\right)^{1/2}\right) \to 0 \qquad (n\to\infty). \end{aligned} \tag{3.31}$$

Recall that $|\mathcal{E}_\infty|$ denotes the number of rays. By density we can consider a collection of sequences

$u_n^{(1)}, \dots, u_n^{(|\mathcal{E}_\infty|)}$ in $C_c^\infty(\mathbb{R})$, one on each of the rays, and choose them to have disjoint supports. Then if we define

$$\widetilde{u}_n := \sum_{i=1}^{|\mathcal{E}_\infty|} u_n^{(i)}.$$

Then with (3.31) we compute

$$\begin{aligned}\widetilde{E}^{(k)} &= \lim_{n\to\infty} \sum_{i=1}^{\mathcal{E}_\infty} E^{(k)}(u_n^{(i)}) \\ &= \lim_{n\to\infty} E^{(k)}\left(\widetilde{u}_n\right) \geq E^{(k)}(\mathbb{R}).\end{aligned}$$

□

Remark 3.3.11. Suppose $\mathcal{G}$ is a locally finite metric graph with at least one ray. Then the inequality

$$\widetilde{E}^{(k)} \leq E^{(k)}(\mathbb{R})$$

can still be shown as in the proof of Lemma 3.3.10 using the test function argument on the half-line. Further using a rescaling argument using a suitable test function supported on the ray we have

$$E^{(k)}(\mathbb{R}) < 0$$

Theorem 3.3.12. *Let $\mathcal{G}$ be a finite metric graph. Assume $m \in L^2 + L^\infty(\mathcal{G})$ satisfies* (3.30)*, then $E^{(k)}$ is strictly subadditive and if*

$$E^{(k)} < E^{(k)}(\mathbb{R})$$

then there exists a minimizer of $E^{(k)}$.

Proof. By Lemma 3.3.3 any minimizing sequence admits a weakly convergent subsequence. By Theorem 3.3.5 the functional is superadditive with respect to the vanishing-compatible sequence of partition of unity and weak limit superadditive. It suffices to prove the strict subadditivity of $E^{(k)}$. As in Theorem 3.3.5 we can argue by contradiction. Assume namely that

$$E_t^{(k)} = tE_1^{(k)}$$

for some $t \in (0,1)$ and let u_n be a minimizing sequence for $E_t^{(k)}$, then in particular we can show

$$\int_{\mathcal{G}} |u_n|^p \,\mathrm{d}x \to 0 \qquad (n \to \infty).$$

But then u_n is a vanishing sequence and passing to a subsequence still denoted by u_n, we deduce with superaddditivity with respect to a sequence of partitions of unity as defined in

Example 2.4.4

$$\begin{aligned}
E_t^{(k)} &= \limsup_{n\to\infty} E^{(k)}(\Psi_n u_n) + \limsup_{n\to\infty} E^{(k)}(\widetilde{\Psi_n} u_n) \\
&\geq \frac{1}{2} \lim_{n\to\infty} \inf_{\substack{\varphi\in H^1 \\ \|u\|_2^2=t,\, \operatorname{supp} u\subset \mathcal{G}\setminus K_n}} \langle Au, u\rangle \\
&\geq -\frac{C}{2} \lim_{n\to\infty} \left(\sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)| + \left(\int_{\mathcal{G}\setminus K_n} |m_2|^2 \,\mathrm{d}x \right)^{1/2} \right) = 0,
\end{aligned}$$

since $\|u_n\|_{H^k} \leq C$ for some $C > 0$ by Lemma 3.3.3. On the other hand, by Lemma 3.3.10 and Remark 3.3.11 we have

$$\Sigma = E^{(k)}(\mathbb{R}) < 0$$

and by contradiction we deduce strict subadditivity.

Hence, the prerequisites of Theorem 3.2.8 and Theorem 3.2.19 are satisfied with $X(\mathcal{G}) = H^k(\mathcal{G})$ and $Y(\mathcal{G}) = \widetilde{C_b^\infty}(\mathcal{G})$. Then the energy inequality in Corollary 3.2.20 is satisfied. In particular we deduce existence of a minimizer of $E^{(k)}(\mathcal{G})$ under the stated assumptions. □

Example 3.3.13. Let $\mathcal{G}$ be a finite metric graph and let $m \in L^2 + L^\infty(\mathcal{G})$ satisfy (3.30). Similarly as in Lemma 3.3.10 we can show

$$\Sigma = \lim_{R\to\infty} \inf_{\substack{\varphi\in D_R(A^m) \\ \|\varphi\|_{L^2}^2=1}} \langle \varphi, A\varphi\rangle_{L^2} = 0.$$

In particular if $\Sigma_0 < 0$, then by Theorem 3.3.5 there exists $\hat{\mu} > 0$, such that for $\mu \in (0, \hat{\mu}]$ there exists a minimizer to $E^{(1)}$. As in [Cac18] one can show due to scaling properties that

$$\Sigma_0^{(\mu,1)} < \Sigma_0 \leq \gamma_p \mu^{\frac{4}{6-p}} = E^{(1)}(\mathbb{R})$$

for some $\gamma_p < 0$ and $0 < \mu \leq (\Sigma_0/\gamma_p)^{\frac{3}{2}-\frac{p}{4}}$. In particular, we can deduce existence of minimizers for $E^{(1)}$ and $0 < \mu \leq (\Sigma_0/\gamma_p)^{\frac{6-p}{4}}$ by Theorem 3.3.12.

3.4 Existence theory for ground states of a stationary NLS with magnetic potential on metric graphs

In this section, we study the NLS energy functional with potentials on more general graphs. We show a decomposition formula for the form associated with the magnetic Schrödinger operator and adapt previous arguments by introducing a suitable sequence of partitions of unity in the case of locally finite metric graphs.

3.4.1 Formulation of the problem

Let $\mathcal{G}$ be a locally finite graph. Consider for $2 < p < 6$ the NLS functional

$$
\begin{aligned}
E_{\text{NLS}}^{(\mathcal{K})}(u) &:= \frac{1}{2}\int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{K}} |u|^p \,\mathrm{d}x \\
&= \frac{1}{2}a^{M,m}(u,u) - \frac{\mu}{p}\int_{\mathcal{K}} |u|^p \,\mathrm{d}x
\end{aligned} \tag{3.32}
$$

where $a^{M,m}$ is the form as defined in §2.3.2, $m \in L^1 + L^\infty(\mathcal{G})$ is a real-valued potential and $\mathcal{K}$ is a not necessarily bounded subgraph of $\mathcal{G}$. Define the corresponding minimization problem

$$
E_{\text{NLS}}^{(\mathcal{K})} := \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} E_{\text{NLS}}^{(\mathcal{K})}(u) \tag{3.33}
$$

with threshold energy

$$
\widetilde{E}_{\text{NLS}}^{(\mathcal{K})} := \sup_{K \Subset \mathcal{G}} \inf_{\substack{u \in H^1(\mathcal{G}) \\ \operatorname{supp} u \subset \mathcal{G}\setminus K, \|u\|_2^2 = 1}} E_{\text{NLS}}^{(\mathcal{K})}(u) \tag{3.34}
$$

similarly as in §3.3.2. We consider two cases:

- *The localized case,* when $\mathcal{K}$ is a bounded subgraph of $\mathcal{G}$;
- *The global case,* when $\mathcal{K} = \mathcal{G}$ is the whole graph. In this case, we drop the superscript and simply define

$$
E_{\text{NLS}}(u) := \frac{1}{2}\int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \,\mathrm{d}x \tag{3.35}
$$

  and for the ground state and threshold energy respectively

$$
E_{\text{NLS}} := \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} E_{\text{NLS}}(u), \tag{3.36}
$$

$$
\widetilde{E}_{\text{NLS}} := \sup_{K \Subset \mathcal{G}} \inf_{\substack{u \in H^1(\mathcal{G}) \\ \operatorname{supp} u \subset \mathcal{G}\setminus K, \|u\|_2^2 = 1}} E_{\text{NLS}}(u). \tag{3.37}
$$

We define quantities analogous to (3.24), (3.25) and (3.26). Let $A^{M,m}$ be the self-adjoint operator associated to the form $a^{M,m}$ as considered in §2.3.2. Given a bounded subgraph K of $\mathcal{G}$ and $R > 0$ recall

$$
\begin{aligned}
D_R &:= \{\varphi \in D(A^{M,m}) | \operatorname{supp}(\varphi) \subset \mathcal{G} \setminus K_R\} \\
\Sigma_R^{M,m} &:= \inf\{\langle \varphi, A^{M,m}\varphi \rangle | \varphi \in D_R, \|\varphi\|_2^2 = 1\},
\end{aligned}
$$

where K_R was defined in (2.23),

$$\begin{aligned} D_0 &:= D(A^{M,m}) \\ \Sigma_0^{M,m} &:= \inf\{\langle\varphi, A^{M,m}\varphi\rangle | \varphi \in D(A^{M,m}), \|\varphi\|_2^2 = 1\} \end{aligned} \tag{3.38}$$

and

$$\Sigma^{M,m} := \lim_{R\to\infty} \Sigma_R = \sup_{R>0} \Sigma_R. \tag{3.39}$$

By §2.4 the quantities $\Sigma_0^{M,m}$ and $\Sigma^{M,m}$ characterize the infimum of the spectrum and essential spectrum of $A^{M,m}$ respectively.

3.4.2 Existence of NLS ground state for a class of Schrödinger operators

3.4.2.1 The localized setting

In the following we study the localized case. We also remark that some of the lemmas will also apply to the global case. For $t > 0$ we define

$$E_t^{(\mathcal{K})} := \inf_{\substack{u\in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = t}} E_{\text{NLS}}^{(\mathcal{K})}(u). \tag{3.40}$$

Lemma 3.4.1. *Let $\mathcal{G}$ be a connected locally finite metric graph. Let $\mathcal{K}$ be a not necessarily bounded subset of $\mathcal{G}$. The functional $E_{NLS}^{(\mathcal{K})}$ under L^2-constraint $\|\cdot\|_{L^2}^2 = 1$ is bounded below for $2 < p < 6$.*

Proof. From the Gagliardo–Nirenberg inequality (2.37) we have

$$\begin{aligned} \int_{\mathcal{K}} |u|^p \,\mathrm{d}x &\le \int_{\mathcal{G}} |u|^p \,\mathrm{d}x \\ &\le \varepsilon \int_{\mathcal{G}} \left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u\right|^2 + m|u|^2 \,\mathrm{d}x + C_\varepsilon \int_{\mathcal{G}} |u|^2 \,\mathrm{d}x \end{aligned}$$

and therefore

$$E_{\text{NLS}}^{(\mathcal{K})}(u) \ge (1-\varepsilon) \int_{\mathcal{G}} \left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u\right|^2 + m|u|^2 \,\mathrm{d}x - C_\varepsilon \ge -C_\varepsilon$$

for all $u \in H^1(\mathcal{G})$ satisfying $\|u\|_2^2 = 1$. □

Lemma 3.4.2. *Let $\mathcal{G}$ be a locally finite, connected metric graph. Assume $A = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m$ admits a ground state, then*

$$E_t^{(\mathcal{K})} = \inf_{\substack{u\in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = t}} E_{NLS}^{(\mathcal{K})} \le \frac{\Sigma_0 t}{2}.$$

The inequality is strict if the ground state does not vanish identically on $\mathcal{K}$

Proof. Assume u is a ground state of $A^{M,m} = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + V$ with $\|u\|_{L^2}^2 = t$, then

$$E_{\text{NLS}}^{(\mathcal{K})}(u) = \frac{\Sigma_0 t}{2} - \frac{\mu}{p}\int_{\mathcal{K}} |u|^p \,\mathrm{d}x \leq \frac{\Sigma_0}{2} t$$

and the inequality is strict if u is not identically vanishing on $\mathcal{K}$. In particular

$$\inf_{\substack{u\in H^1 \\ \|u\|_{L^2}^2 = t}} E_{\text{NLS}}^{(\mathcal{K})}(u) \leq \frac{\Sigma_0 t}{2}$$

with strictness in the inequality if there exists a ground state, which is not identically vanishing on $\mathcal{K}$. □

Lemma 3.4.3. *Let $\mathcal{G}$ be a locally finite, connected metric graph and let $\mathcal{K}$ be any subgraph. Assume $A^{M,m} = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m$ admits a ground state that is not identically vanishing on $\mathcal{K}$, then the functional $E_{NLS}^{(\mathcal{K})}$ is weak limit superadditive, superadditive with respect to the partition of unity in Example 2.4.10 and $t \mapsto E_t$ as defined in* (3.40) *is strictly subadditive.*

Proof. We have

$$\begin{aligned}
\left(\int_{\mathcal{G}} |u'|^2 \mathrm{d}x\right)^{1/2} &- \left(\int_{\mathcal{G}} |M|^2 |u|^2 \,\mathrm{d}x\right)^{1/2} \\
&\leq \left(\int_{\mathcal{G}} \left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u\right|^2 \,\mathrm{d}x\right)^{1/2} \\
&\qquad \leq \left(\int_{\mathcal{G}} |u'|^2 \mathrm{d}x\right)^{1/2} + \left(\int_{\mathcal{G}} |M|^2 |u|^2 \,\mathrm{d}x\right)^{1/2}.
\end{aligned}$$

Hence, if we add a constant to the potential (which we still denote by m), then

$$\|u\|_{2,M,m} = \left(\int_{\mathcal{G}} \left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right) u\right|^2 + m|u|^2 \,\mathrm{d}x\right)^{1/2}$$

defines an equivalent norm on $H^1(\mathcal{G})$.

We proceed as in Theorem 3.3.1. In particular, following the proof of Theorem 3.3.1 the functional E_{NLS} is weak limit superadditive. Superadditivity with respect a vanishing compatible sequence of partitions of unity is inherited by the form property. Consider the sequence $\Psi_n, \widetilde{\Psi}_n$ as defined in Example 2.4.10, then it defines a sequence of a vanishing-compatible sequence of unity satisfying

$$\|\Psi_n'\|_\infty \leq \frac{C}{n}$$

Suppose u_n is a vanishing sequence. Then by Lemma 2.4.15 we have

$$a(u_n, u_n) = a(\Psi_n u_n, \Psi_n u_n) + a(\widetilde{\Psi}_n u_n, \widetilde{\Psi}_n u_n) + o(1) \qquad (n \to \infty).$$

Then as in Theorem 3.3.1 we infer superadditivity with respect to a vanishing compatible sequence of partitions of unity of E_{NLS}.

To show the subadditivity, note that following Theorem 3.3.1

$$t \mapsto E_t^{(\mathcal{K})} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}=1}} E_{\text{NLS}}^{(\mathcal{K})}(u) \tag{3.41}$$

is concave. In particular we have

$$E_t^{(\mathcal{K})} \geq t E_1^{(\mathcal{K})}$$

for $t \in (0,1)$. Suppose for a contradiction

$$E_t^{(\mathcal{K})} = t E_1^{(\mathcal{K})}$$

for some $t \in (0,1)$ and let u_n be a minimizing sequence for E_t, then in particular due to (3.41)

$$\int_{\mathcal{K}} |u_n|^p \, \mathrm{d}x \to 0 \qquad (n \to \infty).$$

Then by density we may assume $u_n \in D(A)$ and we infer

$$\begin{aligned} E_t^{(\mathcal{K})} &= \lim_{n\to\infty} E_{NLS}^{(\mathcal{K})}(u_n) \\ &\geq \frac{1}{2} \limsup_{n\to\infty} \langle A^{M,m} u_n, u_n \rangle \geq \frac{\Sigma_0 t}{2}, \end{aligned}$$

which is a contradiction to the inequality in Lemma 3.4.2. Hence, we have

$$E_t^{(\mathcal{K})} > t E_1^{(\mathcal{K})}$$

and we infer

$$E_t^{(\mathcal{K})} + E_{1-t}^{(\mathcal{K})} > E_1^{(\mathcal{K})}.$$

□

Theorem 3.4.4. *Let $\mathcal{G}$ be a connected, locally finite metric graph. Assume $A^{M,m} = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m$ admits a ground state, which is not identically vanishing on $\mathcal{K}$, then $E_{NLS}^{(\mathcal{K})}$ admits a minimizer for all $\mu > 0$.*

Proof. For $R > 0$ sufficiently large since $\mathcal{K}$ is considered to be bounded

$$\begin{aligned} \inf_{\substack{u \in D_R(A^{M,m}) \\ \|u\|_{L^2}^2=1}} E_{\text{NLS}}^{(\mathcal{K})}(u) &= \inf_{\substack{u \in D_R(A^{M,m}) \\ \|u\|_{L^2}^2=1}} \frac{1}{2}\langle A^{M,m} u, u \rangle \\ &\geq \inf_{\substack{u \in D(A^{M,m}) \\ \|u\|_{L^2}^2=1}} \frac{1}{2}\langle A^{M,m} u, u \rangle = \frac{\Sigma_0}{2}. \end{aligned}$$

In particular with Lemma 3.4.2 we have

$$E_{\mathrm{NLS}}^{(\mathcal{K})} < \lim_{R\to\infty} \inf_{\substack{u\in D_R(A^{M,m})\\ \|u\|_{L^2}^2=1}} E_{\mathrm{NLS}}^{(\mathcal{K})}(u) =: \widetilde{E_{\mathrm{NLS}}^{(\mathcal{K})}}.$$

Due to Lemma 3.4.3 the requirements of Theorem 3.2.8 and 3.2.19 are satisfied and up to a subsequence any minimizing sequence admits a strong limit in L^2 such that the limit achieves the minimum in $E_{\mathrm{NLS}}^{(\mathcal{K})}$. □

Remark 3.4.5.

- If $M \equiv 0$ then we can assume that a ground state of A is nonnegative, since $|u|$ is also a minimizer of the ground state problem. In fact by Hopf's maximum principle positive everywhere and by the boundary point lemma (see [GT01, Lemma 3.4]) if the minimizer would contain a zero x_0 on any edge, then

$$\frac{\partial u}{\partial \nu} u(x_0) > 0$$

which contradicts the Kirchhoff–Neumann conditions. In particular, any ground state of A is not identically vanishing on any subset of $\mathcal{G}$.

- Due to the Theorem 2.4.16 (Persson theory) we have

$$\Sigma_0 = \inf \sigma(A^{M,m}),$$

then $\Sigma_0 < \Sigma$ implies the existence of ground states of A. In particular, $\Sigma_0 < \Sigma$ can replace the condition that A admits a ground state in the previous statement.

3.4.2.2 The global setting $\mathcal{K} = \mathcal{G}$

Consider now the global case, where we consider the functional

$$E_{\mathrm{NLS}}(\varphi) = \frac{1}{2}\int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) \varphi \right|^2 + m|\varphi|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |\varphi|^p \,\mathrm{d}x, \qquad \|\varphi\|_{L^2} = 1.$$

In the global case Lemma 3.4.3 applies since any ground state of the magnetic Schrödinger operator $A = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m$ is not identically zero. In the following we give a criterion for existence of ground states for the corresponding ground state problem of E_{NLS}.

Proposition 3.4.6. *Assume $\mathcal{G}$ is a locally finite, connected metric graph and $\Sigma_0 < \Sigma$. Then there exists $\hat{\mu} > 0$ such that for all $\mu \in (0, \hat{\mu})$*

$$E_{NLS} = \inf_{\varphi\in D(A)} E_{NLS}(\varphi) < \lim_{R\to\infty} \inf_{\varphi\in D_R(A)} E_{NLS}(\varphi) = \widetilde{E}_{NLS}.$$

Proof. Without loss of generality $\Sigma_0 > 0$; otherwise we simply add a constant to the potential m. Let $0 < \varepsilon < 1$ arbitrary, which we will only fix later. With Proposition 2.5.6 we deduce as in

Lemma 3.4.1 that for sufficiently small $\mu > 0$

$$E_{\text{NLS}}(\varphi) \geq \frac{1-\varepsilon}{2}\left(\int_{\mathcal{G}}\left|\left(i\frac{\mathrm{d}}{\mathrm{d}x}+M\right)\varphi\right|^2 + m|\varphi|^2\,\mathrm{d}x\right) - \frac{C\varepsilon}{2}.$$

Then

$$\widetilde{E}_{\text{NLS}} - E_{\text{NLS}} \geq \frac{1-\varepsilon}{2}\Sigma - \frac{C\varepsilon}{2} - \frac{1}{2}\Sigma_0 = \frac{1}{2}(\Sigma - \Sigma_0) - \frac{\varepsilon}{2}\left(\widetilde{C} + \Sigma\right).$$

Since ε can be chosen arbitrarily small, we have for sufficiently small μ

$$\widetilde{E}_{\text{NLS}} > E_{\text{NLS}}.$$

□

Lemma 3.4.7. *Let $\mathcal{G}$ be a locally finite, connected metric graph. Assume $A = \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + V$ admits a ground state, then*

$$E_t = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_{L^2}^2 = t}} E_{NLS}(u) < \frac{\Sigma_0 t}{2}.$$

Proof. Given a ground state $u \in H^2$ we simply compute analogously as in Lemma 3.4.2

$$E_t < \frac{\Sigma_0 t}{2}.$$

□

Lemma 3.4.8. *Assume $\mathcal{G}$ is a locally finite, connected metric graph and $\Sigma_0 < \Sigma$. Then E_{NLS} is weak limit superadditive, superadditive with respect to the sequence of partitions of unity in Example 2.4.4 and $t \mapsto E_t$ defines a strictly subadditive functional.*

Proof. The proof is analogous to the one in Lemma 3.4.3 by simply replacing $\mathcal{K}$ with the whole graph. $\Sigma_0 < \Sigma$ implies by Theorem 2.4.22

$$\inf \sigma\left(\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m\right) < \inf \sigma_{\text{ess}}\left(\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)^2 + m\right).$$

In particular, there exist discrete eigenvalues below the essential spectrum and A admits a ground state. □

Theorem 3.4.9. *Let $\mathcal{G}$ be a locally finite, connected metric graph. Assume $\Sigma_0 < \Sigma$, then there exists $\hat{\mu} > 0$ such that for $\mu \in (0, \hat{\mu})$ the minimization problem*

$$E_{NLS} = \inf_{\substack{\varphi \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} \frac{1}{2}\int_{\mathcal{G}}\left|\left(i\frac{\mathrm{d}}{\mathrm{d}x} + M\right)\varphi\right|^2 + m|\varphi|^2\,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}}|\varphi|^p\,\mathrm{d}x$$

admits a minimizer.

Proof. By Lemma 3.4.8 the requirements of Theorem 3.2.19 are satisfied. Furthermore the energy inequality in Corollary 3.2.20 is satisfied by Proposition 3.4.6 and we infer the statement. □

3.4.3 Sufficient conditions for the threshold condition for the Schrödinger operators without magnetic potentials

The quantities Σ_0 and Σ appeared already previously in §2.4 as the infimum of the spectrum and essential spectrum of the operators considered respectively. Here we obtain criteria for the threshold condition for the operator

$$A = -\Delta + m$$
$$D(A) = H^2(\mathcal{G}).$$

defined on general locally finite metric graphs satisfying a volume growth assumption, which were not previously considered in the literature to best of our knowledge.

Proposition 3.4.10. *Let $\mathcal{G}$ be a locally finite, connected metric graph and let K be a connected, precompact subgraph. We suppose additionally the volume assumption*

$$|K_{2n} \setminus K_n| = o(n^2) \qquad (n \to \infty). \tag{3.42}$$

Assume $\sigma_{ess}(-\Delta + m) \subset [0, \infty)$ and assume additionally either

(i) $m \in L^1(\mathcal{G}) \cap L^2(\mathcal{G})$ and

$$\int_{\mathcal{G}} m \,\mathrm{d}x < 0$$

(ii) or $m < 0$ on $\mathcal{G}$.

Then $\Sigma_0 < \Sigma$ (as defined in (3.38) *and* (3.39)*) and there exists $\hat{\mu} > 0$ such that the minimization problem*

$$E^m_{NLS} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} E^m_{NLS}(u) \tag{3.43}$$

admits a minimizer for $\mu \in (0, \hat{\mu})$.

Proof. Consider as a test function Ψ_n as defined in Example 2.4.10, then we only need to show that for n sufficiently high, the Rayleigh quotient

$$\mathcal{R}[\Psi_n] := \frac{\int_{\mathcal{G}} |\Psi_n'|^2 + m|\Psi_n|^2 \,\mathrm{d}x}{\int_{\mathcal{G}} |\Psi_n|^2 \,\mathrm{d}x} < 0.$$

Indeed, since $\|\Psi_n'\|_\infty^2 \leq O(\frac{1}{n^2})$ as $n \to \infty$ we deduce

$$\|\Psi_n'\|_2^2 \leq \|\Psi_n'\|_\infty^2 |K_{2n} \setminus K_n| \to 0 \qquad (n \to \infty).$$

If $m < 0$ then for sufficiently large n and $\varepsilon > 0$ sufficiently small

$$\int_{\mathcal{G}} m|\Psi_n|^2 \,\mathrm{d}x \leq -\left|\{x \in \mathcal{G} : m(x) \leq -\varepsilon\}\right| \varepsilon < 0.$$

If $\int_{\mathcal{G}} m \,\mathrm{d}x < 0$, then

$$\liminf_{n\to\infty} \int_{\mathcal{G}} m|\Psi_n|^2 \,\mathrm{d}x = \int_{\mathcal{G}} m \,\mathrm{d}x < 0$$

by dominated convergence. In particular for n large enough as in the proof of Proposition 3.3.7

$$\int_{\mathcal{G}} m|\Psi_n|^2 \leq \frac{1}{2} \int_{\mathcal{G}} m \,\mathrm{d}x < 0.$$

We deduce $R[\Psi_n] < 0$ and thus $\inf \sigma(-\Delta + m) < 0$. Then $\Sigma_0 < \Sigma$ and we conclude the existence of minimizers of (3.43) by Theorem 3.4.9. $\square$

We finish the section by giving a criterion for the potential m such that

$$\Sigma = \lim_{n\to\infty} \inf_{\substack{u\in D(A) \\ \|u\|_2^2=1,\ \operatorname{supp} u \subset \mathcal{G}\setminus K_n}} \langle u, Au\rangle \geq 0.$$

This in particular implies

$$\sigma_{\text{ess}}(-\Delta + m) \subset [0, \infty).$$

Consider decaying potentials $m = m_2 + m_\infty$ with $m_2 \in L^2(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ such that

$$\sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)| \to 0 \qquad (n \to \infty). \tag{3.44}$$

Proposition 3.4.11. *Let $\mathcal{G}$ be a locally finite metric graph. Assume $m \in L^2 + L^\infty(\mathcal{G})$ satisfying* (3.44). *Let $A = -\Delta + m$, then*

$$\Sigma = \lim_{n\to\infty} \inf_{\substack{u\in H^{2k}(\mathcal{G}) \\ \|u\|_2^2=1,\ \operatorname{supp} u \subset \mathcal{G}\setminus K_n}} \langle u, Au\rangle_{L^2} \geq 0.$$

Proof. Assume u_n is a minimizing sequence, such that $\|u_n\|_{L^2}^2$, $\operatorname{supp} u \subset \mathcal{G} \setminus K_n$ and

$$\langle u_n, Au_n\rangle_{L^2} \to \Sigma.$$

Then

$$\|u_n\|_{H^1} = \langle u_n, Au_n\rangle_{L^2}^2 + \|u_n\|_2^2$$

is uniformly bounded. Integrating by parts we infer

$$\int_{\mathcal{G}} |u_n'|^2 + m|u_n|^2 \, \mathrm{d}x \geq \int_{\mathcal{G}} |u_n'|^2 \, \mathrm{d}x - \widetilde{C}\left(\left(\int_{\mathcal{G}\setminus K_n} |m|^2 \, \mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right).$$

We have

$$\left(\left(\int_{\mathcal{G}\setminus K_n} |m|^2 \, \mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right) \to 0 \qquad (n\to\infty).$$

Thus,

$$\Sigma = \lim_{n\to\infty} \langle u_n, Au_n\rangle_{L^2} \geq 0.$$

□

Theorem 3.4.12. *Let $\mu > 0$ and $2 < p < 6$. Let $\mathcal{G}$ be a locally finite metric graph with at least one ray, and suppose $m \in L^2 + L^\infty(\mathcal{G})$, then E^m_{NLS} is strictly subadditive and*

$$E^m_{NLS} = \inf_{u\in D(E^V_{NLS})} \frac{1}{2}\int_{\mathcal{G}} |u'|^2 + m|u|^2 \, \mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \, \mathrm{d}x$$

admits a minimizer if

$$E^m_{NLS} < \widetilde{E^0_{NLS}}.$$

Proof. As in Lemma 3.4.3 we have weak limit superadditivity and superadditivity with respect to the partition of unity in Example 2.4.10. For the strict subadditivity, analagous to the approach in the proof of Lemma 3.4.3 it is sufficient to show $E_t < tE_1$ for all $t \in (0,1)$ with E_t defined via

$$t \mapsto E_t := \inf_{\substack{u\in H^1(\mathcal{G})\\ \|u\|_2^2 = t}} E^m_{\mathrm{NLS}}(u).$$

Suppose for a contradiction $E_t = tE_1$ for some $t \in (0,1)$, then as in the proof of Lemma 3.4.3 we infer that a mininizing sequence $u \in D(E^m_{\mathrm{NLS}})$ needs to satisfy

$$\int_{\mathcal{G}} |u_n|^p \, \mathrm{d}x \to 0 \qquad (n\to\infty).$$

Hence, $u_n \rightharpoonup 0$ in $H^1(\mathcal{G})$ and by superadditivity with respect to the partition of unity in Example 2.4.10 and Proposition 3.4.11 we infer

$$E_1 = \lim_{n\to\infty} E^m_{\mathrm{NLS}}(u_n) \geq \widetilde{\Sigma} \geq 0.$$

By Remark 3.3.11 we have

$$E^m_{\mathrm{NLS}} \leq E_{\mathrm{NLS}}(\mathbb{R}) < 0$$

and the statement follows since we have

$$\widetilde{E^m_{\text{NLS}}} = \widetilde{E^0_{\text{NLS}}}$$

due to

$$\left(\left(\int_{\mathcal{G}\setminus K_n} |m_2|^2 \,\mathrm{d}x\right)^{1/2} + \sup_{x\in\mathcal{G}\setminus K_n} |m_\infty(x)|\right) \to 0 \qquad (n\to\infty).$$

□

Example 3.4.13. Let $\mathcal{G}$ be a locally finite, connected noncompact metric graph with at least one ray. Consider the NLS energy functional as considered in [AST16]

$$E_{\text{NLS}}(u,\mathcal{G}) = \int_{\mathcal{G}} |u'|^2 \,\mathrm{d}x - \frac{\mu}{p}\int_{\mathcal{G}} |u|^p \,\mathrm{d}x.$$

Consider the minimization problem

$$E_{\text{NLS}}(\mathcal{G}) := \inf_{\substack{u\in H^1(\mathcal{G})\\ \|u\|_2^2=1}} E_{\text{NLS}}(u,\mathcal{G}). \tag{3.45}$$

Then by Theorem 3.4.12 the functional E_{NLS} satisfies the prerequisites of Theorem 3.2.8 and Theorem 3.2.19. As discussed in Remark 3.3.11 we have

$$\widetilde{E_{\text{NLS}}}(\mathcal{G}) := \lim_{n\to\infty} \inf_{\substack{u\in H^1(\mathcal{G})\\ \|u\|_2^2=1,\,\operatorname{supp} u\subset\mathcal{G}\setminus K_n}} E_{\text{NLS}}(u,\mathcal{G}) \le E_{\text{NLS}}(\mathbb{R}). \tag{3.46}$$

If $\mathcal{G}$ is a finite metric graph we have equality in (3.46) due to Lemma 3.3.10. In particular Corollary 3.2.20 gives a generalization of Theorem 1.2.5 Indeed, in [AST16] it was shown that if $\mathcal{G}$ is finite then minimizers of (3.45) exist if

$$E_{\text{NLS}}(\mathcal{G}) < E_{\text{NLS}}(\mathbb{R}). \tag{3.47}$$

Since (3.46) does not guarantee existence by Corollary 3.2.20, under the assumption (3.47), one cannot necessarily extend this result to general locally finite metric graphs. But as we will see in Example 3.4.17, for a class of infinite tree graphs, one can show the reverse inequality

$$\widetilde{E_{\text{NLS}}}(\mathcal{G}) \ge E_{\text{NLS}}(\mathbb{R}). \tag{3.48}$$

In particular one can derive for such graphs satisfying (3.48) existence of minimizers of $E_{\text{NLS}}(\mathcal{G})$ under assumption (3.47).

3.4.4 Application: Schrödinger operators with magnetic potentials on infinite tree graphs

In certain cases as discussed in [BK13, §2.6] the gauge transform G, as defined below, unitarily transforms the Schrödinger operator with magnetic potential into a Schrödinger operator without magnetic potential, and the NLS functional under gauge transform reduces to a problem without magnetic potential and we may apply the results from §3.4.3.

For infinite tree graphs in the context of locally finite, connected metric graphs it is particularly easy to see this. In this context, let $\mathcal{G}$ be an infinite tree graph. Given a vertex v we can define the gauge transform G radially. More precisely, for any $x \in \mathcal{G}$, let γ be the unique simple path from v to x parametrized by arc length, then

$$G : u(x) \mapsto e^{i \int_{\operatorname{im} \gamma} M \, \mathrm{d}\gamma} u(x).$$

Assume $A^M = (i\frac{\mathrm{d}}{\mathrm{d}x} + M)^2 + m$ admits a ground state. In this particular case since

$$G^{-1} A^{M,m} G = -\Delta + m = A^{0,m},$$

this is equivalent to the assertion that $A^{0,m}$ admits a ground state. Indeed, let u_M be a ground state to A^M, then

$$A^{0,m} G^{-1} u_0 = G^{-1} A^{M,m} u_M = \Sigma G^{-1} u_M$$

and $G^{-1} u_M$ is a ground state of $A^{0,m}$. Then we may assume $u_0 > 0$ by phase invariance and the maximum principle. Then u_M does not vanish anywhere. In particular independent of $M \in H^1 + W^{1,\infty}(\mathcal{G})$

$$\begin{aligned}
\Sigma_0^{M,m} &= \inf_{\substack{u \in D(A^{M,m}) \\ \|u\|_2^2 = 1}} \left\langle A^{M,m} u, u \right\rangle = \inf_{\substack{u \in D(A^{0,m}) \\ \|u\|_2^2 = 1}} \left\langle A^{0,m} u, u \right\rangle =: \Sigma_0 \\
\Sigma_R^{M,m} &= \inf_{\substack{u \in D_R(A^{M,m}) \\ \|u\|_2^2 = 1}} \left\langle A^{M,m} u, u \right\rangle = \inf_{\substack{u \in D_R(A^{0,m}) \\ \|u\|_2^2 = 1}} \left\langle A^{0,m} u, u \right\rangle =: \Sigma_R \\
\Sigma^{M,m} &= \lim_{R \to \infty} \Sigma_R^{M,m} = \lim_{R \to \infty} \Sigma_R =: \Sigma
\end{aligned}$$

and in §3.4.3 we gave sufficient conditions for $\Sigma_0 < \Sigma$.

Proposition 3.4.14. *Assume $\mathcal{G}$ is an infinite tree graph, connected and locally finite. Assume $\mathcal{K}$ is a bounded subgraph of $\mathcal{G}$ and $-\Delta + m$ admits a ground state, then the infimization problem*

$$E_{NLS}^{(\mathcal{K})} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i \frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \, \mathrm{d}x - \frac{\mu}{p} \int_{\mathcal{K}} |u|^p \, \mathrm{d}x$$

admits a minimizer for all $\mu > 0$.

Proof. This follows immediately from Theorem 3.4.4 and the unitary equivalence of the problem in absence of a magnetic potential under the gauge transform. □

Proposition 3.4.15. *Assume $\mathcal{G}$ is an infinite tree graph, locally finite and connected. Assume $\mathcal{K}$ is any unbounded subgraph and $\Sigma_0 < \Sigma$ then there exists $\hat{\mu} > 0$, such that the infimization problem*

$$E_{NLS} = \inf_{\substack{\varphi \in H^1(\mathcal{G}) \\ \|\varphi\|_2^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) \varphi \right|^2 + m|\varphi|^2 \,\mathrm{d}x - \frac{\mu}{p} \int_{\mathcal{K}} |\varphi|^p \,\mathrm{d}x.$$

admits a minimizer for all $\mu \in (0, \hat{\mu})$.

Proof. This follows immediately from Theorem 3.4.9 and the unitary equivalence of the problem in absence of a magnetic potential under the gauge transform □

For decaying potentials in Theorem 2.4.20 we discussed criteria such that $\Sigma_0 < \Sigma$ is satisfied. Indeed, for any given locally finite metric graph, one can construct decaying potentials in the following way:

Example 3.4.16. Let $\mathcal{G}$ be a locally finite, connected graph and K a bounded, connected subgraph. Consider the higher-order Schrödinger operator $A = (-\Delta)^k + m$ with potential m. We define a potential m a.e. via

$$\begin{aligned} m\Big|_{K_1} &\equiv -\frac{1}{2} \\ m\Big|_{K_{2n}\setminus K_n} &\equiv -\frac{1}{2^n|K_{2n} \setminus K_n|}, \quad n \geq 2 \end{aligned}$$

on each "annulus" $K_{2n} \setminus K_n$. Then $m \in L^2 \cap L^1(\mathcal{G})$,

$$\int_{\mathcal{G}} m \,\mathrm{d}\mu = -\sum_{n=0}^{\infty} \frac{1}{2^n} < 0$$

and by Proposition 3.4.11 we infer $\inf \sigma_{\mathrm{ess}}(A) \geq 0$. In particular, if $\mathcal{G}$ is an infinite tree graph satisfying the volume growth assumption (3.42), then the prerequisites in Proposition 3.4.10 are satisfied as well and we have

$$\Sigma_0 < \Sigma.$$

In particular Proposition 3.4.14 and Proposition 3.4.15 can be applied to the functional $E_{\mathrm{NLS}}^{(\mathcal{K})}$ with $\mathcal{K} \subset \mathcal{G}$ and there exists $\hat{\mu} > 0$ such that

$$E_{\mathrm{NLS}}^{(\mathcal{K})} = \inf_{\substack{u \in H^1(\mathcal{G}) \\ \|u\|_2^2 = 1}} \frac{1}{2} \int_{\mathcal{G}} \left| \left(i\frac{\mathrm{d}}{\mathrm{d}x} + M \right) u \right|^2 + m|u|^2 \,\mathrm{d}x - \frac{\mu}{p} \int_{\mathcal{K}} |u|^p \,\mathrm{d}x$$

admits a minimizer for $\mu \in (0, \hat{\mu})$. If $\mathcal{K} \subset \mathcal{G}$ is precompact, then minimizers exist for all $\mu > 0$.

For a certain class of infinite tree graphs we can, in a similar way as in Example 3.3.13, give an explicit $\hat{\mu}$ such that for $\mu \in (0, \hat{\mu}]$ the minimization problem E_{NLS} admits a minimizer.

Example 3.4.17. Consider an *unrooted tree graph* $\mathcal{G}$ as considered for instance in [DST19], i.e. there are no vertices of degree 1 apart of vertices at infinity. Such trees in particular satisfy the (H)-condition formulated in [AST15] in the special case of finite metric graphs:

(H) For every point $x \in \mathcal{G}$, there exist two injective curves $\gamma_1, \gamma_2 : [0, +\infty) \to \mathcal{G}$ parametrized by arc length, with disjoint images except on a discrete set of points, and such that $\gamma_1(0) = \gamma_2(0) = x$.

By rearrangement methods one can show for decaying potentials $m = m_2 + m_\infty$ with $m_2 \in L^2(\mathcal{G})$ and $m_\infty \in L^\infty(\mathcal{G})$ satisfying

$$\sup_{x \in \mathcal{G} \setminus K_n} |m_\infty(x)| \to 0 \qquad (n \to \infty)$$

that

$$\begin{aligned} \widetilde{\Sigma}^{(\mu)} &= \lim_{n\to\infty} \inf_{\substack{u \in H^1(\mathcal{G} \\ \|u\|_2^2 = 1,\, \operatorname{supp} u \subset \mathcal{G} \setminus K_n}} E^m_{\mathrm{NLS}}(u) \\ &\geq \lim_{n\to\infty} \inf_{\substack{u \in H^1(\mathcal{G} \\ \|u\|_2^2 = 1,\, \operatorname{supp} u \subset \mathcal{G} \setminus K_n}} E^0_{\mathrm{NLS}}(u) \geq E_{\mathrm{NLS}}(\mathbb{R}), \end{aligned}$$

where by Remark 3.3.11 one has equality if $\mathcal{G}$ contains a ray.

When $V \equiv 0$, by strictness in the rearrangement inequality in Theorem 2.5.5 one can prove nonexistence results similarly as in [AST15]. On the other hand, under the assumption

$$\Sigma_0 = \inf \sigma(-\Delta + m) < 0,$$

as discussed in Example 3.3.13 we have thus the existence of minimizers of E_{NLS} for

$$\mu \in \left[0, \left(\frac{\Sigma_0}{\gamma_p}\right)^{\frac{6-p}{4}}\right]$$

as in Example 3.3.13.

Remark 3.4.18. The arguments in Example 3.4.17 can be applied to all graphs that satisfy the (H)-condition. One can even consider more general graphs as long they satisfy the following weaker version of the (H)-condition:

($\bar{\mathrm{H}}$) There exists a precompact set $K \subset \mathcal{G}$ such that for every point $x \in \mathcal{G} \setminus K$ each connected component of $\mathcal{G} \setminus \{x\}$ is either unbounded or contains K.

In particular, for each x there exist two injective, simple curves $\gamma_1 : [0, 1] \to \mathcal{G}, \gamma_2 : [0, +\infty) \to \mathcal{G}$ with disjoint images except on a discrete set of points, such that $\gamma_1(0) = x = \gamma_2(0)$ and $\gamma_1(1) \in K$. In particular, this property is satisfied for any finite noncompact graph.

Example 3.4.19. Consider the graph consisting of two half-lines and a pendant edge joined at a single vertex (see Figure 3.2), then the graph satisfies the ($\bar{\mathrm{H}}$)-condition but not the (H)-condition and the existence result from Example 3.4.17 as discussed in Remark 3.4.18 is still applicable.

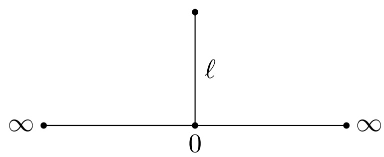


Figure 3.2: Two half-line and a pendant edge. The graph consisting of two half-lines and a pendant edge as an example of a graph that satisfies the ($\bar{\mathrm{H}}$)-condition but not the (H)-condition.

We finish this section by proving Theorem 1.3.4:

Proof of Theorem 1.3.4. Let $\mathcal{G}$ be a locally finite metric tree graph that contains at most finitely many vertices of degree 1. Then there exists a connected, precompact set $K \subset \mathcal{G}$ that contains all vertices of degree 1 by assumption. Consider the set $\overline{\mathcal{G}}$ of points $x \in \mathcal{G}$, such that there exist two injective curves $\gamma_1, \gamma_2 : [0, +\infty) \to \mathcal{G}$ parametrized by arc length, with disjoint images except on a discrete set of points, and such that $\gamma_1(0) = \gamma_2(0) = x$. In particular, if $x \in \overline{\mathcal{G}}$, then

$$\operatorname{im}\gamma_1,\ \operatorname{im}\gamma_2 \subset \overline{\mathcal{G}}.$$

1st Case: $\overline{\mathcal{G}} \neq \emptyset$. Then by assumption $\mathcal{G} \setminus \overline{\mathcal{G}}$ contains at most finitely many connected components. Moreover the connected components are precompact. Otherwise one could construct an injective curve $\gamma_1 : [0, +\infty) \to \mathcal{G} \setminus \overline{\mathcal{G}}$ for all $x \in \mathcal{G} \setminus \overline{\mathcal{G}}$ and since we assumed $\overline{\mathcal{G}} \neq \emptyset$, we can construct $\gamma_2 : [0, +\infty) \to \mathcal{G} \setminus \overline{\mathcal{G}}$. This would then imply that $\mathcal{G} \setminus \overline{\mathcal{G}}$ is necessarily precompact. Since $\mathcal{G}$ is a tree graph, this also implies that each connected component of $\mathcal{G} \setminus \overline{\mathcal{G}}$ contains necessarily a vertex of degree 1. In particular, $\mathcal{G} \setminus \overline{\mathcal{G}}$ admits at most finitely many connected components and is precompact. By construction, $\overline{\mathcal{G}}$ satisfies the (H)-condition and hence $\mathcal{G}$ satisfies the ($\bar{\mathrm{H}}$)-condition. Then as in Example 3.4.17 we have

$$\begin{aligned}\widetilde{\Sigma}^{(\mu)} &= \lim_{n\to\infty} \inf_{\substack{u\in H^1(\mathcal{G} \\ \|u\|_2^2=1,\, \operatorname{supp} u\subset \mathcal{G}\setminus K_n}} E^m_{\mathrm{NLS}}(u) \\ &\geq \lim_{n\to\infty} \inf_{\substack{u\in H^1(\mathcal{G} \\ \|u\|_2^2=1,\, \operatorname{supp} u\subset \mathcal{G}\setminus K_n}} E^0_{\mathrm{NLS}}(u) \geq E_{\mathrm{NLS}}(\mathbb{R})\end{aligned}$$

and we obtain existence of minimizers of E_{NLS} for

$$\mu \in \left[0, \left(\frac{\Sigma_0}{\gamma_p}\right)^{\frac{6-p}{4}}\right].$$

2nd Case: $\overline{\mathcal{G}} = \emptyset$. In particular for each $x \in \mathcal{G}$ there exists only one connected component of $\mathcal{G}$ that contains a vertex at infinity. Assume K is a precompact set that contains all vertices of degree 1, then by assumption for any $x \in \mathcal{G} \setminus K$ the connected components of $\mathcal{G} \setminus \{x\}$ consist of a compact core graph containing all vertices of degree 1 and a half-line. In particular, $\mathcal{G}$ is a finite metric graph and Example 3.3.13 yields the existence of minimizers of E_{NLS} for

$$\mu \in \left[0, \left(\frac{\Sigma_0}{\gamma_p}\right)^{\frac{6-p}{4}}\right].$$

□

Chapter 4

Spectral minimal partitions on graphs

In this chapter we motivate spectral minimal partitions and show their existence, study properties of spectral minimal partitions introduced in §1.2.3 and their corresponding spectral energies. For motivational purposes we discuss the stationary Bose-Einstein condensate equation limiting profiles of solutions and show connections to spectral minimal partitions problems in §4.2. A counterpart for domains can be found for instance in [Tav10, Part I §1], [CTV02], and [CTV03]; the arguments for graphs are loosely based on the respective arguments for domains. In §4.3, existence for a class of spectral minimal partitions is shown using the general existence theory developed in [KKLM21]. In §4.4, which covers the material in [HKMP21a] with only minor changes, we show Theorem 1.3.8 and Theorem 1.3.9. In §4.5, based on [HK21] with only minor changes, we prove interlacing inequalities for spectral minimal energies and show in this context Theorem 1.3.5 and Theorem 1.3.6.

4.1 Overview and definitions

Throughout this chapter we assume $\mathcal{G}$ to be a compact metric graph. Recall from §2.1.4 that $\mathfrak{C}_k = \mathfrak{C}_k(\mathcal{G})$ is the set of connected k-partitions in $\mathcal{G}$ and $\mathfrak{R}_k = \mathfrak{R}_k(\mathcal{G})$ is the set of rigid k-partitions. Let $k \geq 2$ and $\Lambda : \mathfrak{C}_k \to \mathbb{R}$. Then we consider the minimization problem

$$\inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda(\mathcal{P}) \tag{4.1}$$

and we say $\mathcal{P}^*$ is a spectral minimizer of (4.1) if $P^* \in \mathfrak{C}_k$

$$\Lambda(\mathcal{P}^*) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda(\mathcal{P}).$$

We say Λ is lower semi-continuous over a closed subspace A in $\mathfrak{C}_k$, if for

$$\mathcal{P}^{(n)} = (\mathcal{G}_1^{(n)}, \dots, \mathcal{G}_k^{(n)}) \to \mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k),$$

we have

$$\Lambda(\mathcal{P}) \leq \liminf_{n\to\infty} \Lambda(\mathcal{P}^{(n)}),$$

where the partition convergence means that there exists representatives of the canonical cut graphs with $\mathcal{G}_{\mathcal{P}^{(n)}} \to \mathcal{G}_{\mathcal{P}}$ (allowing edge lengths with greater or equal zero in this context; i.e. extending the concept to cut patterns of partitions as introduced in [KKLM21]) in the sense of Definition 2.1.2 (for details see also [KKLM21, §3] regarding the topological issues). If Λ is lower semi-continuous over a closed subspace of $\mathfrak{C}_k$, then the following slightly adapted result from [KKLM21, Theorem 3.13] guarantees existence of minimizers.

Theorem 4.1.1. *Let $k \geq 1$ and let $A \subset \mathfrak{C}_k(\mathcal{G})$. Suppose that the functional $\Lambda : \overline{A} \to \mathbb{R}$ is a lower semi-continuous on A with respect to partition convergence satisfying*

$$\inf\{\Lambda(\mathcal{P}) : \mathcal{P} \in A\}.$$

Suppose in addition that $\Lambda(\mathcal{P}^{(n)}) \to \infty$ whenever there exists clusters $\mathcal{G}^{(n)}$ in $\mathcal{P}^{(n)} \in A$ such that $|\mathcal{G}^{(n)}| \to 0$ as $n \to \infty$, then there is at least one exhaustive k-partition $\mathcal{P}^* \in \overline{A} \cap \mathfrak{C}_k$ realizing

$$\Lambda(\mathcal{P}^*) = \inf\{\Lambda(\mathcal{P}) : \mathcal{P} \in A\}. \tag{4.2}$$

If $A \subset \mathfrak{R}_k(\mathcal{G})$, that is, if we restrict to rigid partitions, then there is at least one exhaustive rigid k-partition $\mathcal{P}^*$ satisfying (4.2).

Let $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ be a connected k-partition in the following. In [KKLM21] the spectral energies

$$\Lambda^N_{k,p}(\mathcal{P}) = \begin{cases} \left(\dfrac{1}{k} \displaystyle\sum_{i=1}^k \mu_2(\mathcal{G}_i)^p \right)^{1/p} & \text{if } p \in (0,\infty), \\ \displaystyle\max_{i=1,\ldots,k} \mu_2(\mathcal{G}_i) & \text{if } p = \infty, \end{cases} \tag{4.3}$$

and

$$\Lambda^D_{k,p}(\mathcal{P}) = \begin{cases} \left(\dfrac{1}{k} \displaystyle\sum_{i=1}^k \lambda_1(\mathcal{G}_i)^p \right)^{1/p} & \text{if } p \in (0,\infty), \\ \displaystyle\max_{i=1,\ldots,k} \lambda_1(\mathcal{G}_i) & \text{if } p = \infty, \end{cases} \tag{4.4}$$

were considered and in [KKLM21, §4] existence of spectral minimizers was shown for

$$\mathcal{L}^{N,r}_{k,p}(\mathcal{G}) = \min_{\mathcal{P}\in\mathfrak{R}_k(\mathcal{G})} \Lambda^N_{k,p}(\mathcal{P}) \quad \text{and} \quad \mathcal{L}^{N,c}_{k,p}(\mathcal{G}) = \min_{\mathcal{P}\in\mathfrak{C}_k(\mathcal{G})} \Lambda^N_{k,p}, (\mathcal{P}) \tag{4.5}$$

the minimum of $\Lambda^N_{k,p}(\mathcal{P})$; and

$$\mathcal{L}^D_{k,p}(\mathcal{G}) = \min_{\mathcal{P}\in\mathfrak{R}_k(\mathcal{G})} \Lambda^D_{k,p}(\mathcal{P}) = \min_{\mathcal{P}\in\mathfrak{C}_k(\mathcal{G})} \Lambda^D_{k,p}(\mathcal{P}) \tag{4.6}$$

the minimum $\Lambda^D_{k,p}(\mathcal{P})$ over all rigid/connected k-partitions, respectively, where we have equality due to [KKLM21, Lemma 4.3]. In §4.2, in the context of the study of k-mixtures of Bose-Einstein condensate equations (c.f. (1.12))

$$\begin{cases} -u_i''(x) + (m_i(x)+\lambda_i)u_i(x) = \mu_i|u_i|^2u_i - \beta\sum_{j\neq i} u_j^2 u_i \\ \displaystyle\sum_{e \text{ incident to } v} \frac{\partial}{\partial\nu} u_i\big|_e(v) = 0, \qquad i = 1,\dots,k. \end{cases} \tag{4.7}$$

other concepts of spectral minimal partitions become relevant. We study solutions $(u_{1,\beta},\dots,u_{k,\beta})$ for (4.7) via the study of Nehari ground states to a corresponding energy functional. In the limit $\beta\to\infty$ in the corresponding solution $(u_{1,\infty},\dots,u_{k,\infty})$ occurs segregation, i.e. $u_{i,\infty}\cdot u_{j,\infty} = 0$ almost everywhere, and the supports of $u_{i,\infty}$ define a partition on $\mathcal{G}$ minimizing the minimal energy $\mathcal{L}^D_{k,4,4}(\mathcal{G})$ (see Theorem 4.2.3), which is a special case of the quantity that we define in the following, in (4.10).

For our purposes we limit ourselves to the case $m_1 \equiv \ldots \equiv m_k \equiv 0$ in §4.3 and define for $\lambda > 0$

$$\|u\|_{1,\lambda} := \left(\|u'\|_2^2 + \lambda\|u\|_2^2\right)^{1/2},$$

which defines an equivalent norm on $H^1(\mathcal{G})$. In §4.3 we consider then the optimal Sobolev constant

$$S_q(\mathcal{G},\mathcal{V}^D) = \inf_{u\in H_0^1(\mathcal{G},\mathcal{V}^D)\setminus\{0\}} S_q(u) := \inf_{u\in H_0^1(\mathcal{G},\mathcal{V}^D)\setminus\{0\}} \frac{\|u\|_{1,\lambda}}{\|u\|_q} \tag{4.8}$$

and study the energy

$$\Lambda^D_{k,q,p}(\mathcal{P}) = \begin{cases} \left(\dfrac{1}{k}\displaystyle\sum_{i=1}^k S_q(\mathcal{G}_i,\partial\mathcal{G}_i)^p\right)^{1/p} & \text{if } p\in(0,\infty), \\ \displaystyle\max_{i=1,\dots,k} S_q(\mathcal{G}_i,\partial\mathcal{G}_i) & \text{if } p=\infty, \end{cases} \tag{4.9}$$

and the corresponding partition problem

$$\mathcal{L}^D_{k,q,p}(\mathcal{G}) = \min_{\mathcal{P}\in\mathfrak{C}_k(\mathcal{G})} \Lambda^D_{k,p}(\mathcal{P}), \tag{4.10}$$

where $\partial\mathcal{G}_i$ is the topological boundary of $\mathcal{G}_i$ in $\mathcal{G}$ as defined in Definition 2.1.17. In §4.3.2 we define a Neumann variant as well. Namely, we define

$$\Lambda^N_{k,q,p}(\mathcal{P}) := \begin{cases} \left(\dfrac{1}{k}\displaystyle\sum_{i=1}^k \mathcal{L}^D_{2,q,\infty}(\mathcal{G}_i)^p\right)^{1/p} & \text{if } p\in(0,\infty), \\ \displaystyle\max_{i=1,\dots,k} \mathcal{L}^D_{2,q,\infty}(\mathcal{G}_i) & \text{if } p=\infty, \end{cases} \tag{4.11}$$

and

$$\mathcal{L}^N_{k,q,p}(\mathcal{G}) = \min_{\mathcal{P}\in\mathfrak{C}_k} \mathcal{L}^N_{k,q,p}(\mathcal{P}). \tag{4.12}$$

We will apply Theorem 4.1.1 for spectral minimal partition problems $\mathcal{L}^N_{k,q,p}(\mathcal{G}), \mathcal{L}^D_{k,qp}(\mathcal{G})$ with the aim to extend the results previously attained in [KKLM21] for (4.6) and (4.5):

Theorem 4.1.2. *Let $\mathcal{G}$ be a compact metric graph, $k \in \mathbb{N}$, $0 < p \leq \infty$ and $1 < q < \infty$, then there exist spectral minimal partitions $\mathcal{P}^D, \mathcal{P}^N$, such that*

$$\mathcal{L}^D_{k,q,p}(\mathcal{G}) = \Lambda^D_{k,q,p}(\mathcal{P}^D)$$
$$\mathcal{L}^N_{k,q,p}(\mathcal{G}) = \Lambda^N_{k,q,p}(\mathcal{P}^N).$$

We return in §4.4 and §4.5 to the spectral minimal partition problems (4.5) and (4.6) and give estimates on the quantities and interlacing inequalities between them. In §4.4 we show spectral inequalities for the quantities in (4.5) and (4.6), which we summarize in §4.4.2. We refer to §1.3.2 for our principal results for §4.4 and §4.5.

4.2 Motivation: stationary Bose–Einstein condensate equation and limiting profiles

In the following we follow §[Tav10, Part §1] closely and will only sketch the arguments in the proofs since we can argue the same way. Consider the system of stationary Bose–Einstein condensate equations ($k \geq 2$)

$$\begin{cases} -u_i''(x) + (m_i(x) + \lambda_i)u_i(x) = \mu_i |u_i|^2 u_i - \beta \sum_{j\neq i} u_j^2 u_i \\ \qquad\qquad u_i \in H^1(\mathcal{G}), \qquad i = 1, \dots, k. \end{cases} \tag{4.13}$$

with $m_i \in L^\infty(\mathcal{G})$, $\lambda_i > -\inf m_i$, $\mu_i > 0$, and $\beta > 0$. We refer to §1.2.3 for the origin of (4.13) in the study of Bose–Einstein condensate and show existence results of solutions in (4.13) and discuss the limiting case $\beta \to \infty$, where the supports of the limiting solutions become disjoint. This so called *phase separation* was previously studied in [CLLL04], [CTV02], [CTV03] and [TV09].

We search for existence of solutions to (4.13) via the study of critical points of the functional

$$J_\beta(u_1,\dots,u_k) = \sum_{i=1}^{k}\left[\frac{1}{2}\int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2\,\mathrm{d}x - \frac{\mu}{4}\int_{\mathcal{G}} |u_i|^4\,\mathrm{d}x\right] + \frac{\beta}{4}\sum_{\substack{i,j=1\\ i\neq j}}^{k}\int_{\mathcal{G}} u_i^2u_j^2\,\mathrm{d}x. \tag{4.14}$$

For $\beta=\infty$ we define

$$J_\infty(u_1,\dots,u_k) = \begin{cases} \displaystyle\sum_{i=1}^{k}\left[\frac{1}{2}\int_{\mathcal{G}} |u_i'|^2 + m_i|u_i|^2\,\mathrm{d}x - \frac{\mu}{4}\int_{\mathcal{G}} |u_i|^4\,\mathrm{d}x\right], & \begin{matrix} u_i\cdot u_j = 0 \text{ a.e.} \\ \text{for all } i\neq j \end{matrix} \\ \infty, & \text{otherwise.} \end{cases} \tag{4.15}$$

Then one way of showing existence of critical points is the consideration of Nehari ground states. We define the Nehari manifold via

$$\begin{aligned} \mathcal{N}_\beta &= \{U=(u_1,\dots,u_k)\in (H^1(\mathcal{G})\setminus\{0\})^k : \partial_{u_i}J_\beta(U)u_i = 0, i=1,\dots,k\} \\ &= \Big\{U=(u_1,\dots,u_k)\in (H^1(\mathcal{G})\setminus\{0\})^k : \\ &\qquad \int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2\,\mathrm{d}x = \mu\int_{\mathcal{G}} u_i^4 - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ i\neq j}}^{k} u_j^2, i=1,\dots,k\Big\}. \end{aligned} \tag{4.16}$$

For $\beta=\infty$ we define

$$\begin{aligned} \mathcal{N}_\infty &= \{U=(u_1,\dots,u_k)\in (H^1(\mathcal{G})\setminus\{0\})^k : u_i\cdot u_j = 0 \text{ a.e. for all } i\neq j, \\ &\qquad \partial_{u_i}J_\infty(U)u_i = 0, i=1,\dots,k\} \\ &= \Big\{U=(u_1,\dots,u_k)\in (H^1(\mathcal{G})\setminus\{0\})^k : u_i\cdot u_j = 0 \text{ a.e. for all } i\neq j \\ &\qquad \int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2\,\mathrm{d}x = \mu\int_{\mathcal{G}} u_i^4, i=1,\dots,k\Big\}. \end{aligned} \tag{4.17}$$

Since by assumption

$$\int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2\,\mathrm{d}x > 0$$

the Nehari manifold $\mathcal{N}_\beta$ necessarily needs to be contained in the Nehari admissible set for $\beta\in(0,\infty)$ via

$$\mathcal{A}_\beta := \left\{U=(u_1,\dots,u_k)\in (H^1(\mathcal{G})\setminus\{0\})^k : \mu\int_{\mathcal{G}} u_i^4 - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ i\neq j}}^{k} u_j^2 > 0, \text{ for } i=\dots,k\right\}. \tag{4.18}$$

and for $\beta = \infty$ via

$$\mathcal{A}_\infty = \{U = (u_1, \dots, u_k) \in (H^1(\mathcal{G}) \setminus \{0\})^k : u_i \cdot u_j = 0 \text{ a.e. for all } i \neq j\}$$

for $\beta = \infty$. We then define for $U = (u_1, \dots, u_k) \in \mathcal{A}_\beta$

$$S_4^\beta(u_1, \dots, u_k) := \sum_{i=1}^k \left(\frac{\left(\int_\mathcal{G} |u_i'|^2 + (m_i + \lambda_i)|u_i|^2 \,\mathrm{d}x\right)^{1/2}}{\left(\int_\mathcal{G} \mu u_i^4 - \int_\mathcal{G} \beta u_i^2 \sum_{\substack{j=1 \\ j\neq i}}^k u_j^2 \,\mathrm{d}x\right)^{1/4}} \right)^4. \tag{4.19}$$

For $\beta = \infty$ we define for $U = (u_1, \dots, u_k) \in \mathcal{A}_\infty$

$$S_4^\infty(u_1, \dots, u_k) := \sum_{i=1}^k \left(\frac{\left(\int_\mathcal{G} |u_i'|^2 + (m_i + \lambda_i)|u_i|^2 \,\mathrm{d}x\right)^{1/2}}{\left(\int_\mathcal{G} \mu u_i^4 \,\mathrm{d}x\right)^{1/4}} \right)^4.$$

In the following we study the existence of minimizers associated to the Nehari ground state energy

$$c_\beta = \inf_{U \in \mathcal{N}_\beta} J_\beta(U) \tag{4.20}$$

for $\beta \in (0, \infty]$ and relate its quantity to a minimization problem associated to S_4^β.

Lemma 4.2.1. *For every $\beta \in (0, \infty)$ we have*

(a) If $U = (u_1, \dots, u_k) \in \mathcal{N}_\beta$, then

$$J_\beta(U) = \frac{1}{4} \sum_{i=1}^k \int_\mathcal{G} |u_i'|^2 + (m_i + \lambda_i)|u_i|^2 \,\mathrm{d}x = \frac{1}{4} \sum_{i=1}^k \int_\mathcal{G} \mu u_i^4 - \int_\mathcal{G} \beta u_i^2 \sum_{\substack{j=1 \\ j\neq i}}^k u_j^2$$

and we have

$$c_\beta = \frac{1}{4} \inf_{U=(u_1,\dots,u_k) \in \mathcal{A}_\beta} S_4^\beta(u_1, \dots, u_k); \tag{4.21}$$

(b) there exists a constant $C > 0$ independent of β such that for all $U = (u_1, \dots, u_k) \in \mathcal{N}_\beta$ we have

$$\|u_i\|_{H^1}, \|u_i\|_4, J_\beta(U) \geq C \qquad \int_\mathcal{G} u_i^4 - \int_\mathcal{G} \beta u_i^2 \sum_{\substack{j=1 \\ j\neq i}}^k u_j^2 \geq C. \tag{4.22}$$

Proof. (a) For each $U = (u_1, \dots, u_k) \in \mathcal{N}_\beta$ and $i = 1, \dots, k$,

$$\frac{1}{4} \int_\mathcal{G} |u_i'|^2 + (m_i + \lambda_i)|u_i|^2 \,\mathrm{d}x = \frac{1}{4} \int_\mathcal{G} u_i^4 - \int_\mathcal{G} \frac{\beta}{4} u_i^2 \sum_{\substack{j=1 \\ i\neq j}}^k u_j^2$$

and we compute

$$J_\beta(U) = \frac{1}{4}\sum_{i=1}^{k}\int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2 \, \mathrm{d}x.$$

Moreover, for any $U = (u_1, \ldots, u_k) \in \mathcal{A}_\beta$ there exists $t_{u_1}, \ldots, t_{u_k} > 0$ such that

$$(t_{u_1}u_1, \ldots, t_{u_k}u_k) \in \mathcal{N}_\beta$$

and we have

$$c_\beta \geq \inf_{u\in\mathcal{A}_\beta} S_4^\beta(U) = \inf_{u\in\mathcal{A}_\beta} S_4^\beta(t_{u_1}u_1, \ldots, t_{u_k}u_k) = \inf_{u\in\mathcal{A}_\beta} J_\beta(t_{u_1}u_1, \ldots, t_{u_k}u_k)) \geq c_\beta.$$

In particular, we infer (4.21).

(b) By assumption

$$\|u_i\|_{H^1}^2 \leq \int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2 \, \mathrm{d}x = \int_{\mathcal{G}} u_i^4 \, \mathrm{d}x - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ i\neq j}}^{k} u_j^2 \, \mathrm{d}x \leq \|u\|_{L^4}^4 \leq C\|u\|_{H^1}^4 \tag{4.23}$$

and we infer

$$\|u\|_{H^1} \geq C^{1/2}.$$

And with (4.23) we infer (4.22).

□

Theorem 4.2.2. *Let $\mathcal{G}$ be a bounded connected graph. Then for $\mu > 0$, $p > 1$ and $\beta > 0$ there exists a critical point $u \in H^2(\mathcal{G})$ of J_β if $\lambda_i > -\inf m_i$ for all $i = 1, \ldots, k$.*

Proof. Consider a minimizing sequence

$$U^{(n)} = (u_1^{(n)}, \ldots, u_k^{(n)}) \in \mathcal{N}_\beta,$$

of (4.22) then by Lemma 4.2.1 (a) there exists $C_1, C_2 > 0$ such that

$$\|u_i^{(n)}\|_{H^1} \leq C_1, \qquad J_\beta(U_n) \leq C_2$$

for all $i = 1, \ldots, k$ and there exists a subsequence still denoted by $u_i^{(n)}$ such that

$$\begin{aligned} u_i^{(n)} &\overset{n\to\infty}{\rightharpoonup} u_i && \text{in } H^1 \\ u_i^{(n)} &\overset{n\to\infty}{\to} u_i && \text{in } L^4. \end{aligned}$$

and we deduce with Lemma 4.2.1 (b), that

$$\int_{\mathcal{G}} |u_i|^4 - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ j\neq i}}^{k} |u_j|^2 = \lim_{n\to\infty} \int_{\mathcal{G}} |u_i^{(n)}|^4 - \int_{\mathcal{G}} \beta |u_i^{(n)}|^2 \sum_{\substack{j=1\\ j\neq i}}^{k} |u_j^{(n)}|^2 \geq C > 0. \tag{4.24}$$

By lower semi-continuity of the norm with respect to weak convergence, then

$$\int_{\mathcal{G}} |u_i'|^2 + (m_i+\lambda_i)|u_i|^2 \,\mathrm{d}x \leq \liminf_{n\to\infty} \int_{\mathcal{G}} |u_i^{(n)\prime}|^2 + (m_i+\lambda_i)|u_i^{(n)}|^2 \,\mathrm{d}x. \tag{4.25}$$

We infer with (4.24), (4.25) and (4.21)

$$c_\beta \leq S_4^\beta(u_1,\dots,u_k) \leq \liminf_{n\to\infty} S_4^\beta(U^{(n)}) = J_\beta(U^{(n)}) = c_\beta.$$

Thus $U=(u_1,\dots,u_i)$ is a minimizer for (4.21) and we infer with Lemma 4.2.1 (a) and (4.24)

$$c_\beta = \int_{\mathcal{G}} \frac{1}{4}\mu u_i^4 - \int_{\mathcal{G}} \frac{\beta}{4} u_i^2 \sum_{\substack{j=1\\ j\neq i}}^{k} u_j^2$$

and we compute

$$\begin{aligned}\left(\int_{\mathcal{G}} \mu u_i^4 - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ j\neq i}}^{k} u_j^2\right)^2 &= 4c_\beta \left(\int_{\mathcal{G}} \mu u_i^4 - \int_{\mathcal{G}} \beta u_i^2 \sum_{\substack{j=1\\ j\neq i}}^{k} u_j^2\right)\\ &= \left(\int_{\mathcal{G}} |u_i|^2 + (m_i+\lambda_i)|u_i|^2 \,\mathrm{d}x\right)^2\end{aligned}$$

and in fact $U=(u_1,\dots,u_k)\in\mathcal{N}_\beta$ is a minimizer of (4.20).

Let $\varphi \in H^1(\mathcal{G})\setminus\{0\}$ fixed but arbitrary. Consider $t\in(-\varepsilon,\varepsilon)$ for $\varepsilon>0$ sufficiently small, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} S_4^{(\beta)}(u_1,\dots,u_i+t\varphi,\dots,u_k) = 0$$

and since $U=(u_1,\dots,u_k)\in\mathcal{N}_\beta$

$$\int_{\mathcal{G}} |u_i|^2 + (m_i+\lambda_i)|u_i^{(n)}|^2 \,\mathrm{d}x = \int_{\mathcal{G}} \mu|u_i|^4 - \int_{\mathcal{G}} \beta|u_i|^2 \sum_{\substack{j=1\\ j\neq i}}^{k} |u_j|^2 \,\mathrm{d}x$$

for all $i=1,\dots,k$ and we infer

$$\int_{\mathcal{G}} u_i'\varphi' \,\mathrm{d}x + (m_i+\lambda_i)u_i\varphi_i \,\mathrm{d}x - \mu_i \int_{\mathcal{G}} |u_i|^2 u_i\varphi + \beta \int \sum_{j\neq i} u_j^2 u_i \varphi \,\mathrm{d}x = 0$$

and $u_1, \dots, u_k$ solves (4.13). The regularity of the solutions follows by elliptic regularity. Since $\varphi \in H^1(\mathcal{G})$ is arbitrary, consider φ supported locally at any vertex $v \in \mathcal{V}$, then by integration by parts we deduce

$$\sum_{e \succ v} \frac{\partial}{\partial \nu} u|_e(v) = \int_{\mathcal{G}} u_i' \varphi' \, \mathrm{d}x + (m_i + \lambda_i) u_i \varphi_i \, \mathrm{d}x - \mu_i \int_{\mathcal{G}} |u_i|^2 u_i \varphi + \beta \int \sum_{j \neq i} u_j^2 u_i \varphi \, \mathrm{d}x = 0 \quad (4.26)$$

and $u \in H^2(\mathcal{G})$. Moreover, since $|u_1| \dots, |u_k|$ is also a minimizer for (4.22) we have $u_1, \dots, u_k \geq 0$, but by Hopf's maximum principle we infer $u_1, \dots, u_k > 0$ since otherwise $u(x_0) = 0$ for any $x_0 \in \mathcal{G}$, without loss of generality $x_0 \in \mathcal{V}$, implies

$$\frac{\partial}{\partial \nu} u_e(x_0) > 0$$

for all edges e incident to x_0 by Hopf's boundary point lemma (see [GT01, Lemma 3.4]), which is in contradiction with (4.26). □

The following result describes the phase separation as $\beta \to \infty$:

Theorem 4.2.3. *Suppose $u_{1,\beta}, \dots, u_{n,\beta}$ are minimizers of (4.22), then there exists a limiting profile $u_{1,\infty}, \dots, u_{k,\infty} \in H^1(\mathcal{G}) \setminus \{0\}$ such that*

$$u_{i,\beta} \overset{\beta \to \infty}{\to} u_{i,\infty} \qquad \textit{in } H^1$$

for all $i = 1, \dots, k$. Furthermore holds

(i) We have

$$c_\beta \to c_\infty \qquad (\beta \to \infty)$$

and $(u_{1,\infty}, \dots, u_{k,\infty}) \in \mathcal{N}_\infty$ minimizes c_∞.

(ii) $\{u_1 > 0\}, \dots, \{u_k > 0\}$ minimizes the equivalent cluster minimization problem

$$c_\infty = \inf_{\substack{\omega_1, \dots, \omega_k \subset \mathcal{G} \\ |\omega_i \cap \omega_j| = 0 \, \textit{for } i \neq j}} \frac{1}{4} \sum_{i=1}^{k} (S_{4,i}(\omega_i))^4$$

where

$$\begin{aligned} S_{4,i}(\omega_i) &:= \inf_{\substack{u \in H_1(\mathcal{G}) \\ \mathrm{supp}(u) \subset \overline{\omega_i}}} S_{4,i}(u) \\ &:= \inf_{\substack{u \in H_1(\mathcal{G}) \\ \mathrm{supp}(u) \subset \overline{\omega_i}}} \frac{\int_{\mathcal{G}} |u'|^2 + (m_i + \lambda)|u|^2 \, \mathrm{d}x}{\int_{\mathcal{G}} |u|^4 \, \mathrm{d}x} \end{aligned}$$

and $S_{4,i}(\{u_i > 0\}) = S_{4,i}(u_i)$ for all $i = 1, \dots, k$.

(iii) if $m = m_1 = \dots = m_k$ and $\lambda = \lambda_1 = \dots = \lambda_k$ for all $i \neq j$, then $(u_{1,\infty}, \dots, u_{k,\infty})$ satisfy

the differential inequalities

$$\begin{gathered}(-\Delta + m + \lambda)u_i \leq \mu|u_{i,\infty}|^2 u_{i,\infty} \\ (-\Delta + m + \lambda)\left(u_{i,\infty} - \sum_{j\neq i} u_{j,\infty}\right) \geq \mu\left(|u_{i,\infty}|^2 u_{i,\infty} - \sum_{j\neq i} |u_{j,\infty}|^2 u_{j,\infty}\right)\end{gathered} \tag{4.27}$$

for all $i = 1, \ldots, k$ in the weak sense.

Remark 4.2.4. The limiting solution $U = (u_{1,\infty}, \ldots, u_{k,\infty})$ as provided in Theorem 4.2.3 satisfies the so-called $\mathcal{S}$-class properties in (4.27). These were already previously considered in [CTV02], [CTV03], [CTV05], [HHT09] among others, and are useful to link spectral minimal partitions to differential equations. Moreover, it was shown that these classes satisfy particularly useful regularity properties.

For graphs similar results hold, despite regularity properties being less of an issue due to the fact that the boundary points are only points, which is for instance reflected in the approach used in [KKLM21], (4.27) is still useful to study existence of solutions of nonlinear eigenvalue equations. In fact, for $k = 2$ due to (4.27) given the limiting solution $U = (u_{1,\infty}, u_{2,\infty})$ as in Theorem 4.2.3 the function $u = u_{1,\infty} - u_{2,\infty}$ satisfies

$$(-\Delta + m + \lambda)u = \mu|u|^2 u$$

in $H^1(\mathcal{G})$ and in fact using elliptic regularity $u \in H^2(\mathcal{G})$ as in the proof of Theorem 4.2.2 (with $\beta = 0$).

Proof of Theorem 4.2.3. By Lemma 4.2.1 (a) we have

$$\frac{1}{4}\sum_{i=1}^{k} \int_{\mathcal{G}} |u_{i,\beta}'|^2 + (m+\lambda)|u_i|^2 \,\mathrm{d}x = c_\beta \leq c_\infty < \infty$$

and for each subsequence we find a subsequence such that

$$\begin{aligned} u_{i,\beta} &\overset{\beta\to\infty}{\rightharpoonup} u_{i,\infty} \qquad \text{in } H^1 \\ u_{i,\beta} &\overset{\beta\to\infty}{\to} u_{i,\infty} \qquad \text{in } L^4 \end{aligned}$$

for each $i = 1, \ldots k$. In particular by Lemma 4.2.1 (b)

$$\int_{\mathcal{G}} |u_{i,\beta}|^4 - \int_{\mathcal{G}} \beta u_{i,\beta}^2 \sum_{\substack{j=1 \\ j\neq i}}^{k} u_{j,\beta}^2 \geq C$$

and we infer

$$\begin{aligned}\int_{\mathcal{G}} u_{i,\infty}^2 \sum_{\substack{j=1\\ j\neq i}}^k u_{j,\infty}^2 &= \lim_{\beta\to\infty} \int_{\mathcal{G}} u_{i,\beta}^2 \sum_{\substack{j=1\\ j\neq i}}^k u_{j,\beta}^2 \\ &\leq \lim_{\beta\to\infty} \frac{1}{\beta}\left(\int_{\mathcal{G}} |u_{i,\beta}|^4 - C\right) = 0.\end{aligned}$$

Hence $u_{i,\infty}\cdot u_{j,\infty} = 0$ a.e. for $i \neq j$. Then with lower semi-continuity of the H^1-norm with respect to weak convergence we infer

$$c_\infty \leq \frac{1}{4}\sum_{i=1}^k \left(S_{4,i}(u_{i,\infty})\right)^4 \leq \lim_{\beta\to\infty} J_\beta(U_{i,\beta}) = \lim_{n\to\infty} c_\beta \leq c_\infty.$$

Then $U_\infty = (u_{1,\infty},\ldots,u_{k,\infty})$ minimizes (4.21) and

$$\lim_{\beta\to\infty} c_\beta = c_\infty.$$

Then as before we infer $U_\infty \in \mathcal{N}_\infty$ and

$$u_{i,\beta} \overset{\beta\to\infty}{\to} u_{i,\infty} \qquad \text{in } H^1.$$

To verify $S_{4,i}(\{u_i>0\}) = S_{4,i}(u_i)$ for each $i=1,\ldots,k$, we proceed similar as before. Since $S_{4,i}(\{u_i>0\}) \leq S_{4,i}(u_i)$ we have

$$c_\infty \leq \inf_{\substack{\omega_1,\ldots,\omega_k\in\mathcal{G}\\ |\omega_i\cap\omega_j|=0 \text{ for } i\neq j}} \frac{1}{4}\sum_{i=1}^k \left(S_{4,i}(\omega_i)\right)^4 \leq \frac{1}{4}\sum_{i=1}^k \left(S_{4,i}(\{u_i>0\})\right)^4 \leq \frac{1}{4}\sum_{i=1}^k \left(S_{4,i}(u_i)\right)^4 = c_\infty$$

and we have $S_{4,i}(\{u_i>0\}) = S_{4,i}(u_i)$ for all $i=1,\ldots,k$ and

$$c_\infty = \inf_{\substack{\omega_1,\ldots,\omega_k\subset\mathcal{G}\\ |\omega_i\cap\omega_j|=0 \text{ for } i\neq j}} \frac{1}{4}\sum_{i=1}^k \left(S_{4,i}(\omega_i)\right)^4.$$

To show the last part of the theorem assume now $m = m_1 = \ldots = m_k$ a.e. for $i \neq j$. Denote in the following

$$\begin{aligned} u_i &= u_{i,\infty} \\ \widehat{u}_i &:= u_{i,\infty} - \sum_{j\neq i} u_{j,\infty}. \end{aligned}$$

Suppose $\varphi > 0$ is an arbitrary function in $H^1(\mathcal{G})$, then we define test functions $U^{(i)} = (v_1^{(i)},\ldots,v_k^{(i)})$ via

$$v_j^{(i)}(t) := \begin{cases} (\widehat{u}_j + t\varphi)^+, & \text{if } j = i \\ (\widehat{u}_j + t\varphi)^-\chi\{u_j>0\}, & \text{if } j \neq i. \end{cases}$$

Then $U^{(i)} \in \mathcal{A}_\infty$ for all $i = 1, \dots, k$ and

$$\frac{1}{4}\sum_{j=1}^{k} S_{4,i}(v_j^{(i)}(t)) - S_{4,i}(u_j) \geq 0.$$

Hence, we have

$$\begin{aligned}
0 &\leq \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}\frac{1}{4}\sum_{j=1}^{k} S_{4,i}(v_j^{(i)}(t)) \\
&= \sum_{j=1}^{k}\int_{\mathcal{G}} \widehat{u}'\varphi'\chi_{\{u_j>0\}} + (m+\lambda)\widehat{u}_i\varphi\chi_{\{u_j>0\}}\,\mathrm{d}x - \mu\int_{\mathcal{G}} |\widehat{u}_i|^2 u_i\varphi\chi_{\{u_j>0\}}\,\mathrm{d}x \\
&= \int_{\mathcal{G}} \widehat{u}'\varphi' + (m+\lambda)\widehat{u}_i\varphi\,\mathrm{d}x - \mu\int_{\mathcal{G}} |\widehat{u}_i|^2 u_i\varphi\,\mathrm{d}x
\end{aligned}$$

where we use Lebesgue's theorem on differentiation under the integral sign and $U = (u_1, \dots, u_k) \in \mathcal{N}_\infty$ in the first step. In particular we infer

$$(-\Delta + m)\left(u_{i,\infty} - \sum_{j\neq i} u_j\right) \geq \mu\left(|u_i|^2 u_i - \sum_{j\neq i}|u_j|^2 u_j\right).$$

On the other hand, suppose now

$$v_j^{(i)}(t) := \begin{cases} u_j, & j \neq i \\ (u_j - t\varphi)^+, & j = i. \end{cases}$$

As in the previous step we infer

$$0 \leq \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0}\frac{1}{4}\sum_{j=1}^{k} S_{4,i}(v_j^{(i)}(t))$$

and we conclude similarly as in the previous step

$$(-\Delta + m + \lambda)u_i \leq \mu|u_i|^2 u_i.$$

This concludes the proof. □

4.3 Existence Results and Spectral Estimates

Theorem 4.2.3 relates the existence of limiting profiles in (4.13) with existence of spectral minimizers. We may generalize this approach using Theorem 4.1.1 to study spectral minimal partition problems

$$\mathcal{L}^D_{k,q,p}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda^D_{k,q,p}(\mathcal{P}), \qquad \mathcal{L}^N_{k,q,p}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda^N_{k,q,p}(\mathcal{P})$$

with $2 \leq q < \infty$ and $\frac{1}{2} < p < \infty$ as defined in §4.1. Theorem 4.2.3 ensures then existence of spectral minimizers for a special spectral minimal partition:

Example 4.3.1. Let $m_1 = \cdots = m_k = 0$ and $\lambda > 0$. Due to Theorem 4.2.3 (ii), the associated faithful partition consisting of clusters associated to the supports of $u_{1,\infty}, \ldots, u_{k,\infty}$, constructed as in Theorem 4.2.3, is then a spectral minimizer of

$$\mathcal{L}^D_{k,4,4}(\mathcal{G}) = \inf_{\mathcal{P}\in\mathfrak{C}_k} \Lambda^D_{k,4,4}(\mathcal{P}).$$

4.3.1 On Dirichlet partitions

We will apply Theorem 4.1.1 to the minimization problem

$$\mathcal{L}^D_{k,q,p}(\mathcal{G}) := \inf_{\mathcal{P}\in\mathfrak{C}_k} \left(\frac{1}{k}\sum_{i=1}^{k}(S_q(\mathcal{G}_i, \partial\mathcal{G}_i))^p\right)^{1/p},$$

where

$$S_q(\mathcal{G}_i, \partial\mathcal{G}_i) := \inf_{u\in H^1_0(\mathcal{G}_i,\partial\mathcal{G}_i)} \frac{\|u\|_{1,\lambda}}{\|u\|^q}.$$

Lemma 4.3.2. *Let $\mathcal{G}_n$ be metric graphs given an underlying combinatorial graph $G = (V; E)$ such that $\mathcal{G}_n \to \mathcal{G}$ and $\mathcal{G}$ is a nontrivial metric graph, i.e. $|\mathcal{G}| \neq 0$, and suppose $\mathcal{V}^D_{\mathcal{G}_n}, \mathcal{V}^D_{\mathcal{G}}$ is associated to the same subset V^D_G of the vertex set on the combinatorial graph G (as defined in §2.1.4), then*

$$S_q(\mathcal{G}_n, \mathcal{V}^D_{\mathcal{G}_n}) \to S_q(\mathcal{G}, \mathcal{V}^D_{\mathcal{G}}) \qquad (n\to\infty).$$

Furthermore, if $|\mathcal{G}_n| \to 0$, then $S_q(\mathcal{G}_n) \to \infty$ as $n \to \infty$.

Remark 4.3.3. Suppose $\mathcal{G}_n \to \mathcal{G}$ as $n \to \infty$, then we suppose that $\mathcal{G}_n, \mathcal{G}$ have the same underlying combinatorial graph and that $\mathcal{V}^D_{\mathcal{G}_n}, \mathcal{V}^D_{\mathcal{G}}$ corresponds to the same subset on the vertex set V^D. This is for instance the case if we consider partition $\mathcal{P}_n = (\mathcal{G}^{(n)}_1, \ldots, \mathcal{G}^{(n)}_k)$, $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$ with $\mathcal{G}_{\mathcal{P}_n} \to \mathcal{G}_{\mathcal{P}}$, where we set the Dirichlet set as a boundary set of the clusters since the boundary set of the partitions as a subset of vertex set of underlying combinatorial graph stay invariant.

Proof of Lemma 4.3.2. Let us identify the underlying combinatorial graph $G = (V; E)$ with the equilateral metric graph for which each edge has length 1. Furthermore, let $\ell_{e,n}, \ell_e$ be the length associated to an edge $e \in E$ for $\mathcal{G}_n$ and $\mathcal{G}$ respectively, then we define for $u \in H_0^1(G, V^D)$

$$S_{q,\boldsymbol{\ell}}(u) := \begin{cases} \dfrac{\left(\sum_{\substack{e\in E\\ \ell_e\neq 0}} \frac{1}{\ell_e}\|u_e'\|_2^2 + \lambda \ell_e \|u_e\|_2^2\right)^{1/2}}{\left(\sum_{\substack{e\in E\\ \ell_e\neq 0}} \ell_e \|u_e\|_q^q\right)^{1/q}}, & (\ell_e = 0 \underset{\text{for all } e\in E}{\Longrightarrow} u_e \equiv \text{const.}) \\ \infty, & \text{otherwise.} \end{cases}$$

By a rescaling argument we deduce

$$S_q(\mathcal{G}_n, \mathcal{V}^D) = \inf_{u\in H_0^1(G,\mathcal{V}^D)} S_{q,\boldsymbol{\ell}_n}(u)$$

By the direct method of the calculus of variation there exists $u_n \in H^1(G, \mathcal{V}^D)$ such that

$$S_q(\mathcal{G}_n, \mathcal{V}^D) = S_{q,\boldsymbol{\ell}_n}(u_n)$$

and since by assumption $|\mathcal{G}| > 0$ there exists an edge $e \in E$ and $C, \varepsilon > 0$ such that

$$C > \ell_e^n \geq \varepsilon > 0$$

for sufficiently large n and

$$\begin{aligned} S_{q,\boldsymbol{\ell}_n}(u_n) &= S_q(\mathcal{G}_n, \mathcal{V}^D_{\mathcal{G}_n}) \\ &\leq \inf_{u\in H_0^1(0,1)\setminus\{0\}} \frac{\left(\frac{1}{\varepsilon}\|u'\|_2^2 + \lambda C\|u\|_2^2\right)^{1/2}}{\|u\|_q} < \infty. \end{aligned}$$

Then for any subsequence of $u_{n,e}$ there exists a weakly convergent subsequence such that

$$u_{n,e} \rightharpoonup u_e \qquad (n \to \infty)$$

weakly in $H^1(0,1)$ for all $e \in E$ such that $\ell_e > 0$. In particular with lower semicontinuity with respect to weak convergence and strong convergence in L^q and L^2 by Rellich-Kondrachov for a subsequence we have

$$\begin{gathered} \|u_e'\|_2^2 \leq \liminf_{n\to\infty} \|u_{n,e}'\|_2^2 \\ \|u_e\|_2^2 = \lim_{n\to\infty} \|u_{n,e}\|_2^2, \|u_e\|_q^q = \lim_{n\to\infty} \|u_{n,e}\|_q^q. \end{gathered}$$

In particular, if $\ell_{n,e} \to 0$ as $n \to \infty$ for any edge, then $u_e \equiv$ const. and we have

$$\liminf_{n\to\infty} S_q(\mathcal{G}_n) = \liminf_{n\to\infty} S_{q,\boldsymbol{\ell}_n}(u_n) \geq \liminf_{n\to\infty} S_{q,\boldsymbol{\ell}}(u) \geq S_q(\mathcal{G}).$$

On the other hand,

$$\limsup_{n\to\infty} S_q(\mathcal{G}_n) \leq \limsup_{n\to\infty} S_{q,\boldsymbol{\ell}_n}(u) = S_{q,\boldsymbol{\ell}}(u) = S_q(\mathcal{G}).$$

Then we have

$$\liminf_{n\to\infty} S_q(\mathcal{G}_n) \geq S_q(\mathcal{G}) \geq \limsup_{n\to\infty} S_q(\mathcal{G}_n)$$

and we infer

$$S_q(\mathcal{G}_n, \mathcal{V}^D) \to S_q(\mathcal{G}, \mathcal{V}^D) \qquad (n \to \infty).$$

□

The following theorem shows the first part of Theorem 4.1.2:

Theorem 4.3.4. *Let $k \in \mathbb{N}$ and $0 < p \leq \infty$ and $1 < q < \infty$, then there exists a spectral minimal partition $\mathcal{P} = (\mathcal{G}_1, \ldots, \mathcal{G}_k)$, such that*

$$\mathcal{L}^D_{k,p}(\mathcal{G}) = \Lambda^D_{k,q,p}(\mathcal{G}).$$

Proof. By Lemma 4.3.2 we have continuity on A with respect to partition convergence. In fact, suppose there exists a cluster $\mathcal{G}_n$ in $\mathcal{P}_n \in A$ such that $|\mathcal{G}_n| \to 0$. For an interval I and $H^1_0(I)$ with at least one Dirichlet end point we have

$$\|u\|_q \leq |I|^{1/q}\|u\|_\infty \leq |I|^{1/q+1/4}\|u\|_{1,\lambda}$$

and we infer

$$S_q(I) \geq \frac{1}{|I|^2}.$$

Then using decreasing rearrangement and Polya-Szego (see Theorem 2.5.5) we infer

$$S_q(\mathcal{G}_n) \geq S_q((0, |\mathcal{G}_n|)) \geq \frac{1}{|\mathcal{G}_n|^2} \to \infty \qquad (n \to \infty).$$

In particular, this implies $\Lambda^D_{k,q,p}(\mathcal{P}_k) \to \infty$ and by Theorem 4.1.1 we infer the existence of a partition $\mathcal{P}$ satisfying

$$\mathcal{L}^D_{k,q,p}(\mathcal{G}) = \Lambda^D_{k,q,p}(\mathcal{P}).$$

□

4.3.2 On Neumann Partitions

We propose an analogue of a Neumann partition problem in this context and will apply Theorem 4.1.1 to the minimization problem

$$\begin{aligned}\mathcal{L}^N_{k,q,p} &:= \inf_{(\mathcal{G}_1,\dots,\mathcal{G}_k)\in\mathfrak{C}_k} \Lambda^N_{k,q,p} := \inf_{(\mathcal{G}_1,\dots,\mathcal{G}_k)\in\mathfrak{C}_k} \left(\frac{1}{k}\sum_{i=1}^k (\mathcal{L}^D_{2,q,\infty}(\mathcal{G}_i))^p\right)^{1/p} \\ &= \inf_{\substack{(\mathcal{G}_1^+,\mathcal{G}_1^-,\dots,\mathcal{G}_k^+,\mathcal{G}_k^-)\in\mathfrak{C}_{2k}\\ G_j^+\sim G_j^- \text{ for all } j=1,\dots,k}} \left(\frac{1}{k}\sum_{i=1}^k \left(\max\left\{S^q(\mathcal{G}_i^+,\partial\mathcal{G}_i^+), S^q(\mathcal{G}_i^-,\mathcal{G}_i^-)\right\}\right)^p\right)^{1/p}.\end{aligned} \tag{4.28}$$

This shows the second part of Theorem 4.1.2 and together with Theorem 4.3.4 concludes the proof.

Theorem 4.3.5. *Let $k \in \mathbb{N}$, $0 < p \le \infty$ and $1 < q < \infty$, then there exists a spectral minimal partition $\mathcal{P} = (\mathcal{G}_1,\dots,\mathcal{G}_k)$, such that*

$$\mathcal{L}^N_{k,q,p}(\mathcal{G}) = \Lambda^N_{k,q,p}(\mathcal{P}).$$

Proof. With (4.28) we have an equivalent minimization problem given a $2k$-partition

$$(\mathcal{G}_1^+,\mathcal{G}_1^-,\dots,\mathcal{G}_k^+,\mathcal{G}_k^-) \in \mathfrak{C}_{2k}(\mathcal{G})$$

such that $\mathcal{G}_i^+$ and $\mathcal{G}_i^-$ are neighbors for all $i = 1,\dots,k$. It is easy to verify that the neighboring conditions are preserved under partition convergence (since the underlying combinatorial graph of the canonical graphs are identical up to vanishing edge lengths) and with Lemma 4.3.2 we infer continuity with respect to partition convergence. And as in the proof of Theorem 4.3.4 we can show that if there exists a sequence of $\mathcal{G}_n$ such that $|\mathcal{G}_n| \to 0$, then

$$\Lambda^N_{k,q,p}(\mathcal{G}_n) \to \infty \qquad (n \to \infty).$$

In particular, we infer existence of minimizers by Theorem 4.1.1. $\square$

We want to give a particular example in the following:

Example 4.3.6. Suppose $\mathcal{G}$ is a compact, finite metric graph and $2 < p \le \infty$ and $\mu = \lambda = 0$, then

$$S_2^2(\mathcal{G}^+) = \lambda_1(\mathcal{G}^+).$$

In particular, since

$$\mu_2(\mathcal{G}) = \mathcal{L}^D_{2,\infty}(\mathcal{G}) = \left(\mathcal{L}^D_{2,2,\infty}(\mathcal{G})\right)^2$$

the expression (4.28) reduces to

$$\left(\mathcal{L}^N_{k,2,2p}(\mathcal{G})\right)^2 = \mathcal{L}^N_{k,p}(\mathcal{G}) = \inf_{(\mathcal{G}_1,\dots,\mathcal{G}_k)\in\mathfrak{C}_k} \left(\frac{1}{k}\sum_{i=1}^k (\mu_2(\mathcal{G}_i))^p\right)^{1/p}$$

By Example 4.3.6 we see that (4.28) generalizes the Neumann partitions associated to $\mathcal{L}^N_{k,p}(\mathcal{G})$ as defined in (4.5).

4.4 Spectral estimates

4.4.1 Preliminaries: Isoperimetric inequalities

The first isoperimetric inequality for metric graphs was discovered by Nicaise 35 years ago; it is sharp, as shown by Friedlander 20 years later. However, it has been observed by several authors that special classes of graphs allow for improved isometric inequalities:

Proposition 4.4.1. *Let $\mathcal{G}$ be any compact connected metric graph. Then the following assertions hold.*

(1) We have

$$\lambda_1(\mathcal{G}) \geq \frac{\pi^2}{4|\mathcal{G}|^2} \qquad \textit{and} \qquad \mu_2(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2},$$

where in the first case $\mathcal{G}$ is equipped with at least one Dirichlet vertex. Equality in either inequality implies that $\mathcal{G}$ is a path graph (interval) of length $|\mathcal{G}|$, with a Dirichlet vertex at exactly one endpoint and the standard (Neumann) condition at the other in the first case, and standard (Neumann) conditions at both endpoints in the second case.

(2) If additionally (possibly upon identifying all Dirichlet vertices) $\mathcal{G}$ is doubly connected, then we have

$$\lambda_1(\mathcal{G}) \geq \frac{\pi^2}{|\mathcal{G}|^2} \qquad \textit{and} \qquad \mu_2(\mathcal{G}) \geq \frac{4\pi^2}{|\mathcal{G}|^2}, \tag{4.29}$$

*In this case, equality is attained only by 2-regular pumpkin chains (second case), or 2-regular pumpkin chains with two edges of equal length attached to one of the endpoints and the degenerate case of an interval with two Dirichlet endpoints (*caterpillar graphs*, first case).*

The inequalities in (1) may be found in [Nic87, Théorème 3.1]. For the characterization of equality, see for example [Fri05, Theorem 1]. For the inequalities in (2) we refer to [BL17a, Theorem 2.1] and [BKKM17, Theorem 3.4 and Lemma 4.3].

4.4.2 Main results: asymptotic behavior of the optimal energies and partitions

We start by summarizing our principal results, which give concrete two-sided bounds on the quantities $\mathcal{L}^D_{k,p}(\mathcal{G})$, $\mathcal{L}^N_{k,p}(\mathcal{G})$ and $\mathcal{L}^{N,c}_{k,p}(\mathcal{G})$, and as a consequence describe their asymptotic behavior, previously summarized in §1.3.2. Actually, we can say more, both about the asymptotic behavior of the clusters of the optimal partitions, and in terms of concrete two-sided bounds on these quantities for finite k. The compact, connected metric graph $\mathcal{G}$ will be fixed throughout, and we recall that $\mathcal{G}$ is taken to have $|\mathcal{E}| \geq 1$ edges, total length L, and $|N|$ vertices of degree one.

Theorem 4.4.2. *Let $p \in [1, \infty]$. Then*

$$\frac{\pi^2}{4kL^2}\left(k^3 + 3(k - \beta - |N|)^3\right) \leq \mathcal{L}^D_{k,p}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\left(k + \left(|\mathcal{E}| - 1 - \left\lfloor \frac{|N|}{2} \right\rfloor\right)\right)^2$$

for all sufficiently large $k \geq 2$, in particular for

$$k \geq \max\left\{\beta + |N|, \frac{L}{\ell_{\min}} + |\mathcal{E}| - 1\right\}.$$

In particular,

$$\mathcal{L}^D_{k,p}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty. \tag{4.30}$$

This theorem will be an immediate consequence of the results of §4.4.3.1 and §4.4.4.1; see in particular Theorems 4.4.10 and 4.4.18. Actually, we can give slightly sharper (but often more involved) lower bounds in some cases; in addition to Theorem 4.4.10 we mention Corollary 4.4.24.

Theorem 4.4.3. *Let $p \in [1, \infty]$. Then*

$$\frac{\pi^2}{L^2}k^2 \leq \mathcal{L}^{N,c}_{k,p}(\mathcal{G}) \leq \mathcal{L}^N_{k,p}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\bigl(k + (|\mathcal{E}| - 1)\bigr)^2. \tag{4.31}$$

for all $k \geq 1$ in the case of the lower bound, and for all sufficiently large k in the case of the upper bound, in particular for $k \geq 5|\mathcal{E}| - 1$. In particular,

$$\mathcal{L}^{N,c}_{k,p}(\mathcal{G}),\, \mathcal{L}^N_{k,p}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty. \tag{4.32}$$

This theorem follows from results in §4.4.3.2 and §4.4.4.2, in particular Theorems 4.4.13 and 4.4.20 (the latter in conjunction with Remark 4.4.21). In this case, it is possible to say a fair amount about when there is equality in the lower bound in (4.31); see Propositions 4.4.15 and 4.4.16.

We can also give a description of the asymptotic behavior of the minimal partitions realizing $\mathcal{L}^D_{k,p}$, $\mathcal{L}^N_{k,p}$ etc. It is perhaps not surprising that for k large enough all clusters become either intervals or stars, just as is the case for both the nodal and the Neumann domains of the k-th eigenfunction of the Laplacian on the whole graph, see [ABBE20, Proposition 7.4]. Our main result states that in fact, for any $p \in [1, \infty]$, asymptotically all clusters are of length of order $1/k$: no clusters can remain too "large".

Theorem 4.4.4. *Fix $p \in [1, \infty]$ and, for each $k \geq 2$, let $\mathcal{P}_k^N$, $\widetilde{\mathcal{P}}_k^N$ and $\mathcal{P}_k^D$ be any admissible partitions realizing $\mathcal{L}_{k,p}^N(\mathcal{G})$, $\mathcal{L}_{k,p}^{N,c}(\mathcal{G})$ and $\mathcal{L}_{k,p}^D(\mathcal{G})$, respectively. Denote the size of the largest cluster of each by $L_{\max}^{N,r}(k)$, $L_{\max}^{N,c}(k)$ and $L_{\max}^D(k)$, respectively. Then*

$$L_{\max}^{N,r}(k),\, L_{\max}^{N,c}(k),\, L_{\max}^D(k) = \mathcal{O}(k^{-1}) \qquad \textit{as } k \to \infty.$$

Remark 4.4.5. One of the main open problems in the theory of spectral minimal partitions for planar domains Ω is the so-called *hexagonal conjecture* that seems to go back to Caffarelli and Lin, see [BHH17, § 10.9.1], which postulates that

$$\lim_{k\to\infty} \frac{\mathcal{L}_{k,p}^D}{k} = \frac{\lambda}{|\Omega|}, \tag{4.33}$$

where λ is the lowest eigenvalue of the Dirichlet Laplacian on a regular hexagon of unit area (regular hexagons being the tesselating planar domains with minimal first Dirichlet eigenvalue). Of course, on graphs, the geometric side of this question disappears: the correct counterparts of hexagons are just intervals. However, Theorems 4.4.2 and 4.4.4 still cover the natural *analytic* counterpart of (4.33), that

$$\lim_{k\to\infty} \frac{\mathcal{L}_{k,p}^D}{k^2} = \frac{\pi^2}{L^2},$$

including the "balancing" statement that in the limit the size of the clusters in the optimal partitions becomes uniform, for every fixed $p \in [1, \infty]$.

Due to parallels between the respective proofs in the Dirichlet and Neumann cases, we will group the lower bounds together in §4.4.3 and the upper bounds in §4.4.4; the proof of Theorem 4.4.4 will be given in §4.4.5, where we also collect a couple of results (improved bounds, Corollary 4.4.24, and a monotonicity statement for $\mathcal{L}_{k,p}^N$ as a function of k for k sufficiently large, Theorem 4.4.25) which follow from Theorem 4.4.4. We also show that this monotonicity result does not necessarily hold for all k, see Example 4.4.26. Finally, we recall that §4.4.6 is devoted to the non-existence of a second term (i.e., term of first order) in the asymptotic expansions (4.30) and (4.32). We also set up one of our examples to give an example that there need not be any second term in the Weyl asymptotics for μ_k (see Remark 4.4.29).

4.4.3 Lower bounds

4.4.3.1 Dirichlet partitions

We first consider lower bounds on the optimal Dirichlet partition energy $\mathcal{L}_{k,p}^D(\mathcal{G})$.

Theorem 4.4.6. *Let $\mathcal{G}$ be a compact and connected metric graph with total length $L > 0$. For any $p \in [1, \infty]$ and any $k \geq 2$, we have*

$$\mathcal{L}^D_{k,p}(\mathcal{G}) \geq \frac{\pi^2 k^2}{4L^2}. \tag{4.34}$$

Equality implies that $\mathcal{G}$ is an equilateral k-star $\mathcal{S}_k$.

Observe that the special case of $p = \infty$ can also be obtained from combining [KKLM21, Prop. 8.4] and [Fri05, Thm. 1].

Proof. Since $\mathcal{L}^D_{k,p}(\mathcal{G})$ is monotonically increasing in $p \in [1, \infty]$ (see [KKLM21, Prop. 6.1]), it suffices to prove (4.37) for $p = 1$ only. We suppose that $\mathcal{G}_1, \dots, \mathcal{G}_k$ are the clusters of an optimal partition associated with $\mathcal{L}^D_{k,1}(\mathcal{G})$; then since each has at least one Dirichlet vertex, we may apply the version of Nicaise' inequality for Dirichlet problems cf. Proposition 4.4.1 to obtain $\lambda_1(\mathcal{G}_i) \geq \pi^2/(4|\mathcal{G}_i|^2)$, $i = 1, \dots, k$. Thus, by Jensen's inequality in discrete form applied to the convex map $x \mapsto x^{-2}$, $x > 0$, we find

$$\mathcal{L}^D_{k,1}(\mathcal{G}) = \frac{1}{k}\sum_{i=1}^{k} \lambda_1(\mathcal{G}_i) \geq \frac{\pi^2}{4}\left(\frac{1}{k}\sum_{i=1}^{k} |\mathcal{G}_i|^{-2}\right) \geq \frac{\pi^2 k^2}{4L^2}.$$

This proves (4.34). For the case of equality, first note that there is equality in Proposition 4.4.1.(1) if and only if $\mathcal{G}_i$ is an interval of length $|\mathcal{G}_i|$, with one Dirichlet and one Neumann endpoint (i.e., vertex); this is an immediate consequence of [Fri05, Lemma 3] together with the variational characterization of λ_1. Moreover, equality in Jensen's inequality implies that $|\mathcal{G}_1| = \ldots = |\mathcal{G}_k| = L/k$. Hence equality in (4.34) (for any $p \geq 1$ and any $k \geq 2$) is only possible if all the $\mathcal{G}_i$ are intervals of length L/k with one Dirichlet and one Neumann endpoint. Since the boundary between neighboring clusters is always marked by a Dirichlet vertex, the only possible connected metric graph that can have these graphs as partition clusters is $\mathcal{S}_k$. □

Remark 4.4.7. The theorem contains the statement that the optimal k-partition of an equilateral k-star $\mathcal{S}_k$, for any $p \in [1, \infty]$, is the expected one, i.e., where each edge is a cluster. More interestingly, this partition reflects the nodal pattern of $\lambda_k(\mathcal{S}_k)$; and $\mathcal{S}_k$ is also the (unique) minimizer of $\lambda_k(\mathcal{G})$ among all graphs of fixed total length, as proved by Friedlander [Fri05]. As with Friedlander's inequality, Theorem 4.4.6 implies in particular that the minimal possible values for $\mathcal{L}^D_{k,p}(\mathcal{G})$ (among all possible graphs $\mathcal{G}$ of given length L) do not exhibit the asymptotic behavior $\pi^2 k^2/L^2$ which would be consistent with the Weyl asymptotics of each fixed graph.

In both cases, the divergence from the Weyl asymptotics is due to the factor of 1/4 appearing in Nicaise' inequality for λ_1, which reflects the case of the interval with only one Dirichlet endpoint. To recover the asymptotically correct value, there needs to be a reasonable "distribution" of Dirichlet vertices in the graph; in particular, an improved inequality can only be valid for sufficiently large k or for special classes of graphs. Before stating our improved estimates, we recall that a connected metric graph is called *doubly connected* if it is not simply connected as a metric space, i.e., if at least two edges need to be deleted in order to make it disconnected. We refer to §4.4.6.1 for a detailed discussion of the asymptotics for equilateral stars.

Definition 4.4.8. Let $\mathcal{G}$ be a compact and connected metric graph. We will call a metric subgraph $\mathcal{G}' \subset \mathcal{G}$ a *doubly connected pendant* of $\mathcal{G}$ if $\mathcal{G}'$ has non-empty interior, $\mathcal{G}'$ is doubly connected and there is exactly one edge $\mathsf{e} \in \mathcal{E}$ of strictly positive length connecting $\mathcal{G}'$ with its complement $\mathcal{G} \setminus \mathcal{G}'$. The set of all doubly connected pendants of $\mathcal{G}$ will be denoted by P_2.

Example 4.4.9. Note that Definition 4.4.8 explicitly requires the existence of a *bridge* (of positive length) as a precondition for the existence of any doubly connected pendants. A dumbbell graph (with non-degenerate handle) has two doubly connected pendants, consisting of its two loops. More generally, an $(m, 1, m)$-pumpkin chain (see [BKKM19, § 5]) has, for $m > 1$, two doubly connected pendants (the two m-pumpkins) but Betti number $2(m-1)$. However, figure-eight graphs and, more generally, flower graphs – indeed, all doubly connected graphs – have *none*.

Note that any two distinct doubly connected pendants are disjoint, and that necessarily the Betti number satisfies $\beta \geq |\mathsf{P}_2|$, as any cycles belonging to different doubly connected pendants are necessarily independent.

Theorem 4.4.10. *Let $\mathcal{G}$ be a compact and connected metric graph with total length $L > 0$, $|N|$ vertices of degree one and $|\mathsf{P}_2|$ doubly connected pendants. Fix $k \geq 2$ and $p \in [1, \infty]$. Then for any $k \geq |N| + |\mathsf{P}_2|$ we have*

$$\mathcal{L}_{k,p}^D(\mathcal{G}) \geq \frac{\pi^2}{4kL^2}\left(k^3 + 3(k - |N| - |\mathsf{P}_2|)^3\right). \tag{4.35}$$

Proof. Without loss of generality, we may assume that $k > |N| + |\mathsf{P}_2|$, since (4.35) reduces to (4.34) for $k = |N| + |\mathsf{P}_2|$. Firstly, as before, by monotonicity it is sufficient to show (4.35) for $p = 1$. So suppose that $\mathcal{P} = \{\mathcal{G}_1, \ldots, \mathcal{G}_k\}$ is an optimal k-partition of $\mathcal{G}$ for $\mathcal{L}_{k,1}^D(\mathcal{G})$; then at most $|N|$ clusters of $\mathcal{P}$ can contain a vertex of degree 1 and at most $|\mathsf{P}_2|$ clusters can contain a doubly connected pendant of $\mathcal{G}$. Suppose

$$j_k \leq |N| + |\mathsf{P}_2| < k$$

of the clusters admit at least one vertex of degree 1 or contain a doubly connected pendant; then after a renumbering if necessary we may assume that $\mathcal{G}_{j_k+1}, \ldots, \mathcal{G}_k$ contain neither a vertex of degree 1 of $\mathcal{G}$ nor a doubly connected pendant of $\mathcal{G}$: in particular, each $\mathcal{G}_i$ for $i > j_k$ has at least two boundary vertices that are thus equipped with a Dirichlet condition, and the graph obtained by merging all these vertices of degree 1 is doubly connected. Therefore, Proposition 4.4.1.(2) is applicable to these clusters, yielding $\lambda_1(\mathcal{G}_i) \geq \pi^2/|\mathcal{G}_i|^2$ for $i > j_k$. Now, define

$$L_k := \sum_{i=1}^{j_k} |\mathcal{G}_i|$$

and note that $L_k < L$ holds, since $j_k < k$. Then, applying Proposition 4.4.1.(1) to the other clusters and using Jensen's inequality as in the proof of Theorem 4.4.6, we see that

$$\begin{aligned}
\mathcal{L}^D_{k,1}(\mathcal{G}) = \Lambda^D_1(\mathcal{P}) &= \frac{\sum_{i=1}^{j_k} 4\lambda_1(\mathcal{G}_i) + \sum_{i=j_k+1}^{k} \lambda_1(\mathcal{G}_i)}{4k} + \frac{3(k-j_k)}{4k}\frac{1}{k-j_k}\sum_{i=j_k+1}^{k} \lambda_1(\mathcal{G}_i) \\
&\geq \frac{1}{4k}\sum_{i=1}^{k}\frac{\pi^2}{|\mathcal{G}_i|^2} + \frac{3(k-j_k)}{4k}\frac{1}{k-j_k}\sum_{i=j_k+1}^{k}\frac{\pi^2}{|\mathcal{G}_i|^2} \\
&\geq \frac{1}{4}\frac{\pi^2 k^2}{L^2} + \frac{3(k-j_k)}{4k}\frac{\pi^2(k-j_k)^2}{(L-L_k)^2} \\
&\geq \frac{1}{4}\frac{\pi^2 k^2}{L^2} + \frac{3(k-j_k)}{4k}\frac{\pi^2(k-j_k)^2}{L^2} \\
&= \frac{\pi^2}{4kL^2}\left(k^3 + 3(k-j_k)^3\right) \\
&\geq \frac{\pi^2}{4kL^2}\left(k^3 + 3(k-|N|-|\mathsf{P}_2|)^3\right).
\end{aligned} \tag{4.36}$$

This proves the claim. □

The lower bound in Theorem 4.4.2 is an immediate consequence of (4.35) and the fact that $\beta \leq |\mathsf{P}_2|$. Also observe that if $\mathcal{G}$ is itself doubly connected, then $|N| = |\mathsf{P}_2| = 0$, whence (4.35) reduces to

$$\mathcal{L}^D_{k,p}(\mathcal{G}) \geq \frac{\pi^2 k^2}{L^2}$$

for all $p \in [1,\infty]$ and $k \geq 2$.

The estimate (4.35) is asymptotically sharp, in the sense that for any value of $p, |N|, |\mathsf{P}_2|$ there exists a value of k and a family of graphs $\mathcal{G}_\varepsilon$ such that, for these values of $p, |N|, |\mathsf{P}_2|, k$ there is equality in (4.35) as $\varepsilon \to 0$; see Remark 4.4.12. From the proof of Theorem 4.4.10 we can characterize the case of equality in (4.35):

Remark 4.4.11. Let us briefly discuss the cases of equality in (4.35). We have already seen in Theorem 4.4.6 that equality holds for $k = |N| + |\mathsf{P}_2|$ if and only if $\mathcal{G}$ is the equilateral k-star. In the case $k > |N| + |\mathsf{P}_2|$ we need to analyze the estimates in (4.36). First of all, note that in this case $\mathcal{L}^D_{k,p}(\mathcal{G}) = \mathcal{L}^D_{k,1}(\mathcal{G})$. Now the equalities in the fourth and sixth steps of (4.36) imply $L_k = 0$ and $|N| + |\mathsf{P}_2| = j_k = 0$. Moreover, equality in Jensen's inequality in the third step yields $|\mathcal{G}_i| = \frac{L}{k}$ for $i = 1, \ldots, k$. Finally, equality in the second step, i.e., in Proposition 4.4.1.(2), implies that every cluster $\mathcal{G}_i$ of an optimal k-partition $\mathcal{P}$ is a *caterpillar graph*, i.e. a 2-regular pumpkin chain of length $\frac{L}{k}$ where one of the two end points (of degree two) is equipped with Dirichlet conditions, see also Figure 4.1. Therefore, equality in (4.35) holds for $k > |N| + |\mathsf{P}_2|$ if and only if $\mathcal{G}$ is obtained by arbitrarily gluing a collection of caterpillar graphs at their Dirichlet vertices so that $\mathcal{G}$ has no vertices of degree one – in particular $\mathcal{G}$ has to be doubly connected.

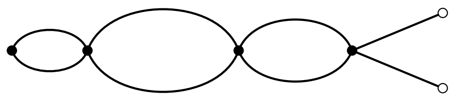


Figure 4.1: Caterpillar graphs. A caterpillar graph with Dirichlet vertices marked in white.

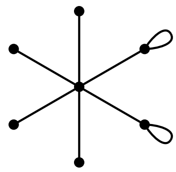


Figure 4.2: Mixed stars and windmill graphs. The graph $\mathcal{W}_{m,n}$ with $m = 2$ and $n = 4$.

Remark 4.4.12. Also note that (4.35) is asymptotically sharp if $|\mathsf{P}_2| > 0$ and $k = |\mathsf{P}_2| + |N|$, in the sense that there exists a family of graphs $\mathcal{G}_\varepsilon$ differing only by their edge lengths, for which there is equality in the limit as $\varepsilon \to 0$. To see this consider, for $m \geq 1$ and $n \geq 0$, an equilateral $m + n$-star graph where m of the degree one vertices are replaced with a loop of sufficiently small length $\varepsilon > 0$; when $n = 0$ these are the graphs considered in [KS18]. The graph $\mathcal{W}_{m,n}$ thus obtained has $|N| = n$ vertices of degree one and $|\mathsf{P}_2| = m$ doubly connected pendants. One can show that for $k = m + n$ an optimal k-partition for $\mathcal{L}^D_{k,p}(\mathcal{W}_{m,n})$ is obtained by cutting through the centre vertex, i.e., it consists of m lasso graphs and n intervals with one Neumann and one Dirichlet vertex. For these graphs and $k = m + n$, the right-hand side of (4.35) is just $\frac{\pi^2 k^2}{4L^2}$, corresponding to the optimal energy $\mathcal{L}^D_{m+n,p}$ of the equilateral $m + n$-star of total length L. If in $\mathcal{W}_{m,n}$ we let the length of the loops tend to zero, then stability of λ_1 with respect to this operation (see [BLS19]) implies that $\mathcal{L}^D_{k,p}(\mathcal{W}_{m,n})$ indeed converges to the right-hand side of (4.35).

4.4.3.2 Neumann partitions

We start with an analogue of Theorem 4.4.6 for Neumann partitions. In comparison with the Dirichlet case, providing a complete description of the graphs for which there is equality seems to be a rather difficult problem.

Theorem 4.4.13. *Let $\mathcal{G}$ be a compact and connected metric graph with total length $L > 0$. For any $p \in [1, \infty]$ and any $k \geq 1$, we have*

$$\mathcal{L}^N_{k,p}(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k,p}(\mathcal{G}) \geq \frac{\pi^2 k^2}{L^2}. \tag{4.37}$$

If $\mathcal{G}$ is not a loop or if $k \geq 2$, then there is equality if and only if there exists a rigid (respectively, a connected) k-partition whose every cluster is an interval of length L/k.

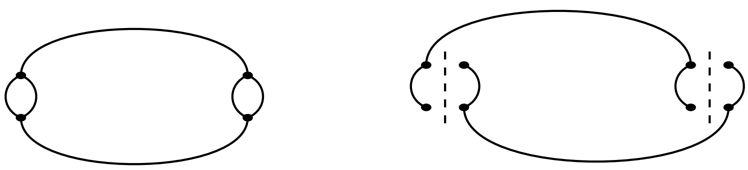


Figure 4.3: Rigid two-partition attaining lower bounds. The graph on the left admits a rigid two-partition into equal intervals (right); thus there is equality in (4.37). We will return to this graph in Example 4.4.26.

Figure 4.4: Connected two-partition attaining lower bounds. The dumbbell graph on the left admits a (non-rigid only) two-partition into equal intervals (right); thus there is equality in the second inequality in (4.37), but the first inequality is strict. Observe that this graph contains an Eulerian path.

See also [KKLM21, §7], where the graphs of Figures 4.3 and 4.4 are considered. Lemma 7.1 of [KKLM21] provides a complement to Theorem 4.4.13: if, for $p = \infty$, there is a k-partition $\mathcal{P}$ of a graph $\mathcal{G}$ whose energy $\Lambda^N_\infty(\mathcal{P})$ equals $\pi^2 k^2/L^2$, then this partition is a minimizer realizing $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G})$, and in particular the minimal energy also equals $\pi^2 k^2/L^2$.

Proof of Theorem 4.4.13. Fix $k \geq 1$. We give the proof for $\mathcal{L}^N_{k,p}$, since the argument for $\mathcal{L}^{N,c}_{k,p}$ is identical (note that due to the statement about equality the statement for $\mathcal{L}^{N,c}_{k,p}(\mathcal{G})$ does not imply the full statement for $\mathcal{L}^N_{k,p}(\mathcal{G})$). As in the proof of Theorem 4.4.6, by monotonicity in p it suffices to prove the inequality for $p = 1$. To this end, we suppose that $\mathcal{G}_1, \dots, \mathcal{G}_k$ are the clusters of an optimal partition associated with $\mathcal{L}^N_{k,1}(\mathcal{G})$, then

$$|\mathcal{G}_1| + \ldots + |\mathcal{G}_k| = L. \tag{4.38}$$

Applying Proposition 4.4.1.(1) to each cluster, we have $\mu_2(\mathcal{G}_i) \geq \pi^2/|\mathcal{G}_i|^2$ for all $i = 1, \dots, k$ and so

$$\mathcal{L}^N_{k,1}(\mathcal{G}) = \frac{1}{k}\sum_{i=1}^k \mu_2(\mathcal{G}_i) \geq \pi^2 \left(\frac{1}{k}\sum_{i=1}^k \frac{1}{|\mathcal{G}_i|^2}\right) \geq \pi^2 \left(\frac{1}{k}\sum_{i=1}^k |\mathcal{G}_i|\right)^{-2} = \frac{\pi^2 k^2}{L^2},$$

where we have applied (4.38) and, as usual, Jensen's inequality.

Equality in (4.37) implies in particular that there is an optimising partition $\{\mathcal{G}_1, \dots, \mathcal{G}_k\}$ yielding equality in the application of Proposition 4.4.1.(1) and Jensen's inequality. This, in turn, requires that the cluster $\mathcal{G}_i$ is an interval of length L/k, for every $i = 1, \dots, k$. □

Remark 4.4.14. Unlike in the Dirichlet case, the condition for equality in the lower bound (4.37) does not prevent the graph from being doubly connected. In other words, we cannot expect an improved version of (4.37) for general doubly connected $\mathcal{G}$. A simple example is given by the loop, for which $\mathcal{L}^N_{k,p}(\mathcal{G}) = \mathcal{L}^{N,c}_{k,p}(\mathcal{G}) = \mathcal{L}^D_{k,p}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$ for all k and all p.

We complement Theorem 4.4.13 with some sufficient conditions for equality which are easy to check.

Proposition 4.4.15. *Suppose that the compact and connected graph $\mathcal{G}$ has an Eulerian path.*

1. *For all $p \in [1,\infty]$ and all $k \geq 1$ there is equality $\mathcal{L}^{N,c}_{k,p}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$ in (4.37).*
2. *If, in addition, for given $k \geq 2$ the girth $\mathfrak{s} \in (0,\infty]$ of $\mathcal{G}$ satisfies $\mathfrak{s} \geq L/k$, then also $\mathcal{L}^N_{k,p}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$ for all $p \in [1,\infty]$.*

For graphs without an Eulerian path, it is still possible for there to be equality for at least some values of k, as the next proposition shows (the graph of Figure 4.3 also provides an example). It seems reasonable to expect that the equality $\mathcal{L}_{k,p}^{N,c}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$ or $\mathcal{L}_{k,p}^{N}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$ for *all* $k \geq 1$ implies that the graph $\mathcal{G}$ has an Eulerian path, but we will not explore this question here.

Proof. Suppose that $\mathcal{G}$ has an Eulerian path. In light of (4.37) and the monotonicity of the optimal energies in p, it suffices to show that under the respective claimed conditions

$$\mathcal{L}_{k,\infty}^{N,c}(\mathcal{G}),\ \mathcal{L}_{k,\infty}^{N}(\mathcal{G}) \leq \frac{\pi^2 k^2}{L^2}.$$

To this end, for $\mathcal{L}_{k,\infty}^{N,c}(\mathcal{G})$ we may easily construct a test k-partition of $\mathcal{G}$ having energy exactly $\pi^2 k^2/L^2$ by cutting the graph along its Eulerian path to create k intervals of length L/k each. For $\mathcal{L}_{k,\infty}^{N}(\mathcal{G})$, we observe that this resulting partition is rigid if $L/k \leq \mathfrak{s}$, since then each cluster may self-intersect at most at its endpoint, which since $k \geq 2$ and $\mathcal{G}$ is connected is necessarily a boundary point. □

We finish this subsection with a complement to the previous proposition, which states that for every graph $\mathcal{G}$ with rationally dependent edge lengths there is a sequence of values k for which there is equality $\mathcal{L}_{k,p}^{N,c}(\mathcal{G}) = \mathcal{L}_{k,p}^{N}(\mathcal{G}) = \frac{\pi^2 k^2}{L^2}$.

Proposition 4.4.16. *Assume that the edge lengths in $\mathcal{G}$ are pairwise rationally dependent, that is, for every pair of edges $\mathsf{e}_1, \mathsf{e}_2 \in \mathcal{E}$ the quotient $|\mathsf{e}_1|/|\mathsf{e}_2|$ is rational. Then there exists some positive integer $m \geq 1$ such that*

$$\mathcal{L}_{jm,p}^{N,c}(\mathcal{G}) = \mathcal{L}_{jm,p}^{N}(\mathcal{G}) = \frac{\pi^2 (jm)^2}{L^2}$$

for any integer $j \geq 1$ and any $p \in [1, \infty]$.

Proof. As $\mathcal{L}_{k,p}^{N}(\mathcal{G}) \geq \mathcal{L}_{k,p}^{N,c}(\mathcal{G})$ both satisfy (4.37) and are monotonically decreasing in $p \in [1, \infty]$ for any $k \geq 1$, it suffices to prove existence of some integer $m \geq 1$ with

$$\mathcal{L}_{jm,\infty}^{N}(\mathcal{G}) \leq \frac{\pi^2 (jm)^2}{L^2}$$

for all $j \geq 1$. First, we observe that the edge lengths are pairwise rationally dependent if and only if there is some positive real number $r > 0$ such that $m_{\mathsf{e}} := |\mathsf{e}|/s$ is an integer for all edges $\mathsf{e} \in \mathcal{E}$. We set

$$m := \sum_{e \in \mathcal{E}} m_e = \frac{L}{r}.$$

For $j \geq 1$ let $\mathcal{P}$ be the rigid jm-partition obtained after cutting through every vertex of $\mathcal{G}$ and then dividing each edge $e \in \mathcal{E}$ into jm_e intervals of equal length s/j, so $\mathcal{P}$ is an equipartition with

$$\mathcal{L}_{jm,\infty}^{N}(\mathcal{G}) \leq \Lambda_{\infty}^{N}(\mathcal{P}) = \frac{\pi^2 j^2}{r^2} = \frac{\pi^2 (jm)^2}{L^2}.$$

This proves the claim. □

Remark 4.4.17. In particular, the previous proposition holds for equilateral graphs, and the proof shows that in this case we may choose m as the cardinality of the edge set in that case.

4.4.4 Upper bounds

4.4.4.1 Dirichlet partitions

We next consider upper bounds on $\mathcal{L}_{k,p}^D(\mathcal{G})$.

Theorem 4.4.18. *Suppose $\mathcal{G}$ is a compact and connected metric graph. Then we have*

$$\mathcal{L}_{k,p}^D(\mathcal{G}) \leq \frac{\pi^2}{L^2}\left(k + \left(|\mathcal{E}| - 1 - \left\lfloor \frac{|N|}{2} \right\rfloor\right)\right)^2 \tag{4.39}$$

for all sufficiently large integers $k \geq 2$ and all $p \in [1, \infty]$, where $|N|$ denotes the number vertices in $\mathcal{G}$ of degree 1. In particular, (4.39) *holds whenever*

$$k \geq \frac{L}{\ell_{\min}} + |\mathcal{E}| - 1,$$

where we recall that $\ell_{\min} = \min_{\mathsf{e}\in\mathcal{E}} |\mathsf{e}|$ is the minimal edge length.

Proof. By monotonicity, it suffices to prove the theorem for $p = \infty$. The proof consists of constructing a "test partition" formed by dividing each edge into a given number of intervals in accordance with its length, where the lengths are suitably chosen.

Without loss of generality, we may assume that $\mathcal{G}$ has at least two edges, otherwise $\mathcal{G}$ would be a cycle or an interval and in both cases (4.39) is obviously satisfied. Let $\mathcal{E}_N$ denote the set of pendant edges in $\mathcal{E}$, i.e those edges containing a vertex of degree one. Note that, since $\mathcal{G}$ has at least two edges and $\mathcal{G}$ is connected, each edge contains at most one vertex of degree one, and thus $|\mathcal{E}_N| = |N|$ holds. Fix an integer $n \geq 1$ large enough, so that $\frac{L}{n} \leq |\mathsf{e}|$ for all $\mathsf{e} \in \mathcal{E}$. Now for each $\mathsf{e} \in \mathcal{E}$ there exists an integer m_e such that

$$m_\mathsf{e} \cdot \frac{L}{n} \leq |\mathsf{e}| < (m_\mathsf{e} + 1)\frac{L}{n}, \tag{4.40}$$

if $\mathsf{e} \in \mathcal{E} \setminus \mathcal{E}_N$ and

$$\frac{2m_\mathsf{e} - 1}{2} \cdot \frac{L}{n} \leq |\mathsf{e}| < \frac{2m_\mathsf{e} + 1}{2} \cdot \frac{L}{n} \tag{4.41}$$

if $\mathsf{e} \in \mathcal{E}_N$. For $\mathsf{e} \in \mathcal{E} \setminus \mathcal{E}_N$ we then partition e into m_e intervals of equal length $\frac{|\mathsf{e}|}{m_\mathsf{e}}$, and for $\mathsf{e} \in \mathcal{E}_N$ we partition e into m_e intervals, so that the interval containing the vertex of degree one has length $\frac{|\mathsf{e}|}{2m_\mathsf{e}+1}$ and the remaining intervals have length $\frac{2|\mathsf{e}|}{2m_\mathsf{e}+1}$. Note that the interval lengths here are chosen so that the first Dirichlet eigenvalue of the longer intervals and the first mixed

Dirichlet–Neumann eigenvalue of the shorter intervals are both equal to $\frac{\pi^2(2m_{\mathsf{e}}+1)^2}{4|\mathsf{e}|^2}$. Let $\mathcal{P}$ be the m-partition thus obtained, where

$$m := \sum_{\mathsf{e}\in\mathcal{E}} m_{\mathsf{e}}.$$

Summing up (4.40) and (4.41) and using $m = \sum_{\mathsf{e}\in\mathcal{E}} m_{\mathsf{e}}$ and $L = \sum_{\mathsf{e}\in\mathcal{E}} |\mathsf{e}|$, we immediately obtain

$$m - \left\lfloor \frac{|N|}{2} \right\rfloor \leq n \leq m + |\mathcal{E}| - 1 - \left\lfloor \frac{|N|}{2} \right\rfloor.$$

By choice of the interval lengths we have

$$\Lambda_\infty^D(\mathcal{P}) \leq \max\left(\max_{1\leq j\leq |N|} \frac{\pi^2(2m_j+1)^2}{4L_j^2}, \max_{|N|+1\leq j\leq |\mathcal{E}|} \frac{\pi^2 m_j^2}{L_j^2} \right) \leq \frac{\pi^2 n^2}{L^2},$$

and thus $\mathcal{L}_{m,\infty}^D(\mathcal{G}) \leq \frac{\pi^2 n^2}{L^2}$. Since $m \geq n - |\mathcal{E}| + 1 + \lfloor \frac{|N|}{2} \rfloor$ and $\mathcal{L}_{k,\infty}^D(\mathcal{G})$ is monotonically increasing in k by [KKLM21, Proposition 4.11], we thus have

$$\mathcal{L}^D_{n-|\mathcal{E}|+1+\lfloor\frac{|N|}{2}\rfloor,\infty}(\mathcal{G}) \leq \frac{\pi^2 n^2}{L^2}.$$

Setting $k := n + |\mathcal{E}| - 1 - \lfloor \frac{|N|}{2} \rfloor$ in the above inequality yields (4.39). $\square$

Remark 4.4.19. It is known that $\mathcal{L}_{k,p}^D(\mathcal{G})$ dominates the k-th lowest eigenvalue μ_k of the Lapacian with standard vertex conditions, cf. [KKLM21, Prop. 8.4]. Hence, in particular, Theorem 4.4.18 yields, for sufficiently large k,

$$\mu_k \leq \frac{\pi^2}{L^2}\left(k - 1 + |\mathcal{E}| - \left\lfloor \frac{|N|}{2} \right\rfloor \right)^2.$$

This estimate can be compared with the upper bound obtained in [BKKM17, Thm. 4.9], which in the present case of Laplacians with no Dirichlet boundary conditions reads

$$\mu_k \leq \frac{\pi^2}{L^2}\left(k - \frac{1}{2} + \frac{3}{2}|\mathcal{E}| - \frac{3}{2}|\mathcal{V}| + \frac{|N|}{2} \right)^2;$$

studying the class of graphs $\mathcal{W}_{m,n}$ (see Example 4.4.9), the latter bound was shown to be asymptotically sharp in [KS18, Theorem 2].

4.4.4.2 Neumann partitions

Our main upper bound in this case reads as follows.

Theorem 4.4.20. *Suppose there exists an n-partition of $\mathcal{G}$ such that every associated cluster $\mathcal{G}_j$ has an Eulerian path, then we have*

$$\mathcal{L}_{k,p}^{N,c}(\mathcal{G}) \leq \mathcal{L}_{k,p}^{N}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\big(k+(n-1)\big)^2$$

for all sufficiently large integers $k \geq 1$ and all $p \in [1,\infty]$. Concretely, we may take $k \geq \max\{4|\mathcal{E}|+n-1, \frac{3L}{2\mathfrak{s}}\}$, where $|\mathcal{E}|$ is the number of edges of $\mathcal{G}$ and $\mathfrak{s} \in (0,\infty]$ its girth.

Remark 4.4.21. Obviously we may always choose n to be the number of edges of $\mathcal{G}$ in Theorem 4.4.20, leading to the bound

$$\mathcal{L}_{k,p}^{N,c}(\mathcal{G}) \leq \mathcal{L}_{k,p}^{N}(\mathcal{G}) \leq \frac{\pi^2}{L^2}\big(k+(|\mathcal{E}|-1)\big)^2.$$

This is valid for all $k \geq 5|E|-1$, as an inspection of the proof shows that $\mathfrak{s}$ may be replaced by the quantity $\max \mathfrak{s}(\mathcal{G}_j)$, where $\mathfrak{s}(\mathcal{G}_j)$ is the girth of $\mathcal{G}_j$, which in the case of each $\mathcal{G}_j$ being an edge is simply ∞. (We still expect this bound on k, like the one in Theorem 4.4.20, to be far from optimal in general.)

Remark 4.4.22. Theorem 4.4.20 can also be used to obtain a different bound on μ_k (and $\mathcal{L}_{k,\infty}^{D}$), cf. Remark 4.4.19, when combined with the interlacing inequalities obtained in [HK21]: there it is shown, using Theorem 4.4.20, that in fact

$$\mu_k(\mathcal{G}) \leq \mathcal{L}_{k,\infty}^{D}(\mathcal{G}) \leq \frac{\pi^2}{L^2}(k+n+\beta-2)^2$$

for all $k \geq \max\{n+1-\beta, 1\}$.

Lemma 4.4.23. *Given an n-partition of $\mathcal{G}$ with associated clusters $\mathcal{G}_1,\dots,\mathcal{G}_n$ we have*

$$\mathcal{L}_{m,p}^{N}(\mathcal{G}) \leq \begin{cases} \left(\displaystyle\sum_{j=1}^{n} \frac{m_j}{m}\mathcal{L}_{m_j,p}^{N}(\mathcal{G}_j)^p\right)^{1/p} & \textit{if } 1 \leq p < \infty, \\ \displaystyle\max_{j=1,\dots,k} \mathcal{L}_{m_j,\infty}^{N}(\mathcal{G}_j) & \textit{if } p = \infty \end{cases}$$

for integers $m_j \geq 1$ and $m = \sum_{j=1}^{n} m_j$. An analogous statement holds for $\mathcal{L}_{m,p}^{N,c}(\mathcal{G})$.

Proof. We restrict ourselves to the case $1 \leq p < \infty$ and rigid partitions, since the other cases can be dealt with analogously. For each j we choose an optimal rigid m_j-partition $\mathcal{P}_j$ of $\mathcal{G}_j$ associated with $\mathcal{L}_{m_j,p}^{N}(\mathcal{G}_j)$ with clusters $\mathcal{G}_j^i$ for $i = 1,\dots,m_j$. We consider the induced rigid m-partition $\mathcal{P}$ of $\mathcal{G}$ given by

$$\mathcal{P} := \bigcup_{j=1}^{n} \mathcal{P}_j.$$

By optimality of $\mathcal{P}_j$ we have

$$m_j \mathcal{L}^N_{m_j,p}(\mathcal{G}_j)^p = \sum_{i=1}^{m_j} \mu_2(\mathcal{G}^i_j)^p.$$

Thus, we obtain

$$\mathcal{L}^N_{m,p}(\mathcal{G}) \leq \Lambda^N_p(\mathcal{P}) = \left(\frac{1}{m} \sum_{j=1}^{n} \sum_{i=1}^{m_j} \mu_2(\mathcal{G}^i_j)^p \right)^{1/p} = \left(\sum_{j=1}^{n} \frac{m_j}{m} \mathcal{L}^N_{m_j,p}(\mathcal{G}_j)^p \right)^{1/p}.$$

This concludes the proof. □

Proof of Theorem 4.4.20. Again, we may restrict ourselves to $\mathcal{L}^N_{k,p}(\mathcal{G})$ and the case $p = \infty$. Similarly to the proof of Theorem 4.4.18, we construct a test partition dividing each Eulerian path into intervals of equal length. Let $k \geq n$ be an arbitrary, sufficiently large integer with $\frac{L}{k} \leq |\mathcal{G}_j|$ for $j = 1, \ldots, n$. For $j = 1, \ldots, n$ there exists an integer $m_j \geq 2$, so that

$$m_j \cdot \frac{L}{k} \leq |\mathcal{G}_j| < (m_j + 1)\frac{L}{k}. \tag{4.42}$$

We set $m := \sum_{j=1}^{n} m_j$. As in the proof of Theorem 4.4.18, it is immediate that

$$m \leq k \leq m + n - 1. \tag{4.43}$$

Since $\mathcal{G}_j$ has an Eulerian path and every cycle in $\mathcal{G}_j$ has length at least

$$\mathfrak{s} \geq \frac{3L}{2k} \geq \frac{m_j + 1}{m_j} \cdot \frac{L}{k} \geq \frac{|\mathcal{G}_j|}{m_j}$$

(if it has any cycles at all), we may apply the result of Proposition 4.4.15 to obtain

$$\mathcal{L}^N_{m_j,\infty}(\mathcal{G}_j) = \frac{\pi^2 m_j^2}{|\mathcal{G}_j|^2}.$$

Thus, Lemma 4.4.23, the previous equality and (4.42) yield

$$\mathcal{L}^N_{m,\infty}(\mathcal{G}) \leq \max_{j=1,\ldots,k} \mathcal{L}^N_{m_j,\infty}(\mathcal{G}_j) = \max_{j=1,\ldots,k} \frac{\pi^2 m_j^2}{|\mathcal{G}_j|^2} \leq \frac{\pi^2 k^2}{L^2}.$$

Since $\mathcal{L}^N_{m,\infty}(\mathcal{G})$ is monotonically increasing in m for sufficiently large m, in particular for $m \geq 4|\mathcal{E}|$ (see [KKLM21, Proposition 4.15] and its proof, and note that under the assumption $k \geq 4|\mathcal{E}| + n - 1$, by (4.43) we also have $m \geq 4|\mathcal{E}|$), we may use (4.43) to conclude

$$\mathcal{L}^N_{k-n+1,\infty}(\mathcal{G}) \leq \mathcal{L}^N_{m,\infty}(\mathcal{G}) \leq \frac{\pi^2 k^2}{L^2}.$$

Finally, replacing k by $k+n-1$ we obtain

$$\mathcal{L}_{k,\infty}^N(\mathcal{G}) \leq \frac{\pi^2(k+n-1)^2}{L^2} = \frac{\pi^2 k^2}{L^2} + \frac{2\pi^2(n-1)k}{L^2} + \frac{\pi^2(n-1)^2}{L^2}.$$

This concludes the proof. □

4.4.5 Asymptotic behavior of the optimal partitions

In this subsection we give the proof of Theorem 4.4.4, which establishes that the maximal cluster size of any optimal partition tends to zero as $k \to \infty$; this relies on the asymptotic behavior of the optimal energies obtained in the previous subsections. We will also give a couple of consequences of this result, as it in turn allows us to refine and sharpen certain statements from the previous subsections.

Proof of Theorem 4.4.4. We first give the proof in the Dirichlet case. Notationally, for any $k \geq 1$ and any $p \in [1,\infty]$ we suppose $\mathcal{P}_{k,p}^* = \{\mathcal{G}_1, \dots, \mathcal{G}_k\}$ to be any admissible k-partition realizing $\mathcal{L}_{k,p}^D(\mathcal{G})$. Fix $p \in [1,\infty]$. As noted in the proof of Theorem 4.4.10, there are at most $|N| + |\mathsf{P}_2|$ clusters of $\mathcal{P}_{k,p}^*$ which contain either a vertex of degree 1 or a doubly connected pendant of $\mathcal{G}$. Denote by $j_k \leq |N| + |\mathsf{P}_2| + 1$ the number of such clusters of $\mathcal{P}_{k,p}^*$, *plus* any cluster of maximal size if there is not already at least one such cluster among them, and suppose without loss of generality that these clusters are numbered $1, \dots, j_k$. Finally, denote by L_k the total length of these j_k clusters; then by construction $L_{\max}^D(k) \leq L_k$. We will prove that in fact $L_k = \mathcal{O}(k^{-1})$ as $k \to \infty$.

Firstly, observe that

$$\Lambda_1^D(\mathcal{P}_{k,p}^*) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty, \tag{4.44}$$

since by monotonicity in p

$$\mathcal{L}_{k,p}^D(\mathcal{G}) = \Lambda_p^D(\mathcal{P}_{k,p}^*) \geq \Lambda_1^D(\mathcal{P}_{k,p}^*) \geq \mathcal{L}_{k,1}^D(\mathcal{G})$$

and both $\mathcal{L}_{k,p}^D(\mathcal{G})$ and $\mathcal{L}_{k,1}^D(\mathcal{G})$ behave like $\frac{\pi^2}{L^2}k^2 + \mathcal{O}(k)$ as $k \to \infty$, by Theorem 4.4.2. Now, with the notation described above, for $k > j_k$, using that $\lambda_1(\mathcal{G}_i) \geq \frac{\pi^2}{4|\mathcal{G}_i|^2}$ for all $i = 1, \dots, j_k$ and $\lambda_1(\mathcal{G}_i) \geq \frac{\pi^2}{|\mathcal{G}_i|^2}$ for all $i = j_k + 1, \dots, k$, the usual argument (see (4.36)) yields

$$\Lambda_1^D(\mathcal{P}_{k,p}^*) \geq \frac{\pi^2}{4}\frac{\pi^2 k^2}{L^2} + \frac{3\pi^2}{4}\frac{(k-j_k)^3}{k(L-L_k)^2}$$

for all $k > j_k$. Suppose now that $L_k \neq \mathcal{O}(k^{-1})$, so that, possibly up to a subsequence, $\lim_{k\to\infty} kL_k = \infty$. We consider the asymptotic behavior of this subsequence of k; our goal is to show that in the asymptotic limit this expression must be larger than allowed by (4.44). Since

j_k remains bounded, the first term in the above estimate converges to zero, and so is certainly of order $\mathcal{O}(1)$, while

$$\frac{(k-j_k)^3}{k(L-L_k)^2} = \frac{k^2}{(L-L_k)^2} + \mathcal{O}(k) \quad \text{as } k \to \infty.$$

But since

$$\frac{k^2}{(L-L_k)^2} = \frac{k^2}{L^2}\frac{1}{(1-\frac{L_k}{L})^2} = \frac{k^2}{L^2}\left(1 + \frac{2}{L}L_k + \mathcal{O}(L_k^2)\right) \quad \text{as } k \to \infty$$

and $\lim_{k\to\infty} kL_k = \infty$ by assumption, this means that

$$\Lambda_1^D(\mathcal{P}_{k,p}^*) \neq \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \quad \text{as } k \to \infty,$$

a contradiction to (4.44).

In the Neumann cases, the argument is similar but simpler owing to the better estimate $\mu_2(\mathcal{G}_i) \geq \frac{\pi^2}{|\mathcal{G}_i|^2}$ for all i. We consider $L_k := L_{\max}^{N,r}(k)$; the case $L_{\max}^{N,c}(k)$ is identical. We fix $p \in [1,\infty]$ and take $\mathcal{P}_{k,p}^* = \{\mathcal{G}_1, \dots, \mathcal{G}_k\}$ to be an optimal k-partition realizing $\mathcal{L}_{k,p}^N(\mathcal{G})$ and suppose that the cluster $\mathcal{G}_1$ has size $|\mathcal{G}_1| = L_{\max}^{N,r}(k)$. As in the Dirichlet case, due to the asymptotics (4.32) of Theorem 4.4.3 we have

$$\Lambda_1^N(\mathcal{P}_{k,p}^*) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \qquad \text{as } k \to \infty. \tag{4.45}$$

On the other hand, for $k \geq 2$,

$$\begin{aligned}\Lambda_1^N(\mathcal{P}_{k,p}^*) &\geq \pi^2\left(\frac{1}{k}|\mathcal{G}_1|^2 + \frac{k-1}{k}\left(\frac{1}{k-1}\sum_{i=2}^{k}|\mathcal{G}_i|^{-2}\right)\right)\\ &\geq \frac{\pi^2}{kL_k} + \pi^2\frac{(k-1)^3}{k(L-L_k)^2}.\end{aligned}$$

Under the assumption that $L_k \neq \mathcal{O}(k^{-1})$, the same argument as in the Dirichlet case now yields that, possibly up to a subsequence, $\Lambda_1^N(\mathcal{P}_{k,p}^*) \neq \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k)$ as $k \to \infty$, contradicting (4.45). □

As a first corollary of Theorem 4.4.4 we obtain an improved version of the lower bound in Theorem 4.4.2 for sufficiently large k; namely, we can drop the term β appearing there.

Corollary 4.4.24. *Let $\mathcal{G}$ be a compact and connected metric graph with total length $L > 0$ and $|N|$ vertices of degree one. Fix $p \in [1,\infty]$. Then there exists $k_0 \geq 2$ such that for all $k \geq k_0$ we have*

$$\mathcal{L}_{k,p}^D(\mathcal{G}) \geq \frac{\pi^2}{4kL^2}\left(k^3 + 3(k-|N|)^3\right).$$

Proof. By monotonicity it is sufficient to prove the assertion for $p = 1$. For $k \geq 2$, we suppose that $\mathcal{P}_k^D$ is an admissible k-partition realizing $\mathcal{L}_{k,1}^D(\mathcal{G})$ and $L_{\max}^D(k)$ is the maximum length of the clusters in $\mathcal{P}_k^D$. By Theorem 4.4.4 we find some $k_0 \geq 2$ such that

$$L^D_{\max}(k) < \ell_{\min}$$

holds for all $k \geq k_0$. In particular, the clusters appearing in $\mathcal{P}_k^D$ are either intervals or stars, where all non-centre vertices are cut points. Let $\mathcal{G}_1, \dots, \mathcal{G}_{|N|}$ be the clusters of $\mathcal{P}_k^D$ that contain the vertices of $\mathcal{G}$ of degree one and let $\mathcal{G}_{|N|+1}, \dots, \mathcal{G}_k$ be the remaining clusters. We then have $\lambda_1(\mathcal{G}_j) = \frac{\pi^2}{4|\mathcal{G}_j|^2}$ for $j = 1, \dots, |N|$ and $\lambda_1(\mathcal{G}_j) \geq \frac{\pi^2}{|\mathcal{G}_j|^2}$ for $j = |N|+1, \dots, k$ by (4.29). Adapting the arguments in (4.36) we obtain

$$\mathcal{L}^D_{k,1}(\mathcal{G}) = \Lambda^D_1(\mathcal{P}^D_k) \geq \frac{\pi^2}{4kL^2}\left(k^3 + 3(k-|N|)^3\right).$$

□

As a second consequence of Theorem 4.4.4 we will prove that, for fixed $p \in [1, \infty]$, $\mathcal{L}^N_{k,p}$ is a monotonically increasing function of k, at least for k sufficiently large.

Note that the monotonicity in the connected case, $\mathcal{L}^{N,c}_{k_2,p}(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k_1,p}(\mathcal{G})$ for all $k_2 \geq k_1 \geq 1$, was established in Proposition 4.11 of [KKLM21], as was Theorem 4.4.25 in the special case $p = \infty$ in [KKLM21, Proposition 4.15] (which was also required in one of the above proofs). In general we cannot necessarily expect $k_0 = 1$, see Example 4.4.26.

Theorem 4.4.25. *Let $\mathcal{G}$ be a compact and connected graph, and fix $p \in [1, \infty]$. Then there exists $k_0 \geq 2$ depending only on $\mathcal{G}$ and p such that*

$$\mathcal{L}^N_{k_2,p}(\mathcal{G}) \geq \mathcal{L}^N_{k_1,p}(\mathcal{G}) \qquad \text{for all } k_2 \geq k_1 \geq k_0.$$

Proof. Since the case $p = \infty$ was treated in [KKLM21], we give the proof for $p \in [1, \infty)$. So fix $p \in [1, \infty)$ and for $k \geq 1$ denote by $\mathcal{P}^*_{k,p} = \{\mathcal{G}_1, \dots, \mathcal{G}_k\}$ any rigid k-partition achieving $\mathcal{L}^N_{k,p}(\mathcal{G})$. By Theorem 4.4.4 there exists some $k_0 = k_0(\mathcal{G}, p)$ such that for every $k \geq k_0$ every cluster of $\mathcal{P}^*_{k,p}$ has length strictly shorter than the shortest edge length of $\mathcal{G}$, and in particular every cluster is a tree, which meets any neighboring cluster of $\mathcal{P}^*_{k,p}$ at a single vertex.

It clearly suffices to prove the theorem for $k_2 = k_1 + 1$. Fix $k \geq k_0 + 1$ and consider $\mathcal{P}^*_{k,p}$; we suppose without loss of generality that

$$\mu_2(\mathcal{G}_k) = \max_{i=1,\dots,k} \mu_2(\mathcal{G}_i) \tag{4.46}$$

and that $\mathcal{G}_{k-1}$ is a neighbor of $\mathcal{G}_k$. We now set $\widetilde{\mathcal{G}}_{k-1} := \mathcal{G}_{k-1} \cup \mathcal{G}_k$; then since $\mathcal{G}_{k-1}$ and $\mathcal{G}_k$ necessarily meet at a single point, by [BKKM19, Theorem 3.10(1)], we have $\mu_2(\widetilde{\mathcal{G}}_{k-1}) \leq \mu_2(\mathcal{G}_{k-1})$. We construct a test $k-1$-partition $\widetilde{\mathcal{P}} := \{\mathcal{G}_1, \dots, \mathcal{G}_{k-2}, \widetilde{\mathcal{G}}_{k-1}\}$ of $\mathcal{G}$; then, again using the fact that $\mathcal{G}_{k-1}$ and $\mathcal{G}_k$ meet at a single point and $\mathcal{P}^*_{k,p}$ was assumed rigid, $\widetilde{\mathcal{P}}$ is a rigid $k-1$-partition of $\mathcal{G}$.

We claim that $\Lambda_p^N(\mathcal{P}_{k,p}^*) \geq \Lambda_p^N(\widetilde{\mathcal{P}})$, from which the conclusion of the theorem in the case $p \in [1,\infty)$ will immediately follow. In fact, this is an elementary calculation using (4.46): it follows from (4.46) that

$$\mu_2(\mathcal{G}_k)^p \geq \frac{1}{k-1}\sum_{i=1}^{k-1} \mu_2(\mathcal{G}_i)^p,$$

and hence

$$\begin{aligned}
\Lambda_p^N(\mathcal{P}_{k,p}^*)^p - \Lambda_p^N(\widetilde{\mathcal{P}})^p &= \frac{1}{k}\sum_{i=1}^{k} \mu_2(\mathcal{G}_i)^p - \frac{1}{k-1}\left(\sum_{i=1}^{k-2} \mu_2(\mathcal{G}_i)^p + \mu_2(\widetilde{\mathcal{G}}_{k-1})^p\right) \\
&= \frac{1}{k}\mu_2(\mathcal{G}_k)^p - \frac{1}{k(k-1)}\sum_{i=1}^{k-2} \mu_2(\mathcal{G}_i)^p + \frac{1}{k}\mu_2(\mathcal{G}_{k-1})^p - \frac{1}{k-1}\mu_2(\widetilde{\mathcal{G}}_{k-1})^p \\
&\geq \frac{1}{k}\mu_2(\mathcal{G}_k)^p - \frac{1}{k(k-1)}\sum_{i=1}^{k-1} \mu_2(\mathcal{G}_i)^p
\end{aligned}$$

since $\mu_2(\mathcal{G}_{k-1}) \geq \mu_2(\widetilde{\mathcal{G}}_{k-1})$. By (4.46), this latter expression is nonnegative, and so we conclude that $\Lambda_p^N(\mathcal{P}_{k,p}^*) \geq \Lambda_p^N(\widetilde{\mathcal{P}})$, as desired. $\square$

Example 4.4.26. We consider the graph $\mathcal{G}$ depicted in Figure 4.3, which in turn was taken from [KKLM21, Example 7.2]; we claim that for this graph $\mathcal{L}_{2,p}^N(\mathcal{G}) < \mathcal{L}_{1,p}^N(\mathcal{G})$ for all $p \in [1,\infty]$, that is, monotonicity in Theorem 4.4.25 fails when $k_1 = 1$ and $k_2 = 2$.

Suppose that $\mathcal{G}$ has total length L and fix $p \in [1,\infty]$. It was already shown in [KKLM21, Example 7.2] that $\mathcal{L}_{2,p}^N(\mathcal{G}) = \frac{4\pi^2}{L^2}$. Next, we note that by definition $\mathcal{L}_{1,p}^N(\mathcal{G}) = \mu_2(\mathcal{G})$. Now by the Band–Lévy inequality, Proposition 4.4.1(2), since $\mathcal{G}$ is not a 2-regular pumpkin chain, we have $\mu_2(\mathcal{G}) > \frac{4\pi^2}{L^2}$. This proves the claimed reverse monotonicity.

4.4.6 Asymptotics on two simple graphs

In the previous subsections, we proved that the minimal energies $\mathcal{L}_{k,p}^{N,D}(\mathcal{G})$ satisfy the Weyl-type asymptotic law

$$\mathcal{L}_{k,p}^{N,D}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + \mathcal{O}(k) \quad \text{as } k \to \infty.$$

In this subsection we are going to discuss the behavior of the first order term $\mathcal{O}(k)$ in this expansion. A natural question to ask is if there exists some $c \in \mathbb{R}$ such that

$$\mathcal{L}_{k,p}^{N,D}(\mathcal{G}) = \frac{\pi^2}{L^2}k^2 + ck + \mathcal{O}(1) \quad \text{as } k \to \infty$$

holds. We are going to show that in general such c does not exist. More precisely, we study the sequence given by

$$c_k := \frac{\mathcal{L}_{k,p}^{N,D}(\mathcal{G}) - \frac{\pi^2 k^2}{L^2}}{k}, \quad k \in \mathbb{N}$$

and give examples where $(c_k)_k$ has a limit points for some given $a \in \mathbb{N}$ (equilateral star graphs with $2a$ edges) or uncountably many limit points (two disjoint path graphs with rationally independent lengths). For simplicity of our discussion, we restrict ourselves to the case $p = \infty$, but note that our techniques may easily be adapted to the case $p \in [1, \infty)$.

4.4.6.1 Equilateral stars

For $m \geq 3$, we consider the equilateral m-star S_m of total length L.

Lemma 4.4.27. *For $j \in \mathbb{N}_0$ we have*

$$\mathcal{L}^D_{jm+1,\infty}(\mathcal{S}_m) = \mu_{jm+1}(\mathcal{S}_m) = \frac{\pi^2 m^2 j^2}{L^2},$$
$$\mathcal{L}^D_{jm+r,\infty}(\mathcal{S}_m) = \mu_{jm+r}(\mathcal{S}_m) = \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}, \quad r = 2, \ldots, m.$$

Proof. The ordered eigenvalues $\mu_k(\mathcal{S}_m)$ of the equilateral m-star $\mathcal{S}_m$ are

$$\mu_{jm+1}(\mathcal{S}_m) = \frac{\pi^2 m^2 j^2}{L^2} \qquad \mu_{jm+r}(\mathcal{S}_m) = \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}, \quad r = 2, \ldots, m \tag{4.47}$$

for $j \in \mathbb{N}_0$ (cf. [Fri05, Example 3]). By [KKLM21, Proposition 8.4] we have $\mu_k(\mathcal{S}_m) \leq \mathcal{L}^D_{k,\infty}(\mathcal{S}_m)$ for $k \in \mathbb{N}$. Therefore it will be sufficient to find respective partitions of $\mathcal{S}_m$ whose energies coincides with the eigenvalues in (4.47) and these partitions will be optimal.
For $k = jm+1$ we consider the partition $\mathcal{P}$ consisting of an equilateral m-star with edge length $\frac{L}{2mj}$, m intervals of length $\frac{L}{2mj}$ each having one Dirichlet and one Neumann vertex and $m(j-1)$ intervals of length $\frac{L}{mj}$ each having two Dirichlet vertices. Then each cluster of $\mathcal{P}$ has the same Dirichlet energy $\frac{\pi^2 m^2 j^2}{L^2}$ and we conclude

$$\mathcal{L}^D_{k,\infty}(\mathcal{S}_m) = \Lambda^D_p(\mathcal{P}) = \frac{\pi^2 m^2 j^2}{L^2}.$$

For $k = mj + r$ with $1 < r \leq m$ we consider a partition $\mathcal{P}$ obtained after cutting through the center vertex of the star, where the first r edges $\mathsf{e}_1, \ldots, \mathsf{e}_r$ are divided into $j+1$ intervals – one of length $\frac{L}{m(2j+1)}$ with one Neumann and one Dirichlet vertex and the other j of length $\frac{2L}{m(2j+1)}$ with two Dirichlet vertices – and the remaining $m-r$ edges $\mathsf{e}_{r+1}, \ldots, \mathsf{e}_m$ are divided into j intervals – one of length $\frac{L}{m(2j-1)}$ with one Neumann and one Dirichlet vertex and the other j of length $\frac{2L}{m(2j-1)}$ with two Dirichlet vertices. The Dirichlet energy of the clusters in $\mathsf{e}_1, \ldots, \mathsf{e}_r$ is $\frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}$ whereas the Dirichlet energy of the clusters in $\mathsf{e}_{r+1}, \ldots, \mathsf{e}_m$ is $\frac{\pi^2 m^2 (j-\frac{1}{2})^2}{L^2}$. We obtain

$$\mathcal{L}^D_{k,\infty}(\mathcal{S}_m) = \Lambda^D_\infty(\mathcal{P}) = \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}.$$

This concludes the proof. $\square$

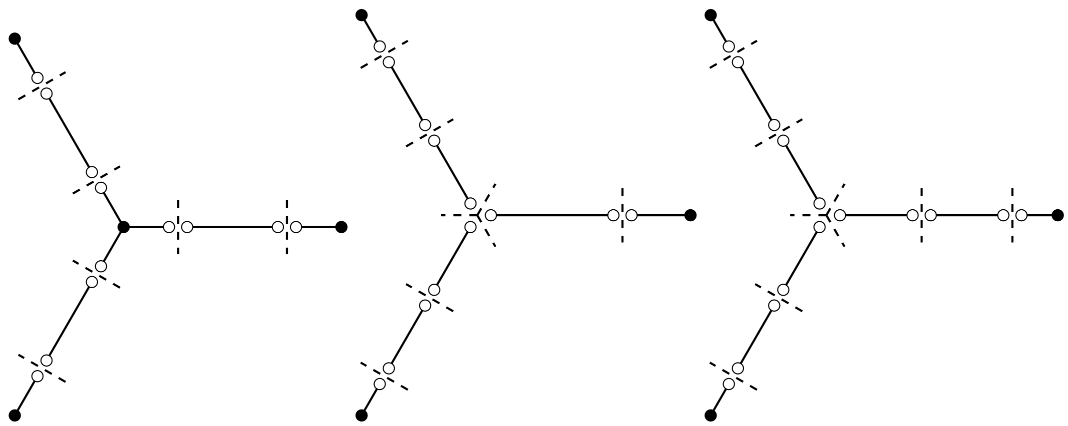


Figure 4.5: Optimal Dirichlet partitions of the three-star. The optimal 7-, 8- and 9-partitions of the 3-star in the proof of Lemma 4.4.27. White vertices denote vertices with Dirichlet conditions.

Proposition 4.4.28. *The limit set of the sequence* $(c_k)_{k\in\mathbb{N}}$ *with*

$$c_k := \frac{\mathcal{L}^D_{k,\infty}(\mathcal{S}_m) - \frac{\pi^2 k^2}{L^2}}{k}, \quad k \in \mathbb{N},$$

is

$$\left\{-\frac{2\pi^2}{L^2}\right\} \cup \left\{\frac{2\pi^2(s-1-\frac{m}{2})}{L^2} \mid s = 1, \dots, m-1\right\}. \tag{4.48}$$

In particular, $(c_k)_{k\in\mathbb{N}}$ *has* $m-1$ *limit points if* m *is even and* m *limit points if* m *is odd.*

Proof. The assertion immediately follows from Lemma 4.4.27 if one considers the subsequences $(c_{k_j})_{j\in\mathbb{N}_0}$ given by $k_j := jm + r$ for $r = 1, \dots, m$ and $j \in \mathbb{N}_0$. Indeed, for $r = 1$, we have

$$k_j c_{k_j} = \frac{\pi^2 m^2 j^2}{L^2} - \frac{\pi^2 k_j^2}{L^2} = \frac{\pi^2}{L^2}\left[(k_j - 1)^2 - k_j^2\right] = \frac{\pi^2}{L^2}(-2k_j + 1)$$

and, thus, $c_{k_j} \to -\frac{2\pi^2}{L^2}$ as $k_j \to \infty$. For $1 < r \le m$, we have

$$\begin{aligned} k_j c_{k_j} = \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2} - \frac{\pi^2 k_j^2}{L^2} &= \frac{\pi^2}{L^2}\left[\left(k_j + \frac{m}{2} - r\right)^2 - k_j^2\right] \\ &= \frac{\pi^2}{L^2}\left[2k_j\left(\frac{m}{2} - r\right) + \left(\frac{m}{2} - r\right)^2\right] \end{aligned}$$

and, thus, $c_{k_j} \to \frac{\pi^2(m-2r)}{L^2}$ as $k_j \to \infty$. Note that, if m is even, the limit point in the second case coincides with the one in the first case for $r = \frac{m}{2} + 1$. $\square$

Remark 4.4.29. Proposition 4.4.28 also shows that, if we write

$$\mu_k(\mathcal{S}_m) = \frac{\pi^2 k^2}{L^2} + c_k k,$$

then the set of points of accumulation of $(c_k)_{k\in\mathbb{N}}$ is exactly (4.48). This is an immediate consequence of the equality $\mathcal{L}^D_{k,\infty}(\mathcal{S}_m) = \mu_k(\mathcal{S}_m)$ for all $k \geq 1$, as shown in Lemma 4.4.27. In particular, we have an explicit example for the non-existence of a second term in the Weyl asymptotics for μ_k.

We now consider the case of Neumann partitions.

Lemma 4.4.30. *For $j \in \mathbb{N}_0$ we have*

$$\mathcal{L}^N_{jm+r,\infty}(\mathcal{S}_m) = \begin{cases} \dfrac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}, & r = 1, \dots, \lfloor \dfrac{m}{2} \rfloor, \\ \dfrac{\pi^2 m^2 (j+1)^2}{L^2}, & r = \lfloor \dfrac{m}{2} \rfloor + 1, \dots, m. \end{cases} \tag{4.49}$$

Proof. We set $k = jm + r$. We first show that Λ^N_∞ is indeed bounded from below by the terms appearing on the right-hand-side of (4.49) respectively. For an arbitrary k-partition $\mathcal{P}$ of $\mathcal{S}_m$, let $\mathcal{P}'$ denote the set of clusters in $\mathcal{P}$ that intersect at least two edges of $\mathcal{S}_m$ and, for each edge e_i of $\mathcal{S}_m$, let $\mathcal{P}_i$ denote the set of clusters in $\mathcal{P}$ that only intersect e_i. Furthermore, let $k' = |\mathcal{P}'|$ and $k_i := |\mathcal{P}_i|$. By choice of k' and k_i, we have $k = k' + \sum_{i=1}^m k_i$ and $k' \leq \frac{m}{2}$, where the latter holds, since each edge of $\mathcal{S}_m$ intersects at most one of the clusters in $\mathcal{P}'$. All clusters in $\mathcal{P}_i$ are intervals, so we may assume that each element of $\mathcal{P}_i$ has the same length ℓ_i. (Note that we only decrease Λ^N_∞ if we adjust the length of the single intervals, so that all off them have the same length.) In particular, we have $\mu_2(\mathcal{G}_i) = \frac{\pi^2}{\ell_i^2}$ for all $\mathcal{G}_i \in \mathcal{P}_i$.

Now, let us first consider the case $1 \leq r \leq \frac{m}{2}$. Without loss of generality, we may assume that $\ell_i > \frac{L}{m(j+\frac{1}{2})}$ holds for $i = 1, \dots, m$ – otherwise, $\Lambda^N_\infty(\mathcal{P}) \geq \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}$ would obviously be satisfied. We obtain

$$\frac{L}{m} \geq \sum_{\mathcal{G}_i \in \mathcal{P}_i} |\mathcal{G}_i| = k_i \ell_i > \frac{k_i L}{m(j+\frac{1}{2})}$$

and, thus, $k_i \leq j$ for $i = 1, \dots m$. This, in turn, implies

$$k' = k - \sum_{i=1}^m k_i \geq jm + r - jm = r \geq 1,$$

i.e. $\mathcal{P}'$ is non-empty. We consider an arbitrary element $\mathcal{G}' \in \mathcal{P}'$. For $i = 1, \dots, m$ with $|\mathsf{e}_i \cap \mathcal{G}'| > 0$ we have

$$|\mathsf{e}_i \cap \mathcal{G}'| = \frac{L}{m} - k_i \ell_i < \frac{L}{m} - \frac{jL}{m(j+\frac{1}{2})} = \frac{L}{2m(j+\frac{1}{2})}.$$

Thus, $\mathcal{G}'$ is a metric star whose maximum length $\ell_{\max}(\mathcal{G}')$ is bounded from above by $\frac{L}{2m(j+\frac{1}{2})}$. We obtain

$$\Lambda^N_\infty(\mathcal{P}) \geq \mu_2(\mathcal{G}') \geq \frac{\pi^2}{4\ell_{\max}(\mathcal{G}')^2} > \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2},$$

where the second step follows from [AC18, Lemma 3.3].

Next, we consider the case $\frac{m}{2} < r \leq m$. First note that $\Lambda_\infty^N(\mathcal{P}) \geq \frac{\pi^2 m^2 (j+1)^2}{L^2}$ is obviously satisfied if $\ell_i \leq \frac{L}{m(j+1)}$ holds. On the other hand, the case $\ell_i > \frac{L}{m(j+1)}$ for all i does not occure, since then following the argumentation of the first case yields $k' \geq r > \frac{m}{2}$, which is a contradiction to $k' \leq \frac{m}{2}$, as we stated in the the beginning of the proof.

Altogether, we have seen that $\mathcal{L}_{k,\infty}^N(\mathcal{S}_m)$ is indeed bounded from below by the terms appearing on the right-hand-side. To show equality, we simply present k-partitions with Neumann energy equal to the right-hand-side – obviously, these partitions are spectral minimal partitions. In the case $1 \leq r < \frac{m}{2}$, we make a choice of r pairs of edges and consider their respective unions $\mathsf{e}_1 \cup \mathsf{e}_2, \ldots, \mathsf{e}_{2r-1} \cup \mathsf{e}_{2r}$; each of these unions is an Eulerian path in $\mathcal{S}_m$. Now let $\mathcal{P}$ be the partition where each of these unions is decomposed into $2j+1$ intervals of equal length $\frac{L}{m(j+\frac{1}{2})}$ and every other edge $\mathsf{e}_i,\ i > 2r$ is decomposed into j intervals of length $\frac{L}{mj}$ (see the decomposition on the left in Figure 4.6). This partition has Neumann energy $\Lambda_\infty^N(\mathcal{P}) = \frac{\pi^2 m^2 (j+\frac{1}{2})^2}{L^2}$. In the case $\frac{m}{2} < r \leq m$, we consider the $jm + r$-partition that decomposes the first r edges into $j+1$ intervals of length $\frac{L}{m(j+1)}$ and the latter $m - r$ edges into j intervals of length $\frac{L}{mj}$ (see the two decompositions on the right in Figure 4.6). Again, this partition has the desired Neumann energy. □

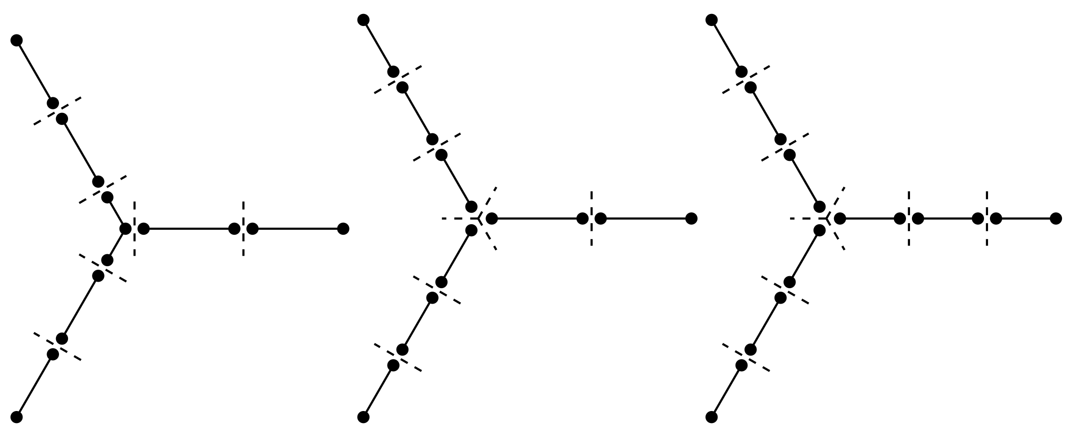


Figure 4.6: Optimal Neumann partitions of the three-star. The optimal 7-, 8- and 9-partitions of the 3-star in the proof of Lemma 4.4.30.

Remark 4.4.31. Note that the spectral minimal partitions in the proof of Lemma 4.4.30 are not unique. For example, another optimal $jm + 1$-partition – whose topology differs from the one presented in the proof – is obtained by decomposing $\mathcal{S}_m$ into one equilateral m-star of total length $\frac{L}{2j+1}$ and jm intervals of length $\frac{L}{m(j+\frac{1}{2})}$ (see Figure 4.7). In fact, this choice seems to be more natural, since each cluster has the same Neumann energy.

Remark 4.4.32. The m-star $\mathcal{S}_m$ can be covered with $\frac{m}{2}$ Eulerian paths, if m is even, and $\frac{m+1}{2}$

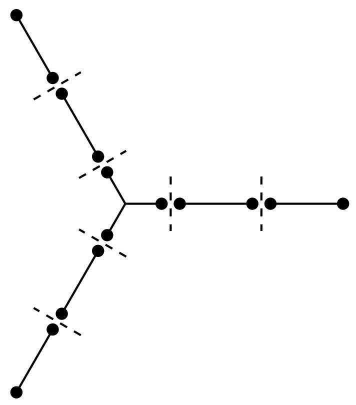


Figure 4.7: Nonuniqueness of the optimal partition of the three-star. A different optimal 7-partitions of the 3-star.

Eulerian paths, if m is odd. Therefore, Theorem 4.4.20 yields the upper bounds

$$\mathcal{L}_{k,\infty}^N(\mathcal{S}_m) \leq \begin{cases} \dfrac{\pi^2(k+\frac{m}{2}-1)^2}{L^2}, & \text{if } m \text{ is even,} \\ \dfrac{\pi^2(k+\frac{m+1}{2}-1)^2}{L^2}, & \text{if } m \text{ is odd.} \end{cases}$$

Lemma 4.4.30 shows that these bounds are actually sharp if m is even and $k = mj+1$, or m is odd and $k = mj + \frac{m+1}{2}$ for $j \in \mathbb{N}_0$ respectively.

Proposition 4.4.33. *The limit set of the sequence $(c_k)_{k\in\mathbb{N}}$ with*

$$c_k := \frac{\mathcal{L}_{k,\infty}^N(\mathcal{S}_m) - \frac{\pi^2 k^2}{L^2}}{k}, \quad k \in \mathbb{N},$$

is

$$\{0\} \cup \left\{ \frac{2\pi^2 s}{L^2} \mid s = 1, \ldots, \frac{m}{2} \right\},$$

if m is even, and

$$\{0\} \cup \left\{ \frac{2\pi^2 s}{L^2} \mid s = 1, \ldots, \frac{m-1}{2} \right\} \cup \left\{ \frac{2\pi^2 (t-\frac{1}{2})}{L^2} \mid t = 1, \ldots, \frac{m-1}{2} \right\}$$

if m is odd. In particular, $(c_k)_{k\in\mathbb{N}}$ has $\frac{m}{2}$ limit points if m is even and m limit points if m is odd.

Proof. This immediately follows from Lemma 4.4.27 if one considers the subsequences $(c_{k_j})_{j\in\mathbb{N}_0}$ given by $k_j := jm + r$ for $r = 1, \ldots, m$ and $j \in \mathbb{N}_0$. Indeed, calculations entirely analogous to the ones in the proof of Proposition 4.4.28 show that $c_{k_j} \to \frac{\pi^2(m-2r)}{L^2}$ as $k_j \to \infty$ for $r = 1, \ldots, \lfloor \frac{m}{2} \rfloor$, while $c_{k_j} \to \frac{\pi^2(2m-2r)}{L^2}$ for $r = \lfloor \frac{m}{2} \rfloor + 1, \ldots, m$. Finally, we remark that if m is even, then the limit points in the two cases coincide (replace r with $r + \frac{m}{2}$), whereas they are distinct if m is odd. $\square$

4.4.6.2 Two disjoint intervals with rationally independent lengths

Let $\mathcal{G}_a = I_1 \sqcup I_a$ be the disjoint union of the intervals $I_1 := [0,1], I_a := [0,a]$ for some $a > 0$.

$$\frac{\pi^2}{(a+1)^2}k^2 \leq \mathcal{L}_{k,\infty}^N(\mathcal{G}_a) \leq \frac{\pi^2}{(a+1)^2}k^2 + \frac{2\pi^2}{(a+1)^2}k + \frac{\pi^2}{(a+1)^2} \tag{4.50}$$

holds for $k \geq 2$ by Theorem 4.4.20. As before, we are interested in the set of points of accumulation of the sequence $(c_k)_{k\geq 2}$ given by

$$c_k = \frac{\mathcal{L}_{k,\infty}^N(\mathcal{G}_a) - \frac{\pi^2 k^2}{(a+1)^2}}{k}, \quad k \geq 2. \tag{4.51}$$

First note that we have

$$0 \leq c_k \leq \frac{2\pi^2}{(a+1)^2}$$

for $k \geq 2$ by (4.50). In fact, we will see that the limit set of $(c_k)_{k\geq 2}$ is the whole interval $[0, \frac{2\pi^2}{(a+1)^2}]$ if a is irrational. In order to show this, let us first compute the minimal energy $\mathcal{L}_{k,\infty}^N(\mathcal{G}_a)$ for $k \geq 2$. Of course, for given $i \in \{1, \dots, k-1\}$, an optimal k-partition of the form $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_i, \mathcal{G}_{i+1}, \dots, \mathcal{G}_k)$ for Λ_∞^N with

$$\mathcal{G}_1, \dots, \mathcal{G}_i \subset I_1, \qquad \mathcal{G}_{i+1}, \dots, \mathcal{G}_k \subset I_a.$$

is obtained by taking each cluster in I_1 of equal length $\frac{1}{i}$ and each cluster in I_a of equal length $\frac{a}{k-i}$, that is,

$$\mathcal{L}_{k,\infty}^N(\mathcal{G}_a) = \min_{1\leq i\leq k-1} \max\left\{\pi^2 i^2, \frac{\pi^2(k-i)^2}{a^2}\right\}. \tag{4.52}$$

Let us further investigate (4.52). One easily sees that

$$\max\left\{\pi^2 i^2, \frac{\pi^2(k-i)^2}{a^2}\right\} = \begin{cases} \dfrac{\pi^2(k-i)^2}{a^2}, & i \leq \left\lfloor \dfrac{k}{a+1} \right\rfloor \\[2ex] \pi^2 i^2, & i \geq \left\lceil \dfrac{k}{a+1} \right\rceil. \end{cases}$$

In particular, we have

$$\begin{aligned} \mathcal{L}_{k,\infty}^N(\mathcal{G}_a) &= \min_{1\leq i\leq k-1} \max\left\{\pi^2 i^2, \frac{\pi^2(k-1)^2}{a^2}\right\} \\ &= \min\left\{\min_{1\leq i\leq \lfloor \frac{k}{a+1}\rfloor} \frac{\pi^2(k-i)^2}{a^2}, \min_{\lceil \frac{k}{a+1}\rceil \leq i\leq k-1} \pi^2 i^2\right\} = \min\left\{\frac{\pi^2\lceil \frac{a}{a+1}k\rceil^2}{a^2}, \pi^2\left(\left\lceil \frac{k}{a+1}\right\rceil\right)^2\right\}. \end{aligned} \tag{4.53}$$

We can treat the asymptotics via study of the orbit of the rotation map $T_\alpha : \mathbb{R}/\mathbb{Z} \to [0,1)$, which is defined via

$$T_\alpha x = x + \alpha \mod 1.$$

It is a well-known fact that the orbits of the map T_α are dense in $[0,1]$ if and only if $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ (see [Dev89, Theorem 3.13]).

Theorem 4.4.34. *Let c_k, $k \geq 2$, be defined as in* (4.51). *If $a \in \mathbb{Q}$, then $(c_k)_{k\geq 2}$ has a finite limit set; if $a \in \mathbb{R} \setminus \mathbb{Q}$, then the limit set of $(c_k)_{k\geq 2}$ is the whole interval $[0, \frac{2\pi^2}{(a+1)^2}]$.*

Proof. Due to (4.53), we have

$$c_k = \min\left\{ \frac{\pi^2\left(\left\lceil \frac{k}{a+1}\right\rceil^2 - \frac{k^2}{(a+1)^2}\right)}{k}, \frac{\pi^2\left(\frac{1}{a}\left\lceil \frac{ak}{a+1}\right\rceil^2 - \frac{k^2}{(a+1)^2}\right)}{k} \right\}. \tag{4.54}$$

We compute

$$\begin{aligned}
\frac{\pi^2\left(\left\lceil \frac{k}{a+1}\right\rceil^2 - \frac{k^2}{(a+1)^2}\right)}{k} &= \frac{\pi^2}{k}\left(\left\lceil \frac{k}{a+1}\right\rceil - \frac{k}{a+1}\right)\left(\left\lceil \frac{k}{a+1}\right\rceil + \frac{k}{a+1}\right) \\
&= \left(\left\lceil \frac{k}{a+1}\right\rceil - \frac{k}{a+1}\right)\left(\frac{2\pi^2}{a+1} + \frac{\pi^2}{k}\left(\left\lceil \frac{k}{a+1}\right\rceil - \frac{k}{a+1}\right)\right) \\
&= T^k_{\frac{a}{a+1}}(0)\left(\frac{2\pi^2}{a+1} + \frac{\pi^2}{k}T^k_{\frac{a}{a+1}}(0)\right) = \frac{2\pi^2}{a+1}T^k_{\frac{a}{a+1}}(0) + o(1) \text{ as } k \to \infty
\end{aligned} \tag{4.55}$$

and

$$\begin{aligned}
\frac{\pi^2\left(\frac{1}{a}\left\lceil \frac{ak}{a+1}\right\rceil^2 - \frac{k^2}{(a+1)^2}\right)}{k} &= \frac{\pi^2}{a^2k}\left(\left\lceil \frac{ak}{a+1}\right\rceil - \frac{ak}{a+1}\right)\left(\left\lceil \frac{ak}{a+1}\right\rceil + \frac{ak}{a+1}\right) \\
&= \left(\left\lceil \frac{ak}{a+1}\right\rceil - \frac{ak}{a+1}\right)\left(\frac{2\pi^2}{a(a+1)} + \frac{\pi^2}{a^2k}\left(\left\lceil \frac{k}{a+1}\right\rceil - \frac{k}{a+1}\right)\right) \\
&= T^k_{\frac{1}{a+1}}(0)\left(\frac{2\pi^2}{a(a+1)} + \frac{\pi^2}{a^2k}T^k_{\frac{1}{a+1}}(0)\right) = \frac{2\pi^2}{a(a+1)}T^k_{\frac{1}{a+1}}(0) + o(1) \text{ as } k \to \infty.
\end{aligned} \tag{4.56}$$

Since the orbits of $T_{\frac{1}{a+1}}$ and $T_{\frac{a}{a+1}}$ are periodic if and only if $a \in \mathbb{Q}$, we deduce that a has a finite limit set if and only if $a \in \mathbb{Q}$. Suppose $a \in \mathbb{R} \setminus \mathbb{Q}$, then

$$\begin{aligned}
T^k_{\frac{1}{a+1}}(0) + T^k_{\frac{a}{a+1}}(0) &= \frac{k}{a+1} - \left\lfloor \frac{k}{a+1}\right\rfloor + \frac{ak}{a+1} - \left\lfloor \frac{ak}{a+1}\right\rfloor \\
&= k - \left\lfloor \frac{k}{a+1}\right\rfloor - \left\lfloor \frac{ak}{a+1}\right\rfloor = \left\lceil \frac{ak}{a+1}\right\rceil - \left\lfloor \frac{ak}{a+1}\right\rfloor = 1.
\end{aligned}$$

Let $x \in [0,1]$. Suppose $(k_n)_{n\in\mathbb{N}}$ is a strictly increasing sequence with

$$\lim_{n\to\infty} T^{k_n}_{\frac{1}{a+1}}(0) = x,$$

then with (4.54), (4.55) and (4.56) for all $k \in \mathbb{N}$ we infer

$$\begin{aligned}\lim_{n\to\infty} c_{k_n} &= \min\left\{\frac{2\pi^2(1-x)}{a+1}, \frac{2\pi^2 x}{a(a+1)}\right\}\\ &= \begin{cases} \dfrac{2\pi^2 x}{a(a+1)}, & x \le \dfrac{a}{a+1}\\[2ex] \dfrac{2\pi^2(1-x)}{a+1}, & x > \dfrac{a}{a+1},\end{cases}\end{aligned}$$

and hence the limit set of $(c_k)_{k\ge2}$ is dense in $[0, \frac{2\pi^2}{(a+1)^2}]$. Since the limit set is clearly closed, we conclude that it equals $[0, \frac{2\pi^2}{(a+1)^2}]$. □

In the Dirichlet case, we may similarly consider the limit set of the sequence $(c_k)_{k\ge2}$ given by

$$c_k = \frac{\mathcal{L}^D_{k,\infty}(\mathcal{G}_a) - \frac{\pi^2 k^2}{(1+a)^2}}{k}, \quad k \ge 2. \tag{4.57}$$

On an interval $I = [0,\ell]$ we have

$$\mathcal{L}^D_{k+1,\infty}(I) = \mathcal{L}^N_{k,\infty}(I), \quad k \ge 2, \tag{4.58}$$

which directly gives us the following result.

Theorem 4.4.35. *Let c_k, $k \ge 2$, be defined as in* (4.57). *If $a \in \mathbb{Q}$, then $(c_k)_{k\ge2}$ has a finite limit set; if $a \in \mathbb{R}\setminus\mathbb{Q}$, then the limit set of $(c_k)_{k\ge2}$ is the interval $[-\frac{4\pi^2}{(a+1)^2}, -\frac{2\pi^2}{(a+1)^2}]$.*

Proof. Using (4.58) yields

$$\mathcal{L}^D_{k+2,\infty}(\mathcal{G}_a) = \mathcal{L}^N_{k,\infty}(\mathcal{G}_a)$$

and, thus,

$$\frac{\mathcal{L}^D_{k+2,\infty}(\mathcal{G}_a) - \frac{\pi^2(k+2)^2}{(1+a)^2}}{k+2} = \frac{k}{k+2}\frac{\mathcal{L}^N_{k,\infty}(\mathcal{G}_a) - \frac{\pi^2k^2}{(a+1)^2}}{k} - 4\frac{\pi^2}{(a+1)^2} + o(1) \qquad \text{as } k \to \infty.$$

The assertion now follows immediately from Theorem 4.4.34. □

4.5 Interlacing results

4.5.1 Results

Our principal objective here is to establish sharp interlacing inequalities linking the quantities $\mathcal{L}^D_{k,\infty}$ and $\mathcal{L}^{N,c}_{k,\infty}$: here and throughout we will suppose $\mathcal{G}$ to be a fixed connected, compact, finite metric graph; β will denote the first Betti number of $\mathcal{G}$, i.e., the number of independent cycles in the graph, and $|N|$ the number of vertices of $\mathcal{G}$ of degree 1, the *leaves*. In this section we will prove Theorem 1.3.5 and Theorem 1.3.6. We recall the statements:

Theorem 4.5.1. *For all $k \in \mathbb{N}$ such that $k \geq \beta$ we have*

$$\left(\mathcal{L}^{N,r}_{k,\infty}(\mathcal{G}) \geq\right) \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^D_{k+1-\beta,\infty}(\mathcal{G}).$$

Theorem 4.5.2. *For all $k \in \mathbb{N}$ such that $k \geq \beta + |N|$ we have*

$$\mathcal{L}^D_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k+1-\beta-|N|,\infty}(\mathcal{G}).$$

A consequence of these inequalities is that we can relate these spectral minimal energies with the eigenvalues of the Laplacian on the whole graph, both with standard conditions at all vertices and with Dirichlet conditions at all vertices. Recall that$\mu_k(\mathcal{G})$ is the k-th eigenvalue of the Laplacian with standard conditions on $\mathcal{G}$ (starting at $\mu_1(\mathcal{G}) = 0$ and counting multiplicities) and $\lambda_k(\mathcal{G}, \mathcal{V}^D)$ the k-th eigenvalue of the Laplacian with Dirichlet conditions at a distinguished set $\mathcal{V}^D$ of Dirichlet vertices and standard conditions on the rest, which we abbreviate to $\lambda^D_k(\mathcal{G}) = \lambda_k(\mathcal{G}, \mathcal{V})$ for when *all* vertices are Dirichlet vertices. Then Corollary 1.19, which we recall in the following is a fairly direct consequence of Theorem 1.3.5:

Corollary 4.5.3. *Let $\mathcal{G}$ be a (connected, compact, finite) metric graph with first Betti number $\beta \geq 0$. Then for all $k \geq \beta + 1$ we have*

$$\lambda^D_k(\mathcal{G}) \geq \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^D_{k+1-\beta,\infty}(\mathcal{G}) \geq \mu_{k+1-\beta}(\mathcal{G}).$$

This, and indeed the principle of interlacing inequalities between such minimal energies, have several natural motivations. For one, rather suprisingly, combining Corollary 1.3.7 with the upper bound on $\mathcal{L}^{N,c}_{k,\infty}$ in Theorem 4.4.18, we obtain a bound which, even as a bound on μ_k, actually turns out to be better for many classes of graphs than the central bound [BKKM17, Theorem 4.9], as we shall see below.

Corollary 4.5.4. *Let $\mathcal{G}$ be a metric graph with first Betti number $\beta \in \mathbb{N}_0$ and total length L, and suppose there exist $n \leq |\mathcal{E}|$* Eulerian paths *covering $\mathcal{G}$, crossing at at most finitely many points. Then for all $k \geq \max\{n + 1 - \beta, 1\}$ we have*

$$\mu_k(\mathcal{G}) \leq \mathcal{L}^D_{k,\infty}(\mathcal{G}) \leq \frac{\pi^2}{L^2}(k + n + \beta - 2)^2. \tag{4.59}$$

But at a more fundamental level a key motivation for Theorems 1.3.5 and 1.3.6 arises from the effect on graph Laplacians, of so-called *surgery* on the graph. Our method of proof of these two theorems, which involves studying *cuts* of a graph and the impact this has on being able to glue together eigenfunctions on different parts of the graph, is intimately related to both the nodal count (and distribution of the nodal domains) of the eigenfunctions, and the number and distribution of the corresponding Neumann domains.

Cutting a graph at a point is a simple operation which changes the topology of the graph and which has a predictable effect on the eigenvalues of the graph, as it represents a finite rank perturbation of the associated Laplacian (see [BKKM19, §3.1 and §4.1]). Cutting a graph at exactly the points x where the k-th standard Laplacian eigenfunction $u_k(x)$ equals 0 leads to a *nodal partition*, the clusters of which are the nodal domains of the eigenfunction. The number and distribution of these has been explored at some length; see for example [ABB18; BBRS12; Ber06]. The Neumann domains arise as the clusters of a partition cut at the points where $u_k'(x) = 0$; the number of Neumann domains behaves similarly as a function of k, at least in the "generic" case where (among other things) all cuts are made away from the vertices [AB19]. Perhaps most notably for us, it has been shown in the generic case that the difference between the number of nodal domains $\nu(k)$ and the number of Neumann domains $\xi(k)$ of u_k satisfies *exactly* the same bounds as the indices appearing in Theorems 1.3.5 and 1.3.6 [AB19, Proposition 3.1(1)] (see also [ABBE20, Proposition 11.2]):

$$1 - \beta \leq \nu(k) - \xi(k) \leq \beta + |N| - 1. \tag{4.60}$$

In fact, (4.60) can also be recovered from our proofs (see Remarks 4.5.7 and 4.5.14). Despite the completely different approaches (here we study cutting and pasting eigenfunctions arising from different minimal partitions, in [AB19] the point of departure being the whole graph eigenfunctions) this hints at a much deeper connection between these spectral minimal partitions and the nodal and Neumann domain patterns of the whole graph eigenfunctions, analogous to or extending the connection between nodal domains and partitions explored in [BBRS12], which will be left to future investigation to explore fully.

Somewhat related is the idea of changing a vertex condition from standard to Dirichlet (or vice versa), another finite rank perturbation which leads to interlacing inequalities between Dirichlet and standard Laplacian eigenvalues. A consequence of the min-max characterization of the eigenvalues is the interlacing inequality which in the notation introduced above reads

$$\lambda_{k+|\mathcal{V}^D|}(\mathcal{G}, \mathcal{V}^D) \geq \mu_{k+|\mathcal{V}^D|}(\mathcal{G}) \geq \lambda_k(\mathcal{G}, \mathcal{V}^D)$$

(again, see [BKKM19, §3.1], or, e.g., [BK13, §3.1.6]). This is reminiscent of, or rather actually at odds with, Friedlander's inequalities between Dirichlet and Neumann Laplacian eigenvalues on domains in $\mathbb{R}^d$, $d \geq 2$ (see [Fri91]), which assert that $\lambda_k(\Omega) \geq \mu_{k+1}(\Omega)$ for all $k \in \mathbb{N}$; in fact the inequality was later shown to be always strict [Fil04]. Similar results also can be obtained for compact manifolds (see [AM12]). On metric graphs this is rather difficult to recover precisely because of the interlacing inequalities, or the related idea that the difference between Dirichlet and standard vertex conditions is somehow "smaller" than the difference between Dirichlet and Neumann boundary conditions. Our Corollary 1.3.7 is a complement to the inequality proved in [Roh17, Theorem 4.1] for *tree graphs* $\mathcal{G}$ (i.e., with $\beta = 0$), which states that

$$\lambda_k(\mathcal{G}) \geq \mu_{k+1}(\mathcal{G}), \qquad k \in \mathbb{N}, \tag{4.61}$$

if we impose Dirichlet conditions on all vertices $\mathcal{V}^D = \mathcal{V}$ of $\mathcal{G}$. Note, however, that (4.61) actually holds under the weaker assumption that Dirichlet conditions only be imposed on the leaves of the tree, with standard conditions at all other vertices; see [BBW15, Lemma 4.5] (with $t = 0$).

Remark 4.5.5. Before proceeding, that for k sufficiently large (how large potentially depending on $\mathcal{G}$), as discussed in [HKMP21a] we actually have $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) = \mathcal{L}^{N}_{k,\infty}(\mathcal{G})$, as the partitions achieving the former infimum will in fact be rigid; for such k, all our results may be adjusted accordingly. In general, however, the class of general connected partitions seems more natural in this context, as, unlike in the rigid case, they do not place potentially artificial restrictions on the locations of the cuts made when forming the partitions. Hence we will not deal with the question of rigidity further.

§4.5.2 is devoted to the proof of Theorem 1.3.5, §4.5.3 to the proof of Theorem 1.3.5; in both cases, at the beginning of the section we include a somewhat less formal explanation of where the respective indices appearing in the inequalities come from. Finally, in §4.5.4 we prove Corollaries 1.3.7 and 4.5.4, give several examples of graphs where the bounds in (4.59) are better than bounds obtained elsewhere, and also study the case of certain *windmill graphs*, introduced in [KS18], where there is equality everywhere in (4.59).

4.5.2 Proof of Theorem 4.5.1

Assume $\mathcal{G}$ is a connected metric graph with first Betti number $\beta = |\mathcal{E}| - |\mathcal{V}| + 1$. We first wish to give an intuitive explanation as to why Theorem 1.3.5 should hold. So let $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k) \in \mathfrak{C}_k(\mathcal{G})$ be an exhaustive k-partition realizing the minimum for $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G})$. Consider any eigenfunctions $u_1, \dots, u_k$ on $\mathcal{G}_1, \dots, \mathcal{G}_k$ associated with $\mu_2(\mathcal{G}_1), \dots, \mu_2(\mathcal{G}_k)$, respectively. We extend each function by zero to obtain an L^2-function on $\mathcal{G}$, which can also be treated as an element of $\bigoplus H^1(e)$, and which we still denote by u_i, $i = 1, \dots, k$. Now since each of these functions necessarily changes sign the sets

$$u_{i,+} = \mathbb{1}_{\{u_i > 0\}} u_i, \qquad u_{i,-} = \mathbb{1}_{\{u_i < 0\}} u_i,$$

$i = 1, \ldots, k$, are all non-empty. Suppose we can *match* these eigenfunctions at the cut vertices in the sense that there exist $\alpha_{1,+}, \alpha_{1,-}, \ldots, \alpha_{k,+}, \alpha_{k,-} \in \mathbb{R} \setminus \{0\}$ such that for all $v \in \mathcal{C}(\mathcal{G}_{\mathcal{P}} : \mathcal{G})$

$$\alpha_{i,\mathrm{sign}(u_i(v_1))} u_i(v_1) = \alpha_{j,\mathrm{sign}(u_j(v_2))} u_j(v_2) \tag{4.62}$$

for all $v_1, v_2 \in \mathcal{C}_v(\mathcal{G}_{\mathcal{P}})$. Then

$$u := \alpha_{1,+} u_{1,+} + \alpha_{1,-} u_{1,-} + \ldots + \alpha_{k,+} u_{k,+} + \alpha_{k,-} u_{k,-} \in H^1(\mathcal{G}). \tag{4.63}$$

How many nodal domains will u have on $\mathcal{G}$? We know that:

1. regarded as a function on the cut graph $\mathcal{G}_{\mathcal{P}}$ it has at least $2k$, since it changes sign on each connected component $\mathcal{G}_i$, $i = 1, \ldots, k$, of $\mathcal{G}_{\mathcal{P}}$;
2. by Lemma 2.1.15 we have
$$k - 1 \leq \mathrm{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) \leq k - 1 + \beta;$$
3. every time we make a cut of $\mathcal{G}$ of rank 1 (cf. Lemma 2.1.8) the number of nodal domains of u considered as a function on the cut graph increases by at most 1.

It follows that $u \in H^1(\mathcal{G})$ admits at least $2k - \mathrm{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) \geq k + 1 - \beta$ nodal domains; moreover, its Rayleigh quotient on each of these nodal domains will be no larger than $\Lambda_k^N(\mathcal{P}) = \max_i \mu_2(\mathcal{G}_i)$. Thus, *if* $u \in H^1(\mathcal{G})$, then we can use the associated nodal partition to obtain

$$\mathcal{L}_{k,\infty}^N(\mathcal{G}) \geq \mathcal{L}_{k,\infty}^{N,c}(\mathcal{G}) \geq \mathcal{L}_{2k-\mathrm{rank}(\mathcal{G}_{\mathcal{P}}:\mathcal{G}),\infty}^D(\mathcal{G}) \geq \mathcal{L}_{k+1-\beta,\infty}^D(\mathcal{G}),$$

which is Theorem 1.3.5. But of course in general we cannot expect the matching conditions (4.62) to hold.

Example 4.5.6. Before proceeding we give a simple example to show that equality is possible in Theorem 1.3.5, that is, that we may have equality

$$\mathcal{L}_{k,\infty}^N(\mathcal{G}) = \mathcal{L}_{k+1-\beta,\infty}^D(\mathcal{G}), \tag{4.64}$$

as well as in the above argument. Consider the equilateral m-star, $m \geq 3$, with m edges of length 1 each. We identify each edge e with the unit interval $[0,1]$, with 0 corresponding to the central vertex. As shown in [HKMP21a, Lemmata 7.1 and 7.4] we have

$$\mathcal{L}_{jm,\infty}^N(\mathcal{S}_m) = \pi^2 j^2 = \mathcal{L}_{jm+1,\infty}^D(\mathcal{S}_m).$$

for all $j \geq 1$. Moreover, in this case there is a nodal partition corresponding to $\mathcal{L}_{jm+1,\infty}^D(\mathcal{S}_m)$, which comes from taking eigenfunctions of the form $u_{e,j}(x) = \cos(\pi j x)$ on each edge $e \simeq [0,1]$.

Note that equality need not hold for integers k not of the form $jm+1$, since for example

$$\mathcal{L}^N_{jm-1,\infty} = \frac{\pi^2 m^2 j^2}{L^2} > \frac{\pi^2 m^2 (j-1/2)^2}{L^2} = \mathcal{L}^D_{jm,\infty}$$

for all $j \geq 1$.

Note that (4.64) also holds for the loop and for the interval, for all $k \geq 1$.

Remark 4.5.7. Suppose u is an eigenfunction, with eigenvalue λ, of the (standard) Laplacian on $\mathcal{G}$, and suppose that considering the total cut of $\mathcal{G}$ at all points where u reaches a local nonzero maximum or minimum generates a partition with $k = \xi(u)$ clusters. (In the language of §4.5.3 and [ABBE20] this means u has $\xi(u)$ *Neumann domains*.) Then λ equals the first nontrivial standard Laplacian eigenvalue on each cluster, with eigenfunction u (see [ABBE20, Lemma 8.1]). Now by construction we can certainly match these restrictions of the eigenfunction at the cut points, in accordance with the above discussion. As we have seen, the resulting Dirichlet partition consists of at least $\xi(u)+1-\beta$ clusters, which in this case are clearly the nodal domains of u. Thus we recover one part of (4.60).

Lemma 4.5.8. *Suppose $\mathcal{G}'$ is a simple cut of $\mathcal{G}$. Suppose $\widetilde{u} \in H^1(\mathcal{G}')$ with nodal partition $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_n)$ with $n \in \mathbb{N}$. Then there exists a function*

$$u \in \operatorname{span}(\widetilde{u}\big|_{\mathcal{G}_1}, \dots, \widetilde{u}\big|_{\mathcal{G}_n}) \cap H^1(\mathcal{G})$$

with at least $n-1$ nodal domains.

Proof. Suppose that v is the unique vertex in $\mathcal{C}(\mathcal{G}' : \mathcal{G})$, and $v_1, v_2 \in \mathcal{V}'$ such that $v = v_1 \cup v_2$. Suppose without loss of generality that $v_1 \in \mathcal{G}_1$ and $v_2 \in \mathcal{G}_2$. Write $\mathcal{G}_i = (\mathcal{V}_i, \mathcal{E}_i)$, $i = 1, \dots, n$.

Case 1: $\widetilde{u}(v_1) = 0$ and $\widetilde{u}(v_2) = 0$. Then since $\widetilde{u}(v_1) = \widetilde{u}(v_2)$ we infer $\widetilde{u} \in H^1(\mathcal{G})$ and we are done since $\widetilde{u}$ admits n connected nodal domains.

Case 2: $\widetilde{u}(v_1) \neq 0 \neq \widetilde{u}(v_2)$. Then there exist $\alpha_1, \alpha_2 \neq 0$ such that

$$\alpha_1 \widetilde{u}(v_1) = \alpha_2 \widetilde{u}(v_2)$$

and we may define

$$u(x) := \begin{cases} \alpha_1 \widetilde{u}(x), & x \in \mathcal{E}_1 \\ \alpha_2 \widetilde{u}(x), & x \in \mathcal{E}_2 \\ \widetilde{u}(x) & \text{otherwise,} \end{cases}$$

so that $u \in H^1(\mathcal{G})$ with $n-1$ nodal domains.

Case 3: Otherwise. Suppose without loss of generality that $\widetilde{u}(v_1) \neq 0$ and $\widetilde{u}(v_2) = 0$. Then we define

$$u(x) := \begin{cases} \widetilde{u}(x), & x \notin \mathcal{G}_1 \\ 0, & \text{otherwise,} \end{cases}$$

and by construction $u \in H^1(\mathcal{G})$ has $n-1$ nodal domains. □

Lemma 4.5.9. *Let $\mathcal{G}$ be a metric graph and $\mathcal{G}'$ a cut of $\mathcal{G}$. Let $r := \operatorname{rank}(\mathcal{G}' : \mathcal{G})$ and $k > r$, then for any k-partition $\mathcal{P}' = (\mathcal{G}'_1, \dots, \mathcal{G}'_k)$ of $\mathcal{G}'$ there exists a $(k-r)$-partition $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_{k-r})$ of $\mathcal{G}$ such that*

$$\Lambda_k^D(\mathcal{P}') \geq \Lambda_{k-r}^D(\mathcal{P}).$$

Proof. By a simple induction argument based on Lemma 2.1.8 it suffices to prove the result for $r = 1$. So suppose $\mathcal{G}'$ is a simple cut of $\mathcal{G}$ and $\mathcal{P}' = (\mathcal{G}'_1, \dots, \mathcal{G}'_k)$ is an arbitrary k-partition of $\mathcal{G}'$. We let $\widetilde{u}_i \in H_0^1(\mathcal{G}'_i, \partial\mathcal{G}'_i)$ be an eigenfunction associated with $\lambda_1(\mathcal{G}'_i)$, $i = 1, \dots, k$, then the function $\widetilde{u}$ such that $\widetilde{u}|_{\mathcal{G}'_i} = \widetilde{u}_i$ for all i belongs to $H^1(\mathcal{G}')$ and has nodal partition exactly $\mathcal{P}'$, and . Then by Lemma 4.5.8 there exists $u \in H^1(\mathcal{G})$ with at least $k-1$ nodal domains such that, likewise, $u|_{\mathcal{G}'_i} = \widetilde{u}_i$ for all i. A simple argument using the nodal partition $\mathcal{P}$ associated with u and fact that $\Lambda_k^D(\mathcal{P}') = \max_i \lambda_1(\mathcal{G}'_i)$ leads to $\Lambda_k^D(\mathcal{P}') \geq \Lambda_{k-r}^D(\mathcal{P})$. □

Corollary 4.5.10. *Let $\mathcal{G}$ be a metric graph and $\mathcal{G}'$ a cut of $\mathcal{G}$, and suppose $r := \operatorname{rank}(\mathcal{G}' : \mathcal{G})$. Then*

$$\mathcal{L}_{k,\infty}^D(\mathcal{G}') \geq \mathcal{L}_{k-r,\infty}^D(\mathcal{G}).$$

Lemma 4.5.11. *Let $\mathcal{G}$ be a metric graph and let $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ be a k-partition with canonical cut graph $\mathcal{G}_{\mathcal{P}}$. Let $r := \operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G})$, then there exists a $(2k-r)$-partition*

$$\mathcal{P}' = (\mathcal{G}_1, \dots, \mathcal{G}_{2k-r})$$

such that

$$\Lambda_k^N(\mathcal{P}) \geq \Lambda_{2k-r}^D(\mathcal{P}').$$

Proof. Suppose $\mathcal{G}_{\mathcal{P}}$ is the canonical cut graph of $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$. Let u_i be an eigenfunction for $\mu_2(\mathcal{G}_i)$ on $\mathcal{G}_i$, $i = 1, \dots, k$. Then u_i necessarily changes sign on $\mathcal{G}_i$ and hence admits at least two nodal domains; denote by $\mathcal{P}_i = (\mathcal{G}_{i,+}, \mathcal{G}_{i,-})$ any exhaustive extension of any corresponding nodal 2-partition of $\mathcal{G}_i$. Then, since $\mu_(\mathcal{G}_i) \geq \max\{\lambda_1(\mathcal{G}_{i,+}), \lambda_1(\mathcal{G}_{i,-})\}$,

$$\Lambda_k^N(\mathcal{P}) \geq \max_{i=1,\dots,k} \max\{\lambda_1(\mathcal{G}_{i,+}), \lambda_1(\mathcal{G}_{i,+})\} \geq \mathcal{L}_{2k,\infty}^D(\mathcal{G}_{\mathcal{P}}) \geq \mathcal{L}_{2k-r,\infty}^D(\mathcal{G}),$$

where the last inequality follows from Corollary 4.5.10. □

We can now give the proof of Theorem 1.3.5.

Proof of Theorem 1.3.5. Let $\mathcal{P}$ be any k-partition of $\mathcal{G}$. By Lemma 2.1.15 we have

$$\operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) \leq k - 1 + \beta$$

and so, applying Lemma 4.5.11, taking the infimum over all such partitions and using the monotonicity of the mapping $j \mapsto \mathcal{L}^D_{j,\infty}(\mathcal{G})$, we obtain

$$\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \geq \mathcal{L}^D_{k+1-\beta,\infty}(\mathcal{G}).$$

$\square$

4.5.3 Proof of Theorem 4.5.2

Just as the basic idea behind Theorem 4.5.1 is gluing together nodal domains of Neumann eigenfunctions of the partition clusters to construct a test partition, here we will be interested in gluing together the so-called *Neumann domains* of the cluster Dirichlet eigenfunctions (see, e.g., [AB19; ABBE20]).

Let us again start with an intuitive explanation of Theorem 4.5.2. We suppose $\mathcal{G}$ is a metric graph with first Betti number β and $|N|$ leaves. We take $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k) \in \mathfrak{C}_k(\mathcal{G})$ to be a fixed exhaustive k-partition of $\mathcal{G}$ and consider the respective first Dirichlet eigenfunctions $u_1, \dots, u_k$ on $\mathcal{G}_1, \dots, \mathcal{G}_k$, associated with $\lambda_1(\mathcal{G}_1), \dots, \lambda_1(\mathcal{G}_k)$ and extended by zero on the rest of $\mathcal{G}$.

We decompose each $\mathcal{G}_i$ by taking the total cut (see Definition 2.1.9) of $\mathcal{G}_i$ at every point, without loss of generality a vertex $v \in \mathcal{V}(\mathcal{G}_i)$, at which u_i attains a nonzero extremum, and thus in particular $\frac{\partial}{\partial\nu}|_e u_i(v) = 0$ on every edge e incident with v. On each connected component $\widetilde{\mathcal{G}}_{i,1}, \dots, \widetilde{\mathcal{G}}_{i,k_i}$, $k_i \geq 1$, the Neumann domains, u_i is the first eigenfunction of the Laplacian with suitable mixed Dirichlet-Neumann conditions, and in particular $\lambda_1(\mathcal{G}_i)$ is still the first eigenvalue of each $\widetilde{\mathcal{G}}_{i,j}$ by a standard variational argument (cf. [BKKM17, Proof of Theorem 3.4], or also [ABBE20, Lemma 8.1] for a similar principle).

Now suppose that, given a cut vertex $v \in \mathcal{C}(\mathcal{G}_\mathcal{P} : \mathcal{G})$, we glue together all the neighboring Neumann domains $\mathcal{G}_{i_1,j_1}, \dots, \mathcal{G}_{i_{k_v},j_{k_v}}$ at v to form a cluster $\mathcal{G}' := \mathcal{G}_{i_1,j_1} \cup \ldots \cup \mathcal{G}_{i_{k_v},j_{k_v}}$; then, by taking a suitable linear combination of $u_{i_1}|_{\mathcal{G}_{i_1,j_1}}, \dots, u_{i_{k_v}}|_{\mathcal{G}_{i_{k_v},j_{k_v}}}$ similarly to (4.63), we obtain a test function on $\mathcal{G}'$, orthogonal to the constant functions for the right choice of coefficients, whose Rayleigh quotient is at most $\max\{\lambda_1(\mathcal{G}_{i_1}), \dots, \lambda_1(\mathcal{G}_{i_{k_v}})\} \leq \Lambda^D_k(\mathcal{P})$.

Gluing such neighboring Neumann domains together at as many different cut vertices as possible (see also Figure 4.8), we may thus construct a partition $\mathcal{P}'$ of $\mathcal{G}$ such that $\Lambda^N(\mathcal{P}') \leq \Lambda^D_k(\mathcal{P})$.

The question is, how many clusters can $\mathcal{P}'$ have? Denote by $\widetilde{\mathcal{P}} = \{\widetilde{G}_{i,j}\}_{i,j}$ the partition of $\mathcal{G}$ which results from making total cuts of the clusters of $\mathcal{P}$ as described above, which will be a finer partition than $\mathcal{P}$ and $\mathcal{P}'$ (in fact, $\mathcal{G}_{\widetilde{\mathcal{P}}}$ will be the common cut of $\mathcal{G}_\mathcal{P}$ and $\mathcal{G}_{\mathcal{P}'}$, cf. Definition 2.1.11). We wish to determine how many clusters must be created when passing from $\mathcal{P}$ to $\widetilde{\mathcal{P}}$, and how many may be lost from $\widetilde{\mathcal{P}}$ to $\mathcal{P}'$.

For the first question, we wish to find a condition that guarantees that a cluster $\mathcal{G}_i$ of $\mathcal{P}$ will yield (at least) two in $\widetilde{\mathcal{P}}$, that is, that it contains at least two Neumann domains. A sufficient condition is that $\mathcal{G}_i$ have at least two Dirichlet (cut) vertices, and that u_i reach an extremum on every *trail* (non-self-intersecting path) in $\mathcal{G}_i$ connecting them. Observe that this need not be the case if the cluster contains a leaf or a cycle of $\mathcal{G}$ (for example if $\mathcal{G}_i$ is an interval with one Dirichlet and one Neumann condition, or lasso with a Dirichlet condition at its degree-one vertex). This motivates the following definition.

Definition 4.5.12. Suppose $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ is a k-partition, $k \geq 2$, of $\mathcal{G}$. We say that a cluster $\mathcal{G}_i$ is *benign* (in $\mathcal{G}$) if it contains neither a vertex of $\mathcal{G}$ of degree one, nor a cycle of $\mathcal{G}$; otherwise, we say it is *malign*.

Observe that any benign cluster of $\mathcal{G}$ must necessarily be a tree each of whose leaves belongs to the cut set $\mathcal{C}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) = \partial\mathcal{P}$, while for malign clusters this is not necessarily the case. We see that if $\mathcal{P}$ has k' malign clusters, then $\widetilde{\mathcal{P}}$ must have at least $2k - k'$.

The next question is how many clusters we may lose going from $\widetilde{\mathcal{P}}$ to $\mathcal{P}'$; the example of Figure 4.8 shows that the answer may be complicated.

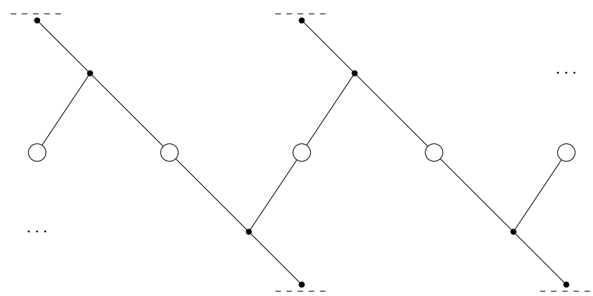


Figure 4.8: Zigzag clusters. A possible cluster of $\mathcal{P}'$ resulting by gluing the corresponding Neumann domains at the cut vertices of $\mathcal{P}$, which are the Dirichlet points (open circles) of the associated eigenfunctions. Observe that while this cluster is composed of a large number of Neumann domains, being constructed in this way it necessarily contains in its interior at least one boundary point of the original Dirichlet partition.

The following lemma formalizes the above reasoning and answers the latter question; the proof of Theorem 4.5.2 will then follow easily.

Lemma 4.5.13. *Let $\mathcal{G}$ be a compact, connected metric graph. Suppose $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ is an exhaustive k-partition, $k \geq 2$, with*

$$\operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}) = k - 1 + r$$

for some $0 \leq r \leq \beta$ and suppose that $\mathcal{P}$ contains at most $1 \leq n \leq k$ malign clusters. Then there exists an exhaustive $k + 1 - n - r$-partition $\mathcal{P}'$ of $\mathcal{G}$ such that

$$\Lambda_k^D(\mathcal{P}) \geq \Lambda_{k+1-n-r}^N(\mathcal{P}').$$

Proof. Let $u_1, \dots, u_k$ be the respective first Dirichlet eigenfunctions on $\mathcal{G}_1, \dots, \mathcal{G}_k$, associated with $\lambda_1(\mathcal{G}_1), \dots, \lambda_1(\mathcal{G}_k)$, identified as functions in $H^1(\mathcal{G})$ via extension by zero. Take $\mathcal{P}'$ to be the partition of $\mathcal{G}$ associated with the cut $\mathcal{G}_{\mathcal{P}'}$ of $\mathcal{G}$ consisting of the total cut of $\mathcal{G}$ at all points where any of the u_i admit a local nonzero extremum. Let $\widetilde{\mathcal{P}}$ be the partition of $\mathcal{G}$ whose clusters are the connected components by the common cut graph of $\mathcal{G}_{\mathcal{P}}$ and $\mathcal{G}_{\mathcal{P}'}$. Then by construction

$$\operatorname{rank}(\mathcal{G}_{\mathcal{P}'} : \mathcal{G}) = \operatorname{rank}(\mathcal{G}_{\widetilde{\mathcal{P}}} : \mathcal{G}) - \operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}).$$

It follows from Lemma 2.1.7 that

$$\operatorname{rank}(\mathcal{G}_{\widetilde{\mathcal{P}}} : \mathcal{G}_{\mathcal{P}'}) = \operatorname{rank}(\mathcal{G}_{\widetilde{\mathcal{P}}} : \mathcal{G}) - \operatorname{rank}(\mathcal{G}_{\mathcal{P}'} : \mathcal{G}) = \operatorname{rank}(\mathcal{G}_{\mathcal{P}} : \mathcal{G}),$$

that is, $\operatorname{rank}(\mathcal{G}_{\widetilde{\mathcal{P}}} : \mathcal{G}_{\mathcal{P}'}) = k - 1 + r$.

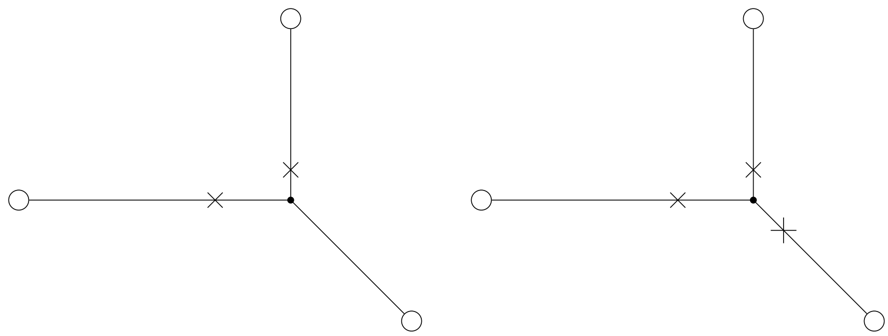


Figure 4.9: On extrema of eigenfunctions. On the left is an example of a possible cluster of $\mathcal{P}$ with nodes (open circles) and local extrema (crosses) of the eigenfunction. Such an eigenfunction may have multiple local extrema within the cluster. However, the local extrema cannot enclose an area as in the image on the right. In particular, any cluster of $\widetilde{\mathcal{P}}$, and thus of $\mathcal{P}'$, necessarily contains a node, that is, a boundary vertex of $\mathcal{P}$.

Next observe that every benign cluster admits at least two Neumann domains and therefore $\widetilde{\mathcal{P}}$ has at least $2k - n$ clusters. Lemma 2.1.8 combined with a simple induction argument shows that $\mathcal{P}'$ has at least $(2k - n) - (k - 1 + r) = k + 1 - n - r$ clusters, since undoing a simple cut (i.e., gluing once) will change the number of connected components of the cut graph by at most one.

We claim that every cluster $\mathcal{G}'$ of $\mathcal{P}'$ satisfies $\mu_2(\mathcal{G}') \leq \Lambda_k^D(\mathcal{P})$, which will complete the proof of the lemma. To this end, fix such a cluster $\mathcal{G}'$ of $\mathcal{P}'$; we first observe that $\mathcal{G}'$ contains at least two clusters of $\widetilde{\mathcal{P}}$, that is, it is formed out of at least two distinct Neumann domains of the eigenfunctions $u_1, \dots, u_k$ (cf. also Figure 4.8). To see this, observe that:

(1) the boundary sets of $\mathcal{P}$ and $\mathcal{P}'$ are disjoint: at any cut vertex of $\mathcal{G}_{\mathcal{P}}$ all the $u_i \in H^1(\mathcal{G})$ satisfy a Dirichlet condition; hence no such point can also be a local nonzero extremum;

(2) by construction, on each cluster of $\widetilde{\mathcal{P}}$ there is exactly one eigenfunction u_i which does not vanish identically, and this eigenfunction does not change sign within the cluster;

(3) no eigenfunction has a strictly positive local minimum or strictly negative local maximum anywhere; hence no eigenfunction can have a Neumann domain strictly contained in a nodal domain (see also Figure 4.9).

If $\mathcal{G}'$ should coincide with a single cluster $\widetilde{\mathcal{G}}$ of $\widetilde{\mathcal{P}}$, then in particular the two must share a boundary set. This means, by construction of $\widetilde{\mathcal{P}}$ and (1), that $\widetilde{\mathcal{G}}$ contains no Dirichlet points, that is, the only eigenfunction u_i (from (2)) which does not vanish identically in $\widetilde{\mathcal{G}}$, cannot have any zeros whatsoever there. But this is a contradiction to (3).

As a result, we can guarantee the existence of a function $\varphi \in H^1(\mathcal{G}')$ such that

$$\int_{\mathcal{G}'} \varphi(x)\,\mathrm{d}x = 0,$$

by taking φ to be a suitable linear combination of the restrictions of $u_i|_{\mathcal{G}'}$, $i = 1, \dots, k$. Then φ is a valid test function for $\mu_2(\mathcal{G}')$ on the one hand, and on the other the Rayleigh quotient of φ cannot exceed $\Lambda_k^D(\mathcal{P}) = \max_{i=1,\dots,k} \lambda_1(\mathcal{G}_i)$. The latter claim follows from a standard argument: by construction, on every nodal domain of φ we have that φ is a multiple of some u_i, and thus its Rayleigh quotient is no larger than the maximum of the Rayleigh quotients of the u_i on the respective nodal domains. Moreover, u_i satisfies either a standard or a Dirichlet condition at every vertex of this nodal domain, treated as a subgraph of $\mathcal{G}'$, and is thus a non-sign-changing classical eigenfunction there, so, as noted earlier, $\lambda_1(\mathcal{G}_i)$ is equal to the Rayleigh quotient of u_i on Ω. □

Proof of Theorem 4.5.2. The theorem will follow immediately from Lemma 4.5.13 once we have shown that any exhaustive partition $\mathcal{P}$ of $\mathcal{G}$ of rank $k-1+r$, $0 \le r \le \beta$, can have at most $n = \beta + |N| - r$ malign clusters.

We first observe that at most $|N|$ clusters can contain at least one leaf of $\mathcal{G}$; it remains to show that at most $\beta - r$ clusters can contain a cycle of $\mathcal{G}$. But this follows if we can show that the (disconnected) canonical cut graph $\mathcal{G}_{\mathcal{P}}$ has Betti number $\beta - r$. This, in turn, follows from a simple induction argument using the definition of r and Lemmata 2.1.8 and 2.1.15: there will exist an intermediate cut of $\mathcal{G}$ rank r which remains connected and has Betti number $\beta - r$; $\mathcal{G}_{\mathcal{P}}$ is then obtained from this intermediate graph by cutting $k-1$ times in such a way that each cut splits off an additional connected component (cluster of $\mathcal{P}$) from the rest of the graph. □

Remark 4.5.14. Let u be an eigenfunction of the Laplacian on $\mathcal{G}$ and $\mathcal{P}$ be its nodal partition with $k = \nu(u)$ nodal domains (clusters). We know that on each the restriction of u to each cluster coincides with the corresponding first eigenfunction on that cluster, with Dirichlet conditions at the boundary points. Then by construction, the partition $\mathcal{P}'$ in Lemma 4.5.13 coincides with the partition of $\mathcal{G}$ into the Neumann domains of u. The proof of Theorem 1.3.5 in particular ensures that this partition contains at least

$$\xi(u) \ge \nu(u) + 1 - \beta - |N| \tag{4.65}$$

clusters, the Neumann domains of u. Combining (4.65) and Remark 4.5.7, we recover (4.60).

4.5.4 Application: Spectral inequalities

In this section we will prove Corollary 4.5.3, relating the interlacing inequalities of Theorems 4.5.1 and 4.5.2 to the eigenvalues of the Laplacian on the whole graph $\mathcal{G}$ with Dirichlet and standard vertex conditions. Afterwards, we will discuss their relation with concrete estimates on the optimal energies $\mathcal{L}^D_{k,\infty}(\mathcal{G})$, $\mathcal{L}^N_{k,\infty}(\mathcal{G})$ in terms of geometric and topological properties of $\mathcal{G}$; complementary estimates were obtained in §4.4. We recall that $\lambda_k(\mathcal{G},\mathcal{V}) =: \lambda_k(\mathcal{G})$ and $\mu_k(\mathcal{G})$ are, respectively, the k-th eigenvalue, counted with multiplicities, of the Laplacian with Dirichlet conditions at *all* vertices of $\mathcal{G}$ (which thus reduces to a disjoint union of n intervals), and of the Laplacian with standard conditions at all vertices of $\mathcal{G}$.

Proof of Corollary 4.5.3. We clearly only have to prove the first and the last inequalities, the middle one being contained in Theorem 4.5.1. For the first inequality, $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \le \lambda_k(\mathcal{G})$, we observe, firstly, that for any finite interval $I \subset \mathbb{R}$ and $j \in \mathbb{N}$, $\lambda_j(I) = \mu_{j+1}(I)$.

We suppose that for each $i = 1,\dots,n$,

$$j_i := \max\{j \ge 0 : \lambda_j(e_i) \le \lambda_k(\mathcal{G})\},$$

so that the collection $\{\lambda_\ell(e_i) : 1 \le \ell \le j_i\}$ gives exactly the first k eigenvalues $\lambda_1(\mathcal{G}),\dots,\lambda_k(\mathcal{G})$, counted with multiplicities (if $\lambda_k(\mathcal{G})$ is multiple, meaning at least two edges have the same eigenvalue corresponding to $\lambda_k(\mathcal{G})$, then we arbitrarily choose a certain number to be excluded in order to guarantee that $\{\lambda_\ell(e_i) : 1 \le \ell \le j_i\}$ does in fact consist of exactly k elements, the largest of which is $\lambda_k(\mathcal{G})$).

For each $i = 1,\dots,n$ for which $j_i \ge 1$, we partition the edge e_i into j_i equal subintervals $e_{i,1},\dots,e_{i,j_i}$, each of which is a nodal domain for the eigenfunctions of $\lambda_{j_i}(e_i)$, so that, with our first observation, $\mu_2(e_{i,1}) = \ldots = \mu_2(e_{i,j_i}) = \lambda_1(e_{i,1}) = \lambda_{j_i}(e_i)$. Since $\sum_{i=1}^n j_i = k$, the (non-exhaustive) partition $\mathcal{P} := \{e_{i,\ell} : 1 \le \ell \le j_i,\ 1 \le i \le n\}$ is a k-partition of $\mathcal{G}$ such that

$$\Lambda^N_k(\mathcal{P}) = \max_{i,\ell} \mu_2(e_{i,\ell}) = \max_i \lambda_{j_i}(e_i) = \lambda_k(\mathcal{G}).$$

The inequality now follows extending the partition to an exhaustive partition that does not increase the energy (due to surgery principles; see e.g. [KKMM16, Lemma 2.3]). The last inequality,

$$\mu_k(\mathcal{G}) \le \mathcal{L}^D_{k,\infty}(\mathcal{G}),$$

follows from a standard argument involving the min-max characterization of $\mu_k(\mathcal{G})$, see also [KKLM21, Proposition 8.4] for a detailed proof. □

We now turn to Corollary 4.5.4. We first recall that [HKMP21a] derived, among other things, both upper and lower bounds for the quantities $\mathcal{L}^D_{k,\infty}(\mathcal{G})$ and $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G})$, namely

$$\frac{\pi^2}{L^2}k^2 \le \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G}) \le \frac{\pi^2}{L^2}\big(k+n-1\big)^2 \tag{4.66}$$

Figure 4.10: Two pumpkins connected by an edge. A graph given by two 3-pumpkins connected by an edge. The graph admits an Eulerian path seen on the right side.

and

$$\frac{\pi^2}{4kL^2}\left(k^3+3(k-|\mathsf{P}_2|-|N|)^3\right) \le \mathcal{L}_{k,\infty}^D(\mathcal{G}) \le \frac{\pi^2}{L^2}\left(k+\left(|\mathcal{E}|-1-\left\lfloor\frac{|N|}{2}\right\rfloor\right)\right)^2 \qquad (4.67)$$

for all sufficiently large k depending on $\mathcal{G}$; see [HKMP21a, Theorems 4.5, 4.9, 5.1 and 5.3] (note that the proof of the upper bound in (4.66), given for $\mathcal{L}_{k,p}^N(\mathcal{G})$, works for $\mathcal{L}_{k,p}^{N,c}(\mathcal{G})$ whenever $k \ge n$, that is, (4.66) is valid for all $k \ge n$). Here $|\mathsf{P}_2| \le \beta$ is the number of *doubly connected pendants* of $\mathcal{G}$ and $n \le |\mathcal{E}|$ is any number for which there exists an n-partition of $\mathcal{G}$ each of whose clusters consists of a single *Eulerian path*.

Proof of Corollary 4.5.4. This is an immediate consequence of the upper bound in (4.66) and Corollary 4.5.3. □

We observe that our inequality (4.59), which we reproduce here for the sake of convenience,

$$\mu_k(\mathcal{G}) \le \mathcal{L}_{k,\infty}^D(\mathcal{G}) \le \frac{\pi^2}{L^2}(k+n+\beta-2)^2$$

involves rather different quantities from the upper bound in (4.67), as well as what is possibly the best general upper bound on $\mu_k(\mathcal{G})$ to date, namely [BKKM17, Theorem 4.9]

$$\mu_k(\mathcal{G}) \le \frac{\pi^2}{L^2}(k+\tfrac{3}{2}\beta+\tfrac{1}{2}|N|-2)^2 \qquad (4.68)$$

for all $k \ge 1$ (see also [Ari16, Theorem 1.2] for an earlier iteration). We finish with a few examples which show that at least for some graphs our bound (4.59) can be better than (4.67) and even (4.68). Note, however, that the corresponding lower bound coming from Theorem 4.5.1 and (4.66),

$$\mathcal{L}_{k,\infty}^D(\mathcal{G}) \ge \frac{\pi^2}{L^2}(k-1-\beta-|N|)^2,$$

will not in general be better than the lower bound in (4.67), at least for large k, as one can see by comparing the respective coefficients of the k term in the bounds. It would be interesting to understand what the optimal coefficients might look like.

Example 4.5.15. We consider the *pumpkin dumbbell* depicted in Figure 4.10, consisting of two 3-pumpkins connected by an edge (interestingly, the relative edge lengths are irrelevant for these bounds). Then by Corollary 4.5.4 we have $\mathcal{L}_{k,\infty}^D(\mathcal{G}) \le \frac{\pi^2}{L^2}(k+4)^2$ for all $k \ge 1$, while since $|\mathcal{E}| = 7$ and $|N| = 0$ the upper bound in (4.67) reads $\mathcal{L}_{k,\infty}^D(\mathcal{G}) \le \frac{\pi^2}{L^2}(k+7)^2$ (for sufficiently large k). Introducing thicker pumpkins would lead to the same conclusion, that (4.59) is better.

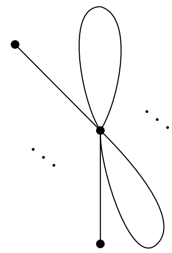


Figure 4.11: Stower graphs. Stower graphs as an example of a class of graphs for which (4.59) is better than (4.68)

.

Example 4.5.16. The bound on $\mu_k(\mathcal{G})$ in (4.59) is better than (4.68) for all flower graphs (where $|N| = 0$ and $n = 1$), and more generally *stower graphs* (flowers with a finite number of pendant edges attached to the central vertex, i.e., a union of a flower and a star; see Figure 4.11). These were introduced in [BL17a], where they played a major role in the minimization of $\mu_2(\mathcal{G})$ among various classes of graphs. There exist such stower graphs with any $\beta \geq 1$ and $|N| \geq 1$ pendant edges, while we certainly have $n \leq \lceil \frac{|N|}{2} \rceil$, leading to the assertion that (4.59) is better. Finally, the respective upper bounds coincide for star graphs for which $|N|$ is even, since then $\beta = 0$ and $n = \frac{|N|}{2}$.

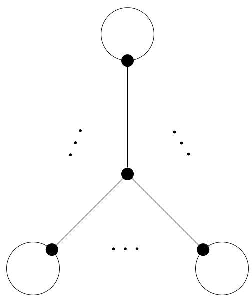


Figure 4.12: Windmill graph. Windmill graphs are examples of graphs for which the upper estimate in (4.68) is attained. As it turns out this is also the case in (4.59) when the graph has an even number of pendant lassos.

Example 4.5.17. Let $\mathcal{G}$ be a *windmill graph* $\mathcal{W}^{2m}$, $m \geq 1$, which consists of $2m$ lassos(*blades*) glued together at a central vertex (see Figure 4.12); we assume that all the loops have a common length $\ell > 0$ and the bridges a common length $s > 0$. It was shown in [KS18] that, if the ratio $\ell/s = 4$, then there is equality in (4.68) for any number of blades. In particular, since $\beta = 2m$,

$$\mu_k(\mathcal{W}^{2m}) = \frac{\pi^2}{L^2}(k + 3m - 2)^2$$

for all $k \geq 1$. Note that $\mathcal{W}^{2m}$ can be partitioned into $n = m$ clusters, each consisting of exactly two blades glued together (like the dumbbell pumpkin of Figure 4.10 but with loops in place of the 3-pumpkins). This means that the upper bound in (4.59) is also equal to $\frac{\pi^2}{L^2}(k + 3m - 2)^2$;

hence we have equality everywhere,

$$\mu_k(\mathcal{W}^{2m}) = \mathcal{L}^D_{k,\infty}(\mathcal{W}^{2m}) = \mathcal{L}^{N,c}_{k-1+\beta,\infty}(\mathcal{W}^{2m}) = \frac{\pi^2}{L^2}(k+3m-2)^2$$

for all $k \geq 1$. In particular, Theorem 4.5.1 is sharp for windmill graphs $\mathcal{W}^{2m}$ for which $\ell/s = 4$.

Very recently, all graphs which attain the upper estimate in (4.68) were classified in [Ser21]. We leave it as an open question whether similar results can be shown for the inequalities obtained in this section especially for Theorem 4.5.1.

4.6 On the Monotonicity of spectral minimal energies

The spectral minimal partitions $\mathcal{L}^D_{k,p}(\mathcal{G}), \mathcal{L}^N_{k,p}(\mathcal{G})$ as defined in §4.1 exhibit some monotonicity properties we will con. Let $\Omega \subset \mathbb{R}^N$ for some $n \in \mathbb{N}$. In [CTV05] was shown existence of minimizers of the spectral minimal partitions that

$$\mathcal{L}_{k,p}(\Omega) := \inf_{\substack{\Omega_1,\ldots,\Omega_k \text{ open, connected} \\ |\Omega_i \cap \Omega_j|=0 \text{ for } i\neq j}} \Lambda_p(\mathcal{P})$$

with

$$\Lambda_p(\Omega_1,\ldots,\Omega_k) = \begin{cases} \left(\frac{1}{k}\sum_{i=1}^k \lambda_1(\Omega_i)\right)^{1/p}, & p<\infty \\ \max\{\lambda_1(\Omega_1),\ldots,\lambda_1(\Omega_k)\}, & p=\infty \end{cases}$$

where $\lambda_1(\Omega_i)$ is the first nontrivial eigenvalue of $-\Delta$ on Ω_i with Dirichlet condition at $\partial\Omega_i$. In particularly, it was shown that $\mathcal{L}_{k,p}(\Omega)$ is monotonic increasing in p and k. For metric graphs we have following analogy of [KKLM21, Proposition 6.1]:

Proposition 4.6.1. *For all $1 \leq p_1 \leq p_2 \leq \infty$, we have*

$$\mathcal{L}^N_{k,q,p_1}(\mathcal{G}) \leq \mathcal{L}^N_{k,q,p_2}(\mathcal{G}) \leq k^{\frac{1}{p_1}-\frac{1}{p_2}}\mathcal{L}^N_{k,q,p_2}(\mathcal{G})$$

and

$$\mathcal{L}^D_{k,q,p_1}(\mathcal{G}) \leq \mathcal{L}^D_{k,q,p_2}(\mathcal{G}) \leq k^{\frac{1}{p_1}-\frac{1}{p_2}}\mathcal{L}^D_{k,q,p_1}(\mathcal{G}).$$

Moreover, $p \mapsto \mathcal{L}^N_{k,q,p}(\mathcal{G})$ and $p \mapsto \mathcal{L}^D_{k,q,p}(\mathcal{G})$ are continuous and monotonically increasing in $p \in [1,\infty]$.

Proof. For simplicity we only give the proof for $\mathcal{L}^N_{k,q,p}$; the other case follows analogous. Let $\mathcal{P}$ be any connected k-partition, then with Hölder inequality we infer

$$\Lambda^N_{k,q,p_1}(\mathcal{P}) \leq \Lambda^N_{k,q,p_2}(\mathcal{P}) \leq k^{\frac{1}{p_1}-\frac{1}{p_2}}\Lambda^N_{k,q,p_1}(\mathcal{P}).$$

We then have from the definition

$$\mathcal{L}^N_{k,q,p_1}(\mathcal{G}) \le \mathcal{L}^N_{k,q,p_2}(\mathcal{G}) \le k^{\frac{1}{p_1}-\frac{1}{p_2}} \mathcal{L}^N_{k,q,p_1}(\mathcal{G}).$$

Thus, we infer

$$\left|\mathcal{L}^N_{k,q,p_2}(\mathcal{G}) - \mathcal{L}^N_{k,q,p_1}(\mathcal{G})\right| \le k^{\frac{1}{p_1}-\frac{1}{p_2}} \sup_{p\in[1,\infty]} \mathcal{L}^N_{k,q,p_1}$$

and since $\mathcal{L}^N_{k,q,p_1}(\mathcal{G}) \le \mathcal{L}^N_{k,q,\infty}(\mathcal{G})$ is uniformly bounded, we infer that $p \mapsto \mathcal{L}^N_{k,q,p}(\mathcal{G})$ is continuous. □

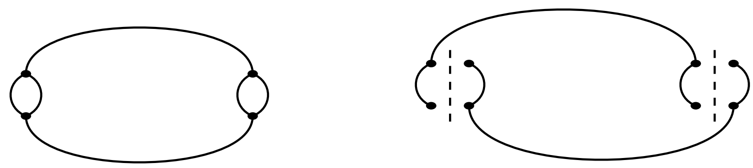


Figure 4.13: Counterexample for monotonicity in the Neumann case. The graph on the left admits a rigid two-partition into equal intervals (right); thus there is equality in the lower bound (4.37). We will return to this graph in Example 4.4.26 to show that we do not necessarily have monotonicity in k in the Neumann case.

However, monotonocity in k is not so clear in the Neumann cases.

Example 4.6.2. Consider the graph $\mathcal{G}$ in Figure 4.13, then we have

$$\mu_2(\mathcal{G}) = \mathcal{L}^D_{2,\infty}(\mathcal{G}) = \mathcal{L}^{N,r}_{1,\infty} > \mathcal{L}^{N,c}_{1,\infty} = \mathcal{L}^{N,c}_{2,\infty}(\mathcal{G}) = \mathcal{L}^{N,r}_{2,\infty}(\mathcal{G}). \tag{4.69}$$

In fact, as Figure 4.13 shows that there exists a rigid two-partition into equal intervals, then by Theorem 4.4.13 we have

$$\mathcal{L}^{N,r}_{2,\infty} = \frac{4\pi^2}{|\mathcal{G}|^2},$$

but by Proposition 4.4.1 we have $\mu_2(\mathcal{G}) > \frac{\pi^2}{|\mathcal{G}|^2}$ and we infer (4.69). However $k \mapsto \mathcal{L}^D_{k,\infty}(\mathcal{G})$ is still monotonic as the following statement shows.

Theorem 4.6.3. *Let $\mathcal{G}$ be a metric graph, then for $k \ge 1$*

$$k \mapsto \mathcal{L}^D_{k,\infty}(\mathcal{G}) \quad \textit{and} \quad k \mapsto \mathcal{L}^{N,c}_{k,\infty}(\mathcal{G})$$

are monotonically increasing in k. Moreover for $k \ge \beta + 1$ also

$$k \mapsto \mathcal{L}^N_{k,\infty}(\mathcal{G})$$

is monotonically increasing.

Proof. Let us first deal with the case of connected partitions. Suppose $\mathcal{P} = (\mathcal{G}_1, \dots, \mathcal{G}_k)$ is a k-partition, then given a non-exhaustive connected partition one can always find a exhaustive partition with the same number of clusters which does not increase the spectral energy and we can restrict ourselves to non-exhaustive connected partitions. Consequentially, if we take any partition $\mathcal{P}'$ consisting of the elements $\mathcal{G}_1, \dots, \mathcal{G}_k$ we have

$$\Lambda^N_{k,\infty}(\mathcal{P}) \geq \Lambda^N_{k,\infty}(\mathcal{P}') \text{ and } \Lambda^D_{k,\infty}(\mathcal{P}) \geq \Lambda^D_{k,\infty}(\mathcal{P}')$$

respectively. Hence, $\mathcal{L}^{N,c}_{k,\infty}(\mathcal{G})$ and $\mathcal{L}^D_{k,\infty}(\mathcal{G})$ is monotonous for all $k \geq 1$.

This procedure does not however apply in the same way to rigid partitions. However, when there is $k > \beta$ at least two partition elements are necessarily only connected by a pendant graph, then by the surgery principle [BKKM19, Theorem 3.10 (2)] we can glue together two graphs at one vertex and the resulting graph does not increase the spectral energy. $\square$

Chapter 5

On Pleijel's theorem for metric graphs

In this chapter we present Pleijel type theorems for differential operators on metric graphs. In particular, we show our results from §1.3.3. In §5.1 we present the principal setting and introduce the operators we consider. §5.2 is a prelimary section regarding results such as an estimate of the first eigenvalues of the operators considered and the characterization of variational eigenvalues of the p-Laplacian and Weyl asymptotics. In §5.3 we prove Pleijel's theorem for general Schrödinger operators on metric graphs that we introduce in §5.1, which shows in particular Theorem 1.3.10. In the particular case, for the free Laplacian with standard conditions at all vertices we present refined results in §5.4 and show in particular Theorem 1.3.11. This chapter corresponds to the joint work [HKMP21b], which we present here with only minor modifications, such as comments to related subjects considered in the thesis.

5.1 General setting

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a compact metric graph throughout this chapter. In what follows we will give a description of the operators we will be considering in the context of our main results in §1.3.3. Note that all we will need for the results there are certain more or less abstract properties which these operators satisfy. We first consider a possible relaxation of the continuity condition at the vertices to allow for *weighted* continuity encoded in a nonnegative vector of edge weights $w_{\mathsf{v}} \in \mathbb{R}_{>0}^{\deg(\mathsf{v})}$, $\mathsf{v} \in V$, i.e.,

$$w_{\mathsf{e},\mathsf{v}} f_{\mathsf{e}}(\mathsf{v}) = w_{\mathsf{f},\mathsf{v}} f_{\mathsf{f}}(\mathsf{v}) \quad \text{if } \mathsf{v} \in \mathsf{e} \cap \mathsf{f}. \tag{5.1}$$

Indeed, in this case we can define, in a natural way, a space $H^1_w(\mathcal{G})$ of edgewise H^1-functions that satisfy (5.1) at the vertices. Note that while functions in $H^1_w(\mathcal{G})$ may be discontinuous at the vertices, they can only change sign at a vertex, i.e., take on positive and negative values in any neighborhood of a vertex, if they are zero at that vertex.

We then define, for $q \in L^1(\mathcal{G})$ and a matrix $\mathcal{B} \in M_{2|E|\times 2|E|}(\mathbb{C})$ consisting of block matrices

$\mathcal{B}_{\mathsf{vw}} \in \mathbb{C}^{\deg(\mathsf{v})\times\deg(\mathsf{w})}$ for all $\mathsf{v},\mathsf{w} \in V$ the quadratic form

$$\begin{aligned} a(f) &:= \int_{\mathcal{G}} \left(|f'(x)|^2 + q(x)|f(x)|^2\right) \mathrm{d}x + \sum_{\mathsf{v},\mathsf{w}\in V} (\mathcal{B}_{\mathsf{vw}} f(\mathsf{w}), f(\mathsf{v}))_{\mathbb{C}^{\deg(\mathsf{v})}} , \\ D(a) &:= H^1_w(\mathcal{G}), \end{aligned} \tag{5.2}$$

where for each $\mathsf{v},\mathsf{w} \in V$, $\mathcal{B}_{\mathsf{vw}}$ is a $\deg(\mathsf{v}) \times \deg(\mathsf{w})$-matrix, and for $\mathsf{v} \in V$, $f(\mathsf{v}) = (f_{\mathsf{e}}(\mathsf{v}))_{\mathsf{e}\in E_{\mathsf{v}}}$. If we want to emphasise the dependence on the potential and the vertex conditions, then we will also write

$$a_{q,\mathcal{B},w} \qquad \text{in place of just } a.$$

At any rate, it follows from the theory presented in [Mug14, §6.5] that this form is bounded and elliptic; hence the associated operator $A = A(q,\mathcal{B},w)$ is (minus) the generator of an analytic, strongly continuous semigroup on $L^2(\mathcal{G})$. This semigroup is of trace class and therefore A has pure point spectrum.

If in particular q is real-valued and $\mathcal{B}$ is Hermitian for all $\mathsf{v} \in V$, then a is a closed quadratic form, hence $A(q,\mathcal{B},w)$ is a self-adjoint operator that is bounded from below. This setting includes, as special cases, realizations of the Laplacian on $\mathcal{G}$ with so-called standard conditions (continuity across vertices, all normal derivatives sum up to 0), i.e. with domain contained in $W^{2,1}(\mathcal{G})$ as defined in §2.2.2, corresponding to $q \equiv 0$, $\mathcal{B} = 0$ and $w \equiv 1$, as well as (standard) delta couplings (continuity across vertices, at each vertex the sum of all normal derivatives equals a multiple of the point evaluation at the same vertex), where $q \equiv 0$, $w \equiv 1$ and $\mathcal{B}$ is a diagonal matrix with respect to the canonical basis of $\mathbb{C}^{2|E|}$.

Now, because $u^+ \in H^1_w(\mathcal{G})$ for all $u \in H^1_w(\mathcal{G})$ due to positivity of the edge weights w, it is known, cf. [Mug14, Theorem 6.85], that the semigroup is positive if and only if so is the semigroup generated by each $-\mathcal{B}$ (this is in particular the case if $\mathcal{B}$ is diagonal, which covers delta couplings, including weighted versions thereof). In this context, we refer to the condition (5.1) and the weighted Kirchhoff–Robin-type condition associated with the matrix $\mathcal{B}$ collectively as *positivity preserving* vertex conditions. Finally, all these assertions remain valid if, for some $\mathcal{V}^D \subset \mathcal{V}$ (where possibly, trivially, $\mathcal{V}^D = \emptyset$), we consider the operator $A(q,\mathcal{B},w,\mathcal{V}^D)$ associated with the restriction of the form a to $H^1_{0,w}(\mathcal{G},\mathcal{V}^D)$, the space of all functions in $H^1_w(\mathcal{G})$ that vanish on the vertices in $\mathcal{V}^D$ (in this case, of course, we only require that $\mathcal{B}_{\mathsf{vw}}$ be defined for $\mathsf{v},\mathsf{w} \in \mathcal{V}\setminus\mathcal{V}^D$). Finally, let

$$H^1_0(\mathcal{G}) := H^1_0(\mathcal{G};\mathcal{V}^D) \tag{5.3}$$

denote the space of globally H^1-functions which vanish at *all* vertices, which is clearly contained in the domain of the considered forms.

The Schrödinger operators associated with these classes of forms were thoroughly studied in [Kur19].

In all these cases, the discrete spectrum of $A(q, \mathcal{B}, w, \mathcal{V}^D)$ consists of real eigenvalues $\lambda_n(q, A, w, \mathcal{V}^D)$ repeated according to their finite multiplicities, characterized minimax principles (c.f. §2.3.3 for the related minimax principle for Schrödinger operators), which diverge to $+\infty$ as $n \to \infty$, and whose eigenfunctions may be chosen to be real and to form an orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of $L^2(\mathcal{G})$. (We mostly avoid this heavy notation and simply write $\lambda_n(\mathcal{G}) := \lambda_n(q, \mathcal{B}, w, \mathcal{V}^D)$.)

Suitably adapting the proof of [Mug07, Proposition 3.7.(1)] to the case of $w \not\equiv 1$ and $q \not\equiv 0$, one can easily prove that the associated semigroup, if positive, is additionally irreducible if there is no point in V_0 whose removal would disconnect $\mathcal{G}$. Hence, by the Kreĭn–Rutman Theorem (c.f. [Hen06, Theorem 1.2.6] and the references therein), we deduce that the first eigenspace is one-dimensional and spanned by a positive function (the Perron eigenfunction) ψ_1: i.e., $\psi_1(x) > 0$ for a.e. $x \in \mathcal{G}$. Indeed, more holds: it was proved in [Kur19] that a strong maximum principle holds, namely the Perron eigenfunction vanishes only at the vertices in $\mathcal{V}^D$. This was proved in [Kur19] for the case of block-diagonal $\mathcal{B}$ (corresponding to the case of local vertex conditions) only; here we restrict ourselves to this case.

We will denote by $\lambda_n^D = \lambda_n^D(\mathcal{G})$ the n-th lowest eigenvalue (counting multiplicities) of the Schrödinger operator with potential q and Dirichlet conditions at *all* vertices of $\mathcal{G}$, that is, whose form domain is $H_0^1(\mathcal{G})$; in this case the graph decomposes into a disjoint collection of intervals, moreover, the associated sesquilinear form is exactly (5.2) restricted to $H_0^1(\mathcal{G})$. We note the following eigenvalue interlacing result for future reference. This is an immediate variant of interlacing results stated in [BK13, Chapter 3.1.6] (cf. also [BKKM19, §4.1]).

Lemma 5.1.1. *With the above assumptions and notation, for all $n \geq |V| + 1$ we have*

$$\lambda_{n-|V|}^D(\mathcal{G}) \leq \lambda_n(\mathcal{G}) \leq \lambda_n^D(\mathcal{G}).$$

Proof. Both inequalities are an immediate consequence of the min-max characterization of the respective eigenvalues and the fact that the forms agree on $H_0^1(\mathcal{G})$, the latter in conjunction with the inclusion of the form domains $H_0^1(\mathcal{G}) \subset D(a)$, the former in conjunction with the fact that the quotient space $D(a)/H_0^1(\mathcal{G})$ is at most $|V|$-dimensional. □

5.2 Preliminary results

In this preliminary section we show some preliminary results that we require for our main results (see §1.3.3). In §5.2.1 we show an estimate for the first eigenvalue of the Schrödinger operators we consider. In §5.2.2 we review the construction of the variational eigenvalues of the p-Laplacian (with standard vertex conditions, that is, continuity and an appropriate p-version of the Kirchhoff condition) and show the Weyl asymptotics of the p-Laplacian, an adapted version of the Weyl asymptotics (c.f. in Lemma 5.3.5) for the second-order operators considered.

5.2.1 An estimate on the first eigenvalue of general Schrödinger operators

In this preliminary section we give an estimate on the first eigenvalue $\lambda_1(\mathcal{G})$ of any Schrödinger operator $A = A(q, \mathcal{B}, w, V_0)$ of the form introduced in §5.1, on any compact metric graph. We impose the following assumptions in this chapter.

Assumption 5.2.1. *$\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a compact, connected metric graph with underlying combinatorial graph $G = (V, E)$ and edge lengths ℓ_{e}, $\mathsf{e} \in E$; we set $\ell_{\min} := \min_{\mathsf{e}\in E} \ell_{\mathsf{e}}$. We also fix a (possibly empty) set $\mathcal{V}^D \subset \mathcal{V}$ and a potential $q \in L^1(\mathcal{G})$ with $q \geq q_{\min}$ for some $q_{\min} \in \mathbb{R}$, and suppose $\mathcal{B}$ is a Hermitian $2|E| \times 2|E|$-matrix such that the semigroup $(e^{-t\mathcal{B}})_{t\geq 0}$ is positive and $(w_{\mathsf{v}})_{\mathsf{v}\in V} \in \mathbb{R}^{2|E|}$ is a vector such that $w_{\mathsf{v}} \in \mathbb{R}_+^{\deg(\mathsf{v})}$ for all $\mathsf{v} \in V$.*

Estimates of this level seem to be new at this level of generality and may be of some independent interest, although there is considerable room for improvement. In practice we will take Assumption 5.2.1; however, the following statement and proof is also valid for general $q \in L^1(\mathcal{G})$, not necessarily bounded from below. The proof also shows that the norm $\|q\|_1$ may be replaced by $\|q_+\|_1$, the norm of the positive part of q (this is a trivial consequence of the variational characterization of λ_1).

Proposition 5.2.2. *Keeping the notation of §5.1 and §5.3, under Assumption 5.2.1 we have*

$$\lambda_1(\mathcal{G}) \leq \left(\frac{\pi|E|}{|\mathcal{G}|} + \|q\|_1\right)^2 - \|q\|_1^2. \tag{5.4}$$

Note that $\frac{|\mathcal{G}|}{|E|}$ is exactly the average edge length of $\mathcal{G}$. If $q \equiv 0$, a similar but stronger inequality was obtained in [KKMM16, Theorem 4.2].

Proof. We first observe that the inequality

$$\|f\|_\infty^2 \leq 2\|f'\|_2\|f\|_2 \tag{5.5}$$

is valid for all $f \in H_0^1(\mathcal{G})$: indeed, fixing any edge e, identified with the interval $[0, \ell_{\mathsf{e}}]$, and any $x \in (0, \ell_{\mathsf{e}})$, by the fundamental theorem of calculus and the Cauchy–Schwarz inequality, since $f(0) = 0$ we have

$$|f(x)|^2 = \int_0^x \left(|f(t)|^2\right)' \,\mathrm{d}t \leq 2\int_0^x |f'(t)||f(t)| \,\mathrm{d}t \leq 2\|f'\|_2\|f\|_2.$$

Now suppose that $f \in H_0^1(\mathcal{G})$ satisfies $\|f\|_2 = 1$, then by (5.5)

$$\lambda_1(\mathcal{G}) \leq \int_{\mathcal{G}} |f'(x)|^2 + q(x)|f(x)|^2 \,\mathrm{d}x \leq \|f'\|_2^2 + 2\|q\|_1\|f'\|_2.$$

Taking the infimum over all such functions f yields

$$\lambda_1(\mathcal{G}) \leq \lambda_1^D(0) + 2\lambda_1^D(0)^{1/2}\|q\|_1,$$

where $\lambda_1^D(0)$ is the Dirichlet Laplacian on $\mathcal{G}$, i.e., with zero potential and Dirichlet conditions at all vertices of $\mathcal{G}$ (that is, the Dirichlet Laplacian on the collection of $|E|$ disjoint intervals comprising the edges of $\mathcal{G}$). Now at least one edge of $\mathcal{G}$ has length at least $|\mathcal{G}|/|E|$; and so $\lambda_1^D(0) \le \pi^2|E|^2/|\mathcal{G}|^2$. This yields (5.4). □

5.2.2 Weyl's law for the p-Laplacian on metric graphs

The goal of this section is, firstly, to recall briefly the construction of the variational eigenvalues of the p-Laplacian (with standard vertex conditions, that is, continuity and an appropriate p-version of the Kirchhoff condition); this is well known on intervals and domains, and nothing changes in the case of metric graphs (see also [DR16]); secondly, we will show that the Weyl asymptotics known for the p-Laplacian eigenvalues on the interval also holds on metric graphs. This is a simple application of Dirichlet–Neumann bracketing.

We recall that the n-th variational eigenvalue of the p-Laplacian on a graph $\mathcal{G}$ with standard vertex conditions, $p \in (1,\infty)$, may be characterized variationally in terms of the Krasnosel'skii genus. More precisely, analogously to [BD03, Section 5], see also [DR02, Section 3], we consider the manifold

$$\mathcal{S} := \left\{ f \in W^{1,p}(\mathcal{G}) : \|f\|^p_{L^p(\mathcal{G})} = 1 \right\},$$

and for a closed, symmetric, non-empty set $\mathcal{A} \subset \mathcal{S}$ its Krasnosel'skii genus $\gamma(\mathcal{A}) \in \mathbb{N}$ by

$$\gamma(\mathcal{A}) := \inf\{k \in \mathbb{N} : \text{ there exists } \Phi : \mathcal{A} \to \mathbb{S}^k \text{ continuous and odd}\},$$

(or $\gamma(\mathcal{A}) = \infty$ if this infimum is infinite). Here $\mathbb{S}^k$ denotes the unit sphere in $\mathbb{R}^k$ for $k \in \mathbb{N}$ and a map $\Phi : \mathcal{A} \to \mathbb{S}^k$ is called *odd* if $\Phi(-f) = -\Phi(f)$ holds for all $f \in \mathcal{A}$. Finally, for every $n \in \mathbb{N}$ we set $\mathcal{F}_n := \{\mathcal{A} \subset \mathcal{S} : \gamma(\mathcal{A}) \ge n\}$. Then we may define the n-th variational eigenvalue $\lambda_{n,p}(\mathcal{G})$ of the p-Laplacian on $\mathcal{G}$ with standard vertex conditions by

$$\lambda_{n,p}(\mathcal{G}) = \inf_{\mathcal{A}\in\mathcal{F}_n} \sup_{f\in\mathcal{A}} \int_{\mathcal{G}} |f'(x)|^p \,\mathrm{d}x. \tag{5.6}$$

That this does indeed give rise to an infinite sequence of eigenvalues on any compact metric graph $\mathcal{G}$ follows from the same argument as the one used in [BD03], see also [DR00; DR02]. While *a priori* $(\lambda_{n,p}(\mathcal{G}))_{n\in\mathbb{N}}$ is just a sequence of critical points of a certain functional, mimicking the proof of [BR08, Theorem 2.1] one can show by known methods that each such *variational eigenvalue* is actually associated with an eigenfunction in the following weak sense.

Lemma 5.2.3. *For each $n \in \mathbb{N}$ there exists a (so-called Carathéodory) eigenfunction associated with $\lambda = \lambda_{n,p}(\mathcal{G})$, i.e., a non-zero solution $\psi_{n,p} = u$ of the system*

$$\begin{aligned} u' &= |v|^{\frac{1}{p-1}} \operatorname{sgn} v \\ v' &= -\lambda |u|^{p-1} \operatorname{sgn} u. \end{aligned}$$

such that u and v satisfy the continuity and Kirchhoff-type vertex conditions, respectively. In particular, $\psi_{n,p}$ is a real, absolutely continuous function, and so is $|\psi_{n,p}|^{p-1}\operatorname{sgn}\psi_{n,p}$.

In particular, and with the terminology of [BR08]: like on intervals with Dirichlet or Neumann boundary conditions, each variational eigenvalue is a Carathéodory eigenvalue, too.

We also define the corresponding eigenvalues in the case that all vertices of $\mathcal{G}$ are equipped with either a Dirichlet or a Neumann condition, in which case $\mathcal{G}$ decomposes into the disjoint union of $|E|$ edges, or intervals; this obviously includes the case $|E| = 1$ where $\mathcal{G}$ is just a (bounded) interval itself. We define the natural analogues of $\mathcal{S}$, namely

$$\mathcal{S}^D := \left\{ f \in W_0^{1,p}(\mathcal{G}) : \|f\|^p_{L^p(\mathcal{G})} = 1 \right\},$$
$$\mathcal{S}^N := \left\{ f \in \bigoplus_{\mathsf{e}\in E} W^{1,p}(0,\ell_\mathsf{e}) : \|f\|^p_{L^p(\mathcal{G})} = 1 \right\},$$

where $W_0^{1,p}(\mathcal{G})$ is, analogously to $H_0^1(\mathcal{G}) := H^1(\mathcal{G}; V)$ in (5.3), the space of all functions in $W^{1,p}(\mathcal{G})$ vanishing at *all* vertices, and $\bigoplus_{\mathsf{e}\in E} W^{1,p}(0,\ell_\mathsf{e})$ is to be identified with a superset of $W^{1,p}(\mathcal{G})$ in the obvious way. Then, defining the Krasnosel'skii genus in the same way as above, and finally

$$\mathcal{F}_n^{D,N} := \{\mathcal{A} \subset \mathcal{S}^{D,N} : \gamma(\mathcal{A}) \geq n\},$$

we define the respective n-th variational eigenvalues by

$$\lambda_{n,p}^{D,N}(\mathcal{G}) = \inf_{\mathcal{A}\in\mathcal{F}_n^{D,N}} \sup_{f\in\mathcal{A}} \int_{\mathcal{G}} |f'(x)|^p \,\mathrm{d}x. \tag{5.7}$$

Again, it is easy to see that in both cases there is a sequence of eigenvalues; this is proved explicitly in [LE11, Theorems 3.3 and 3.4] for the p-Laplacian on intervals (but it makes no difference if we consider a disjoint union of intervals). We may also consider eigenvalues $\lambda_{n,p}^D(\mathcal{G}; V_0)$ with a Dirichlet condition imposed at some subset V_0 of the vertices and standard conditions at the rest; all the definitions are analogous and we do not go into details.

The following Dirichlet–Neumann bracketing principle is an immediate consequence of the respective eigenvalue definitions.

Lemma 5.2.4. *Fix $p \in (1,\infty)$ and $\mathcal{G}$. With the notation introduced above, we have*

$$\lambda_{n,p}^N(\mathcal{G}) \leq \lambda_{n,p}(\mathcal{G}) \leq \lambda_{n,p}^D(\mathcal{G})$$

for all $n \geq 1$.

Proof. We observe that $\mathcal{S}^D \subset \mathcal{S} \subset \mathcal{S}^N$, whence $\mathcal{F}_n^D \subset \mathcal{F}_n \subset \mathcal{F}_n^N$. The statement is now an immediate consequence of the characterizations (5.6) and (5.7). □

Theorem 5.2.5 (Weyl asymptotics). *Fix $p \in (1, \infty)$ and suppose the graph $\mathcal{G}$ has total length $|\mathcal{G}|$. Then the n-th variational eigenvalue $\lambda_n(\mathcal{G})$ satisfies*

$$\lambda_{n,p}(\mathcal{G}) = (p-1)\left(\frac{\pi_p}{|\mathcal{G}|}\right)^p n^p + o(n^p) \qquad \text{as } n \to \infty, \tag{5.8}$$

where we recall $\pi_p = \frac{2\pi}{p\sin(\frac{\pi}{p})}$.

A corresponding Weyl asymptotics for the Dirichlet p-Laplacian on general domains in $\mathbb{R}^n$ was established only very recently, see [Maz19].

Proof. We first observe that the Weyl asymptotics (5.8) holds for the p-Laplacian on an interval with both Dirichlet and Neumann boundary conditions (see [LE11, Theorems 3.3 and 3.4]. Hence it also holds in the case that $\mathcal{G}$ is a disjoint collection of intervals, equivalently, for any graph $\mathcal{G}$ it holds for $\lambda^N_{n,p}(\mathcal{G})$ and $\lambda^D_{n,p}(\mathcal{G})$. The conclusion of the theorem now follows immediately from Lemma 5.2.4. □

5.3 Pleijel's theorem for Schrödinger operators on metric graphs

Our main result in this chapter is a variation of Pleijel's theorem for metric graphs. Under Assumption 5.2.1 we will consider the operator associated with the form $a_{q,A,w}$ introduced in Section 5.1. In this section we fix once and for all an (*a priori* arbitrary) eigenbasis of this operator.

Definition 5.3.1. Let $(\psi_n)_{n\in\mathbb{N}}$ be an orthonormal sequence of eigenfunctions $(\psi_n)_{n\in\mathbb{N}}$ with associated eigenvalues $(\lambda_n)_{n\in\mathbb{N}}$ of the Schrödinger operator $A(q, \mathcal{B}, w, V_0)$ associated with the form $a_{q,\mathcal{B},w}$. As already mentioned in the introduction, the *nodal domains* of any eigenfunction ψ_k are the respective closures in the metric space $\mathcal{G}$ of connected components of the sets $\{\psi_k \neq 0\}$. We occasionally denote by $\mathcal{G}_1, \dots, \mathcal{G}_{\nu_k}$ the nodal domains themselves, and by $\partial\mathcal{G}_i$ the topological boundary of $\mathcal{G}_i$ in $\mathcal{G}$. We denote the nodal count of this sequence by $(\nu_n)_{n\in\mathbb{N}}$.

The following simple example demonstrates that, contrary to the previously mentioned generic case, the nodal domains of an eigenfunction might not exhaust the whole graph; and an eigenfunction might have the same sign on two adjacent nodal domains.

Example 5.3.2. We consider the equilateral 4-star; more precisely, we take $\mathcal{G}$ to consist of four edges $\mathsf{e}_1, \dots, \mathsf{e}_4$, each of length 1 and identified with the interval $[0, 1]$, joined at a common vertex of degree four (identified with 0 on each edge), and with the other four vertices each being of degree one. An eigenfunction φ with respect to the eigenvalue $\frac{\pi^2}{4}$ of the Laplacian on $\mathcal{G}$ with standard vertex conditions is given by $\varphi(x) = \sin(\frac{\pi}{2}x)$ on e_1 and e_2 respectively, $\varphi(x) = -2\sin(\frac{\pi}{2}x)$ on e_3 and $\varphi(x) = 0$ on e_4. The three nodal domains of φ are the (closed) edges e_1, e_2 and e_3. Clearly, they do not cover the whole graph $\mathcal{G}$. Moreover, although the nodal domains e_1 and e_2 are adjacent, φ has the same sign on both.

A priori the sequence $\nu_k \in \mathbb{N}$, including the points of accumulation, can depend on the precise choice of basis, see Example 5.4.5 below, unless suitable assumptions on the edge lengths $(\ell_\mathsf{e})_{\mathsf{e}\in E}$ and the graph topology are imposed that force all eigenvalues to be simple.

Furthermore, here and throughout, given a sequence $(a_n)_{n\in\mathbb{N}} \subset \mathbb{R}$, we will write

$$\operatorname{acc}\{a_n : n \in \mathbb{N}\}$$

to denote its set of points of accumulation. With this we are now ready to formulate our first main theorem.

Theorem 5.3.3. *For all quantum graphs satisfying Assumption 5.2.1, the nodal count $(\nu_n)_{n\in\mathbb{N}}$ satisfies for any choice of basis of eigenfunctions*

$$\operatorname{acc}\left\{\tfrac{\nu_n}{n} : n \in \mathbb{N}\right\} \subset \left\{\frac{\sum_{\mathsf{e}\in E_0}\ell_\mathsf{e}}{|\mathcal{G}|} : E \supset E_0 \textit{ is a nonempty set of edges}\right\}. \tag{5.9}$$

In particular, $\operatorname{acc}\left\{\tfrac{\nu_n}{n} : n \in \mathbb{N}\right\}$ *is a finite set, and*

$$0 < \frac{\ell_{\min}}{|\mathcal{G}|} \le \liminf_{n\to\infty}\frac{\nu_n}{n} \le \limsup_{n\to\infty}\frac{\nu_n}{n} \le 1. \tag{5.10}$$

While the right-hand side of (5.9) does not depend on the parameters $q, \mathcal{B}, w$, the set inclusion in (5.9) is sharp in the case of a graph consisting of just one interval. Indeed, recall that on intervals, in the case of Sturm–Liouville problems, $\nu_n = n$ for all $n \in \mathbb{N}$ (see [Hin05]).

As mentioned in the introduction, the key driving force behind the potential appearance of a non-trivial set of points of accumulation of $\frac{\nu_n}{n}$ between 0 and 1 here is the failure of the unique continuation principle, as evidenced by the following characterization.

Proposition 5.3.4. *Under Assumption 5.2.1 we have*

$$\operatorname{acc}\left\{\tfrac{\nu_n}{n} : n \in \mathbb{N}\right\} = \operatorname{acc}\left\{\frac{|\mathit{supp}\,\psi_n|}{|\mathcal{G}|} : n \in \mathbb{N}\right\}.$$

The proof of Theorem 5.3.3 and Proposition 5.3.4 is based on the following principles, the proofs of which, in turn, are postponed to Subsection 5.3.1.

Lemma 5.3.5 (Weyl asymptotics)**.** *We have*

$$\lambda_n(\mathcal{G}) = \frac{\pi^2}{|\mathcal{G}|^2}n^2 + o(n^2) \qquad \textit{as } n \to \infty. \tag{5.11}$$

Lemma 5.3.6 (Relationship between ν_n and λ_n)**.** *Suppose in addition to Assumption 5.2.1 that $q_{\min} = 0$. Then, there exists $n_0 \in \mathbb{N}$ depending only on the metric graph $\mathcal{G}$ and the potential $0 \le q \in L^1(\mathcal{G})$ such that, for all $n \ge n_0$,*

$$|supp\, \psi_n| \cdot \frac{\lambda_n(\mathcal{G})^{1/2} - \|q\|_1}{\pi} - (2|E| - 1)|V| \le \nu_n \le |supp\, \psi_n| \cdot \frac{\lambda_n(\mathcal{G})^{1/2}}{\pi} + |V|. \tag{5.12}$$

In particular,

$$\nu_n = |supp\, \psi_n| \cdot \frac{\lambda_n(\mathcal{G})^{1/2}}{\pi} + O(1) \qquad \text{as } n \to \infty. \tag{5.13}$$

These two lemmata are logically independent of each other; in particular, in (5.12) we explicitly do not use the Weyl asymptotics to estimate λ_n. Lemma 5.3.5 in particular can be refined significantly for specific types of vertex conditions and potentials; for example, in the case of the Laplacian with standard vertex conditions and if $\mathcal{G}$ is not a cycle, then we may strengthen (5.11) to

$$\left(n - \frac{|N| + \beta}{2}\right)^2 \frac{\pi^2}{|\mathcal{G}|^2} \le \lambda_n(\mathcal{G}) \le \left(n - 2 + \beta + \frac{|N| + \beta}{2}\right)^2 \frac{\pi^2}{|\mathcal{G}|^2},$$

where $|N|$ is the number of degree one vertices and β is the first Betti number (number of independent cycles) of the graph, as follows from [BKKM17, Theorems 4.7 and 4.9]. More generally, if $q \in L^\infty(\mathcal{G})$, then we may obtain the two-sided estimate

$$(n - c_1)^2 \frac{\pi^2}{|\mathcal{G}|^2} \le \lambda_n(\mathcal{G}) \le (n + c_2)^2 \frac{\pi^2}{|\mathcal{G}|^2} \qquad \text{for all } n \in \mathbb{N}$$

for constants $c_1, c_2 > 0$ depending only on $\mathcal{G}$ and $\|q\|_\infty$; this is a consequence of Lemma 5.1.1 and a simple variational argument bounding q in terms of the constant potential $\|q\|_\infty$, and zero.

Let us now show how Lemmata 5.3.5 and 5.3.6 lead to the proofs of the main results. To prove Proposition 5.3.4, if we combine (5.13) and (5.11), then we obtain the asymptotic behavior

$$\nu_n = \frac{|\mathrm{supp}\, \psi_n|}{|\mathcal{G}|} n + o(n) \qquad \text{as } n \to \infty, \tag{5.14}$$

if $q \ge 0$. This in turn, immediately yields the result claimed in Proposition 5.3.4 for arbitrary lower bounded potentials, since the eigenvalue problem $Au = \lambda u$ is equivalent to the shifted eigenvalue problem $(A - q_{min})u = (\lambda - q_{\min})u$, where the potential $q - q_{\min} \in L^1(\mathcal{G})$ associated with the shifted Schrödinger operator $A - q_{min}$ is nonnegative.

The other ingredient in the proof of Theorem 5.3.3 is the following "weak" unique continuation principle, whose proof will also be given in Subsection 5.3.1; Theorem 5.3.3 is a direct consequence of (5.14) and (5.15).

Lemma 5.3.7 (Possible values of $|\mathrm{supp}\, \psi_n|$)**.** *Under Assumption 5.2.1, we have, for all $n \in \mathbb{N}$:*

(i) There exists some non-empty subset $E_0 = E_0(n) \subset E$ such that supp $\psi_n = \bigcup_{\mathsf{e} \in E_0} \mathsf{e}$; in

particular,

$$\Big\{|\mathit{supp}\,\psi_n| : n \in \mathbb{N}\Big\} \subset \left\{ \sum_{\mathsf{e}\in E_0} \ell_{\mathsf{e}} : E_0 \subset E \textit{ is a nonempty set of edges} \right\}. \tag{5.15}$$

(ii) If e *is some edge of* $\mathcal{G}$ *with* $\mathsf{e} \subset \mathit{supp}\,\psi_n$ *and* $\mathsf{v} \in V \setminus V_0$ *is a vertex incident to* e*, then* e *is a loop or there is a second edge* $\mathsf{f} \neq \mathsf{e}$ *incident to* v *with* $\mathsf{f} \subset \mathit{supp}\,\psi$*.*

Remark 5.3.8. Note that Lemma 5.3.7 gives additional information on the geometric structure of the supports of the eigenfunctions ψ_n. For instance part (ii) implies that – for sufficiently large n – supp ψ_n contains a cycle or a path that connects two vertices that are in V_0 or of degree one. In particular we find that, if n is sufficiently large and e is an edge of $\mathcal{G}$ with supp $\psi_n = \mathsf{e}$, then $|E| = 1$ or e is a loop.

As a consequence of the observations in Remark 5.3.8, part (i) of Lemma 5.3.7 and Proposition 5.3.4 we obtain the following

Corollary 5.3.9. *Under Assumption 5.2.1, if*

$$\frac{\ell_{\min}}{|\mathcal{G}|} = \liminf_{n\to\infty} \frac{\nu_n}{n}$$

holds, then $|E| = 1$ *or there is a loop in* $\mathcal{G}$ *of length* $\ell_{\min}$*.*

5.3.1 Proofs of the lemmata

Here we give the proofs of the three main auxiliary results, Lemmata 5.3.5, 5.3.6 and 5.3.7 which, combined, yield Theorem 5.3.3. We suppose throughout, without further comment, that Assumption 5.2.1 holds.

Proof of Lemma 5.3.5. This is an immediate consequence of Lemma 5.1.1, together with the fact that the eigenvalues of the operator associated with the restriction of the form $a_{q,\mathcal{B},w}$ to $H^1_0(\mathcal{G})$, that is, with Dirichlet boundary conditions everywhere, satisfy the usual Weyl asymptotics on any bounded interval and thus any finite union of disjoint intervals, see, e.g., [AM87, Lemma 2.1]. □

The second, Lemma 5.3.6, is in turn based on the principle that $\lambda_n(\mathcal{G})$ is always the first eigenvalue of any nodal domain of ψ_n, and as a consequence, that the maximal size of any nodal domain converges to zero as $n \to \infty$.

Lemma 5.3.10. *Given* $n \in \mathbb{N}$*, the eigenvalue* $\lambda_n(\mathcal{G})$*, and the associated eigenfunction* ψ_n*, with nodal domains* $\mathcal{G}_1, \dots, \mathcal{G}_{\nu_n}$*, for each* $j = 1, \dots, \nu_n$ *we have*

$$\lambda_n(\mathcal{G}) = \lambda_1(\mathcal{G}_j),$$

where the operator associated with the latter eigenvalue has Dirichlet conditions at all the boundary points of $\mathcal{G}_j$ corresponding to zeros of ψ_n (but the same vertex conditions as before at the interior vertices of $\mathcal{G}_j$, and the same potential q restricted to $\mathcal{G}_j$).

Proof. Suppose without loss of generality that $\psi_n \geq 0$ in $\mathcal{G}_j$, with strict inequality except at the Dirichlet vertices of $\mathcal{G}_j$, and set $\varphi_n := \psi_n \chi_{\mathcal{G}_j}$; in a slight abuse of notation, we will identify φ_n with its restriction to $\mathcal{G}_j$ in $L^2(\mathcal{G}_j)$. We observe that φ_n is an edgewise solution of the eigenvalue equation on the edges of $\mathcal{G}_j$ that satisfies Dirichlet conditions at the boundary points of $\mathcal{G}_j$ and the same vertex conditions as ψ_n at the interior vertices of $\mathcal{G}_j$; moreover, the corresponding eigenvalue, which we can read off the eigenvalue equation, is $\lambda_n(\mathcal{G})$.

That is, $\lambda_n(\mathcal{G})$ is an eigenvalue of $\mathcal{G}_j$, i.e., $\lambda_n(\mathcal{G}) = \lambda_k(\mathcal{G}_j)$ for some $k \geq 1$; moreover, its eigenfunction φ_n is, by construction, strictly positive in $\mathcal{G}_j$ except at boundary points of $\mathcal{G}_j$ and any interior Dirichlet vertices. By [Kur19, Theorem 3], it is possible to choose the first eigenfunction φ_1 of $\lambda_1(\mathcal{G}_j)$ to have this property. Hence the L^2-scalar product of φ_n and φ_1 is strictly positive. Orthogonality of eigenfunctions on $\mathcal{G}_j$ belonging to different eigenspaces implies that $\lambda_n(\mathcal{G}) = \lambda_1(\mathcal{G}_j)$. (In fact, we could even infer $\varphi_n = c\varphi_1$ for some $c > 0$, since the eigenspace corresponding to $\lambda_1(\mathcal{G}_j)$ has dimension 1, but we do not need this.) □

The other ingredient we need for the proof of Lemma 5.3.6 is an estimate on the first eigenvalue of any operator $A(q, \mathcal{B}, w, V_0)$ on any compact, connected graph (which in practice will be one of the nodal domains of ψ_n), which is given in Proposition 5.2.2 in §5.2.1. This proposition, when applied to the nodal domains $\mathcal{G}_j$ of ψ_n upon invoking Lemma 5.3.10, leads to the following estimate on the size of $\mathcal{G}_j$.

Lemma 5.3.11. *For all $n \in \mathbb{N}$, for all nodal domains $\mathcal{G}_j$, $j = 1, \dots, \nu_n$, we have*

$$|\mathcal{G}_j| \leq \frac{2\pi|E|}{\sqrt{\lambda_n(\mathcal{G}) + \|q\|_1^2} - \|q\|_1}. \tag{5.16}$$

In particular, if $\lambda_n(\mathcal{G})$ is sufficiently large; explicitly, if

$$\lambda_n(\mathcal{G}) > \left(\frac{2\pi|E|}{\ell_{\min}} + \|q\|_1\right)^2 - \|q\|_1^2,$$

then no nodal domain can contain more than one vertex of $\mathcal{G}$.

Proof. Fix a nodal domain $\mathcal{G}_j$; then $\mathcal{G}_j$ certainly cannot have more than $2|E|$ edges (note that it could contain both ends of a given edge in $\mathcal{G}$ without containing the whole edge). Now by Lemma 5.3.10, we have $\lambda_n(\mathcal{G}) = \lambda_1(\mathcal{G}_j)$; combining this with the estimate (5.4) applied to $\mathcal{G}_j$ yields

$$\lambda_n(\mathcal{G}) \leq \left(\frac{2\pi|E|}{|\mathcal{G}_j|} + \|q\|_1\right)^2 - \|q\|_1^2.$$

Rearranging yields (5.16). If $\lambda_n(\mathcal{G})$ is sufficiently large as stated, then $|\mathcal{G}_j| < \ell_{\min}$ for all j, meaning no nodal domain can contain an entire edge. □

Remark 5.3.12. The proof shows that if $\mathcal{G}_j$ is an interval, then, since we may take $|E(\mathcal{G}_j)| = 1$ in (5.4), (5.16) may be improved to

$$|\mathcal{G}_j| \le \frac{\pi}{\sqrt{\lambda_n(\mathcal{G}) + \|q\|_1^2} - \|q\|_1}. \tag{5.17}$$

Proof of Lemma 5.3.6. Firstly observe that by definition of the nodal domains, for any $n \in \mathbb{N}$, we have

$$|\operatorname{supp} \psi_n| = \sum_{j=1}^{\nu_n} |\mathcal{G}_j|.$$

Now note that $\lambda_n(\mathcal{G}) \to \infty$ (this follows from the compactness of the resolvent and the semi-boundedness of the form $a_{q,\mathcal{B},w}$, but can also be obtained as a consequence of Lemma 5.3.5). Hence, by Lemma 5.3.11 there exists some $n_0 \in \mathbb{N}$, which may be chosen to depend only on the metric graph $\mathcal{G}$ and q, such that the interior of each nodal domain $\mathcal{G}_j$ contains at most one vertex of $\mathcal{G}$, for all $n \ge n_0$. For such n, we suppose the nodal domains are ordered in such a way that, for some $m \le |V|$, $\mathcal{G}_1, \dots, \mathcal{G}_m$ each contain exactly one vertex in their respective interiors, while $\mathcal{G}_{m+1}, \dots, \mathcal{G}_{\nu_n}$ are all intervals; in particular, for all $j \ge m+1$, by Lemma 5.3.10, $\lambda_n(\mathcal{G}) = \lambda_1(\mathcal{G}_j)$. Now on the one hand, since $q \ge 0$, $\lambda_1(\mathcal{G}_j) \ge \pi^2/|\mathcal{G}_j|^2$, whence

$$|\mathcal{G}_j| \ge \frac{\pi}{\lambda_n(\mathcal{G})^{1/2}}.$$

On the other hand, using (5.17), for such nodal domains we also have, supposing without loss of generality that $\lambda_{n_0} > \|q\|_1^2$,

$$|\mathcal{G}_j| \le \frac{\pi}{\sqrt{\lambda_n(\mathcal{G}) + \|q\|_1^2} - \|q\|_1} \le \frac{\pi}{\lambda_n(\mathcal{G})^{1/2} - \|q\|_1}.$$

Summing over j, we obtain the two-sided estimate

$$(\nu_n - m) \cdot \frac{\pi}{\lambda_n(\mathcal{G})^{1/2}} + \sum_{j=1}^{m} |\mathcal{G}_j| \le |\operatorname{supp} \psi_n| \le (\nu_n - m) \cdot \frac{\pi}{\lambda_n(\mathcal{G})^{1/2} - \|q\|_1} + \sum_{j=1}^{m} |\mathcal{G}_j|. \tag{5.18}$$

Invoking (5.16), we may estimate the size of the first m nodal domains by

$$0 \le \sum_{j=1}^{m} |\mathcal{G}_j| \le \frac{2\pi |E| m}{\lambda_n(\mathcal{G})^{1/2} - \|q\|_1}.$$

Using this in (5.18) and rearranging yields

$$|\operatorname{supp} \psi_n| \cdot \frac{\lambda_n(\mathcal{G})^{1/2} - \|q\|_1}{\pi} - (2|E| - 1)m \le \nu_n \le |\operatorname{supp} \psi_n| \cdot \frac{\lambda_n(\mathcal{G})^{1/2}}{\pi} + m. \tag{5.19}$$

Observing that (5.19) is monotonic in m and using $m \le |V|$ yields (5.12). □

Let us finally turn to Lemma 5.3.7. The main tool in its proof is a result in Sturm–Liouville theory that is likely to be already known; we provide a proof, since we could not find an appropriate reference in the literature.

Lemma 5.3.13. *If $I \subset \mathbb{R}$ is an open interval containing 0, $q \in L^1(I)$, and $u \in W^{2,1}_{loc}(I) \hookrightarrow C^1(I)$ is a distributional solution of $-u'' + qu = 0$ such that $u(0) = u'(0) = 0$, then $u = 0$ in I.*

Proof. For any $x \in [0, \infty) \cap I$, we have

$$|u'(x)| = \left| \int_0^x u''(s)\,\mathrm{d}s \right| \leq \int_0^x |q(s)u(s)|\,\mathrm{d}s$$

and

$$|u(x)| = \left| \int_0^x u'(x)\,\mathrm{d}s \right| \leq \int_0^x |u'(x)|\,\mathrm{d}s.$$

Summing the two inequalities yields

$$|u(x)| + |u'(x)| \leq \int_0^x |u'(s)| + |q(s)u(s)|\,\mathrm{d}s \leq \int_0^x (1 + |q(s)|)(|u(s)| + |u'(s)|)\,\mathrm{d}s;$$

it now follows from Grönwall's Lemma that $|u(x)| + |u'(x)| = 0$; we thus conclude that $u(x) = 0$ for all $x \in [0, \infty) \cap I$ and hence all $x \in I$. □

Proof of Lemma 5.3.7. For part (i), it suffices to prove the following unique continuation statement: if any eigenfunction ψ_n has a zero at some point x_0 in the interior of an edge, then either $\psi_n \equiv 0$ in a neighborhood of x_0 or $\psi_n'(x_0) \neq 0$. This, in turn, follows from Lemma 5.3.13, applied to ψ_n with a suitably adjusted q.

We prove part (ii) by contradiction using similar arguments: suppose that e is not a loop and that ψ_n vanishes on all edges incident to $\mathsf{v} \in \mathcal{V} \setminus \mathcal{V}^D$ with $\mathsf{f} \neq \mathsf{e}$. The vertex conditions associated with the operator $A(q, \mathcal{B}, w, V_0)$ yield $\psi_{\mathsf{e},n}(\mathsf{v}) = 0$ and $\psi'_{\mathsf{e},n}(\mathsf{v}) = 0$ where $\psi_{\mathsf{e},n}$ denotes the restriction of ψ_n to e. But then, as in the proof of part (i), Grönwall's Lemma yields that $\psi_{n,\mathsf{e}}$ vanishes in a neighborhood about v if $\lambda_n - q_{\min} \geq 0$ and therefore e is not a subset of $\operatorname{supp} \psi_n$. □

5.4 A stronger Pleijel's Theorem for the Laplacian with standard vertex conditions

We consider the free Laplacian with standard conditions at all vertices, i.e., throughout this section, we suppose, in addition to Assumption 5.2.1, that $q \equiv 0$, $\mathcal{B} = 0$, $\mathsf{w} \equiv 1$, $V_0 = \emptyset$. In this case we can say somewhat more.

The principal result of [BL17b] (see Theorem 3.6 and Remark 3.7 there) states that, given a fixed graph topology without loops, the set of edge length vectors for which all eigenvalues of the corresponding graph are simple and all eigenfunctions do not vanish in the vertices, is of the second Baire category (i.e., it is a countable intersection of open dense sets). As a consequence of Proposition 5.3.4 above we obtain $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$ in this case; however, this could also be concluded using the main result in [GSW04] which states that $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$ holds in the generic case where no eigenfunctions vanish at any vertices of the loop-free graph. Nevertheless, for future reference, we state our observation in the following

Theorem 5.4.1 ([BL17b; GSW04]). *If $\mathcal{G}$ does not contain any loops, then the set of edge length vectors in $\mathbb{R}_+^{|E|}$ for which, for the corresponding graph with the given topology and these edge lengths, all eigenvalues are simple and $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$, is of the second Baire category (i.e., is a countable intersection of open dense sets).*

Put differently, in the case of standard vertex conditions and no potential, "almost all" graphs (in the usual sense of holding generically and being loop-free) have all eigenvalues simple, and satisfy $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$.

Here we wish to say more about the "non-generic" cases. The following theorem states that for graphs with pairwise commensurable edge lengths, at least $\limsup_{n\to\infty} \frac{\nu}{n} = 1$ holds and thus the upper bound in Theorem 5.3.3 is sharp.

Theorem 5.4.2. *If the edge lengths of $\mathcal{G}$ are pairwise commensurable, then for every choice of orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of the Laplacian with standard vertex conditions we have $\limsup_{n\to\infty} \frac{\nu_n}{n} = 1$.*

Actually, we expect that on *any* graph $\mathcal{G}$ there exists a choice of (standard Laplacian) eigenfunctions for which $\limsup_{n\to\infty} \frac{\nu_n}{n} = 1$. This would be an immediate consequence of the following conjecture together with Proposition 5.3.4.

Conjecture 5.4.3. *Let, as usual, $\mathcal{G}$ be a compact, connected metric graph and let $(\psi_n)_{n\in\mathbb{N}}$ be an orthonormal basis of $L^2(\mathcal{G})$ consisting of eigenfunction of the Laplacian with standard vertex conditions on $\mathcal{G}$. Then there exists a subsequence $(\psi_{n_k})_{k\in\mathbb{N}}$ such that no eigenfunction ψ_{n_k} vanishes identically on any edge of $\mathcal{G}$.*

Remark 5.4.4. It follows from Theorem 5.4.1 that the conjecture is true generically; it is also true in the case where all edge lengths are pairwise commensurable, by Theorem 5.4.2. A counterexample would hence require a graph to have at least two rationally independent edge lengths. Additionally, topological constraints exist, too: it follows from [Ser20, Lemma 2.7 and Corollary 2.8] that so-called *lasso trees* (i.e., graphs that can be constructed by attaching at most one loop to any leaf of a tree) cannot be counterexamples, either.

Before giving the proof of Theorem 5.4.2, we will give a simple example which shows that the sequence $\frac{\nu_n}{n}$, and even its set of points of accumulation, can depend on the choice of the basis of eigenfunctions ψ_n.

Example 5.4.5. Consider again the equilateral 4-star from Example 5.3.2. Then there are two families of eigenfunctions (and corresponding eigenvalues):

- Eigenfunctions which are invariant under permutation of the edges; up to scalar multiples these are of the form $\varphi_k(x) = \cos(\pi k x)$, $k \in \mathbb{N}$, on each edge $\mathsf{e}_j \simeq [0,1]$, with corresponding eigenvalues $\pi^2 k^2$, each of which has multiplicity one.
- Eigenfunctions which vanish at the central vertex: the corresponding eigenvalues, $\pi^2(k-\frac{1}{2})^2$, $k \in \mathbb{N}$, all have multiplicity three. Any function φ in the eigenspace has the form $c_j \sin(\pi(k-\frac{1}{2})x)$ on each edge e_j, where the coefficients $c_j = c_j(\varphi) \in \mathbb{R}$ are chosen in such a way that the Kirchhoff condition is satisfied at the vertex.

We present two different choices for the c_j, which give rise to two different families of orthogonal bases with different nodal counts. To keep the presentation more compact and easier to read, we present these choices in table form:

	c_1	c_2	c_3	c_4
φ_1	1	-1	0	0
φ_2	0	0	1	-1
φ_3	1	1	-1	-1

	c_1	c_2	c_3	c_4
φ_1	1	-1	0	0
φ_2	1	1	-2	0
φ_3	1	1	1	-3

Thus, for example, in the second case, for each $k \in \mathbb{N}$ there is an eigenfunction $\varphi_3 = \varphi_3(k)$ which takes the form $\sin(2\pi(k-1)x)$ on each of e_1, e_2 and e_3, and $-3\sin(2\pi(k-1)x)$ on e_4. The orthogonality of $\varphi_1, \varphi_2, \varphi_3$ within each family is easy to check, as we simply require that the respective row vectors have inner product zero with each other; while the Kirchhoff condition is satisfied as long as the sum of the entries in each vector is zero. (The eigenfunctions will not have norm one, but this is obviously just a question of rescaling.) Now in the first family, there are two eigenfunctions each supported on two different edges and one supported on all four; in the second family, the second eigenfunction is supported on three edges rather than two. It follows from Proposition 5.3.4 (also taking into account the nature of the eigenfunctions not vanishing on the central vertex) that in the first case the set of points of accumulation of the sequence $\frac{\nu_n}{n}$ is $\{\frac{1}{2}, 1\}$ and in the second case it is $\{\frac{1}{2}, \frac{3}{4}, 1\}$.

Proof of Theorem 5.4.2. By inserting dummy vertices as necessary, we may assume that the graph is in fact equilateral; after rescaling if necessary, we may also assume without loss of generality that each edge has length 1. The following proof is essentially based on the possibility of considering all eigenfunctions as linear combinations of full frequency eigenfunctions on each edge, more precisely for each $k \in \mathbb{N}$ it is known that $4\pi^2 k^2$ is an eigenvalue of multiplicity $\beta + 1$, where β is the first Betti number of $\mathcal{G}$; we refer to §6.4 and the references therein for details. A basis of the corresponding eigenspace is obtained by choosing the following functions:

- the function $\varphi_k \in H^1(\mathcal{G})$ given by $\varphi_k(x) = \cos(2\pi k x)$ on each edge $\mathsf{e} \simeq [0,1]$;

- and, given a specific choice of independent cycles $\mathcal{C}_1, \dots, \mathcal{C}_\beta$ with associated edge sets $E_1, \dots, E_\beta$ (i.e. $\mathcal{C}_j = \bigcup_{\mathsf{e} \in E_j} \mathsf{e}$), the functions $\varphi_{k,j} \in H^1(\mathcal{G})$ given by $\varphi_{k,j}(x) = \sin(2\pi k x)$ on each edge $\mathsf{e} \simeq [0,1]$ in E_j and $\varphi_{k,j} = 0$ on each edge $\mathsf{e} \in E \setminus E_j$.

We point out that these linearly independent eigenfunctions are not necessarily orthogonal, but that will not be needed for the following argument. We also observe that, while the eigenfunctions $\varphi_{k,1}, \dots, \varphi_{k,\beta}$ vanish at all the vertices of $\mathcal{G}$, the eigenfunction φ_k is non-zero at all vertices.

Now let $\psi_{n_0}, \dots, \psi_{n_0+\beta}$ denote the eigenfunctions appearing in the given orthonormal basis associated with the eigenvalue $4\pi^2 k^2$ for some $n_0 = n_0(k)$. Then, we may write each of these eigenfunctions as a linear combination of $\varphi_k, \varphi_{k,1}, \dots, \varphi_{k,\beta}$ and, since $\psi_{n_0}, \dots, \psi_{n_0+\beta}$ are linearly independent, the coefficient corresponding to φ_k appearing in these linear combinations has to be non-zero for at least one ψ_{n_0+l}, $l = l(k) \in \{0, 1, \dots, \beta\}$. By our previous observations on the vanishing and non-vanishing behavior of $\varphi_k, \varphi_{k,1}, \dots, \varphi_{k,\beta}$ at the vertices of $\mathcal{G}$, we conclude that ψ_{n_0+l} is non-zero in the vertices of $\mathcal{G}$. Putting $n_k = n_0(k) + l(k)$ we obtain a subsequence $(\psi_{n_k})_{k \in \mathbb{N}}$ with $\operatorname{supp} \psi_{n_k} = \mathcal{G}$ for all k. That $\limsup_{n\to\infty} \frac{\nu_n}{n} = 1$ now follows immediately from Theorem 5.3.3 and Proposition 5.3.4. $\square$

In the proof of Theorem 5.4.2, given a cycle with pairwise commensurable edge lengths, we constructed a sequence of eigenfunctions whose support was said cycle. Using Proposition 5.3.4 we can obtain the following result as a by-product:

Proposition 5.4.6. *If $\mathcal{G}$ contains a cycle $\mathcal{C}$ with corresponding edge set E_0, so that the lengths of the edges in E_0 are pairwise commensurable, then the orthonormal basis of eigenfunctions of $\mathcal{G}$ may be chosen so that $\frac{\sum_{\mathsf{e} \in E_0} \ell_\mathsf{e}}{|\mathcal{G}|}$ is a point of accumulation of $\frac{\nu_n}{n}$. In particular, if $\mathcal{G}$ contains a loop of length ℓ, then ℓ may be chosen so that $\frac{\ell}{|\mathcal{G}|}$ is a point of accumulation of $\frac{\nu_n}{n}$. In particular, the lower estimate of* (5.10) *is sharp whenever $\ell_{\min}$ is realized by a loop of $\mathcal{G}$.*

Proposition 5.4.6 has two obvious consequences which are nevertheless worth stating explicitly. First given any $\varepsilon > 0$ there exists a graph $\mathcal{G}$ such that for this graph $\liminf_{n\to\infty} \frac{\nu_n}{n} < \varepsilon$. Secondly, if $\mathcal{G}$ is neither a tree nor a itself a cycle and has pairwise commensurable edge lengths, then there exists a orthonormal basis so that $\liminf_{n\to\infty} \frac{\nu_n}{n} < 1$ holds. This is not necessarily true if the graph is a tree: indeed, the following example shows that there are trees with pairwise commensurable edge lengths where any eigenfunction of the Laplacian with standard conditions is supported on the whole tree, which in turn yields, by Proposition 5.3.4, that $\lim_{n\to\infty} \frac{\nu_n}{n} = 1$ holds for any orthonormal basis of eigenfunctions.

Example 5.4.7. Consider the 3-star $\mathcal{G}$ consisting of three edges $\mathsf{e}_1, \mathsf{e}_2, \mathsf{e}_3$ of edge lengths ℓ_1, ℓ_2, ℓ_3 respectively. An eigenfunction $\varphi = (\varphi_1, \varphi_2, \varphi_3)$ corresponding to some eigenvalue $\lambda > 0$ is of the form $\varphi_j(x) = c_j \cos(\sqrt{\lambda} x)$ on the edge $\mathsf{e}_j \simeq [0, \ell_j]$ where ℓ_j corresponds to the centre vertex of the star. If φ vanished on some edge e_i, we would obtain $c_i = 0$ and $c_j \neq 0$ for $j \neq i$. Then continuity in the centre vertex yields $0 = \varphi_j(\ell_j)$ for $j \neq i$ and, thus $0 = \cos(\ell_j \sqrt{\lambda})$. Therefore there is some $m_j \in \mathbb{N}$ such that $\ell_j\sqrt{\lambda} = \pi(m_j - \frac{1}{2})$. This yields

$$\frac{\ell_k}{\ell_j}(2m_k - 1) = 2m_j - 1 \tag{5.20}$$

for $k, j \neq i$. Now we choose $\ell_1 = 1$, $\ell_2 = 2$ and $\ell_3 = 4$. Suppose without loss of generality that $\ell_k > \ell_j$ in (5.20). Then, with our choice of the edge lengths, (5.20) clearly leads to a contradiction, since the left-hand side is an even integer, whereas the right-hand side is odd. Therefore all eigenfunctions on the 3-star with edge lengths 1, 2 and 4 must be supported on the whole graph.

Remark 5.4.8. Theorem 5.4.1 and Proposition 5.4.6 also hold if any mix of delta couplings and Dirichlet conditions is imposed at some vertices, although for the former we still need a certain additional genericity assumption (coming from [BL17b, Theorem 3.6]) on the delta couplings. In the former case the proof is essentially identical; in the latter case we may directly construct eigenfunctions supported on the cycle out of suitably adjusted sine curves, which in particular vanish at all vertices and thus satisfy all possible delta couplings there. We expect Proposition 5.4.6 to hold for many tree graphs as well, although here the situation is more complicated, as Example 5.4.7 shows.

We finish this section with a discussion of the case of equality in (5.9). Recall that a metric graph $\mathcal{G}$ is called a *flower graph* if all its edges are loops. If, in addition, $\mathcal{G}$ has only two edges, then we call it a *figure eight graph*.

Proposition 5.4.9. *In addition to Assumption 5.2.1, suppose that $q \equiv 0$, $\mathcal{B} = 0$, $\mathsf{w} \equiv 1$, $V_0 = \emptyset$. Then there exists an orthonormal basis $(\psi_n)_{n\in\mathbb{N}}$ of eigenfunctions so that for each non-empty subset $E_0 \subset E$ there is a subsequence $(\psi_{n_k})_{k\in\mathbb{N}}$ with*

$$\mathit{supp}\,\psi_{n_k} = \bigcup_{\mathsf{e}\in E_0} \mathsf{e}, \qquad k \in \mathbb{N}$$

if and only if one the following cases occurs:

(i) $\mathcal{G}$ is an interval or a cycle;

(ii) $\mathcal{G}$ is a figure eight graph;

(iii) $\mathcal{G}$ is a flower graph with pairwise commensurable edge lengths.

In particular, for any of these graphs, for this choice of an orthonormal basis, equality holds in (5.9).

Before we give a proof of Proposition 5.4.9 we point out there may be other graphs for which there is equality (5.9), as the following example will show. In particular it will demonstrate that a full characterization of equality in (5.9) would have to incorporate both the local and global combinatorial and metric structure of the graph, and would therefore be too technically complicated to be treated here.

Example 5.4.10. Consider the $[3,2]$-pumpkin chain $\mathcal{G}$ that consists of two vertices v_1 and v_2, three parallel edges $\mathsf{e}_1, \mathsf{e}_2, \mathsf{e}_3$ of equal length 1 each connecting the two vertices, and one pendant loop e_4 of length 1 attached to the vertex v_2; see Figure 5.1.

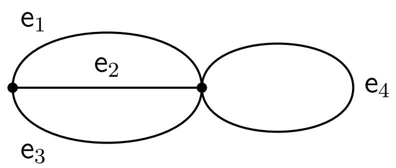


Figure 5.1: Pumpkin chain. The $[3,2]$-pumpkin chain $\mathcal{G}$.

In the spirit of [BKKM19, Lemma 5.4] we choose an orthonormal basis of eigenfunctions consisting of (i) *longitudinal functions*, functions that are radially symmetric with respect to the vertex v_1, and (ii) *transversal functions*, functions whose support is contained in one of the pumpkins $\mathsf{e}_1 \cup \mathsf{e}_2 \cup \mathsf{e}_3$ or e_4. The infinite orthonormal subsequence of longitudinal eigenfunctions corresponds to a 1-dimensional Sturm–Liouville problem; these eigenfunctions are therefore supported on the whole graph (see [BKKM19, §5.2] for details). For $k \in \mathbb{N}$ the transversal eigenfunctions supported on e_4 are given by $\varphi(x) = \sin(2\pi kx)$ for $x \in \mathsf{e}_4 \simeq [0,1]$. The transversal eigenfunctions φ with support in $\mathsf{e}_1 \cup \mathsf{e}_2 \cup \mathsf{e}_3$ are given by $\varphi(x) = c_j \sin(\pi kx)$ for $x \in \mathsf{e}_j \simeq [0,1]$, $j = 1,2,3$ and constants $c_j \in \mathbb{R}$ with $c_1 + c_2 + c_3 = 0$. By choosing $(c_1, c_2, c_3) = (1,1,-2)$ and $(c_1, c_2, c_3) = (1,-1,0)$ respectively we obtain – after normalisation – an orthonormal basis of eigenfunctions, and by Proposition 5.3.4 the set of points of accumulation of the sequence $\frac{\nu_n}{n}$ is $\{\frac{1}{4}, \frac{1}{2}, \frac{3}{4}, 1\}$, which coincides with set of values $\frac{\sum_{\mathsf{e} \in E_0} \ell_{\mathsf{e}}}{|\mathcal{G}|}$ for nonempty subsets $E_0 \subset E$. Note, however, that there is no possible choice of eigenfunctions supported on, say, $\mathsf{e}_1 \cup \mathsf{e}_4$; thus there is no contradiction to Proposition 5.4.9.

Proof of Proposition 5.4.9. Clearly the statement is true if $\mathcal{G}$ has only one edge, so we may assume that $\mathcal{G}$ has at least two edges.

Suppose first that there exists an orthonormal basis of eigenfunctions as stated in Proposition 5.4.9. Then, in particular, for each edge of $\mathcal{G}$ there is a sequence of eigenfunctions supported exactly on that edge. From Lemma 5.3.7 and the following Remark 5.3.8 we infer that each edge is a loop and therefore $\mathcal{G}$ is a flower graph. If $\mathcal{G}$ has two edges, then we are clearly in case (ii).

It remains to show that the edge lengths of $\mathcal{G}$ are pairwise commensurable if $\mathcal{G}$ has at least three edges. Let $\mathsf{e}_1 \neq \mathsf{e}_2$ be any two edges of $\mathcal{G}$. Then, by assumption, there is an eigenfunction φ with associated eigenvalue $\lambda > 0$ for which $\operatorname{supp}\varphi = \mathsf{e}_1 \cup \mathsf{e}_2$. Since φ vanishes on all edges different from e_1 and e_2 and is continuous in the centre vertex v of the flower, we obtain $\varphi(\mathsf{v}) = 0$. Therefore there exist $a_1, a_2 \in \mathbb{R} \setminus \{0\}$ such that $\varphi(x) = a_j \sin(\sqrt{\lambda}x)$ for $j = 1,2$ and $x \in \mathsf{e}_j \simeq [0, \ell_{\mathsf{e}_j}]$. Then $\varphi(\mathsf{v}) = 0$ yields $\sin(\sqrt{\lambda}\ell_{\mathsf{e}_j}) = 0$, and thus, for $j = 1,2$, there exists some $k_j \in \mathbb{N}$ such that $\sqrt{\lambda}\ell_{m_j} = \pi k_j$. We obtain $\frac{\ell_{\mathsf{e}_1}}{\ell_{\mathsf{e}_2}} = \frac{k_1}{k_2} \in \mathbb{Q}$; hence ℓ_{e_1} and ℓ_{e_2} are commensurable.

Finally, we show that for each of the graphs in (i), (ii) and (iii) there does indeed exist an orthonormal basis of eigenfunctions with the claimed properties. Such a basis obviously exists for an interval or cycle. For a figure eight graph such a basis can be constructed following arguments similar to the ones used in Example 5.4.10. So suppose $\mathcal{G}$ is a flower graph with pairwise commensurable edge lengths. Then there exist $a > 0$ and $m_{\mathsf{e}} \in \mathbb{N}$ with $\ell_{\mathsf{e}} = am_{\mathsf{e}}$ for all $\mathsf{e} \in E$. It is sufficient to show that for each subset $E_0 \subset E$ there is an infinite sequence of eigenfunctions associated with pairwise different eigenvalues that are supported on $\bigcup_{\mathsf{e}\in E_0} \mathsf{e}$. Indeed such a sequence exists: for $k \in \mathbb{N}$ there is an eigenfunction φ_k associated with the eigenvalue $\frac{4\pi^2 k^2}{a^2}$ given by $\varphi_k(x) = \sin(\frac{2\pi k}{a}x)$ for $x \in \mathsf{e} \simeq [0, \ell_{\mathsf{e}}]$ on $\mathsf{e} \in E_0$ and $\varphi_k = 0$ on $\mathsf{e} \in E \setminus E_0$. $\square$

5.5 Pleijel's theorem for the p-Laplacian

In this last section we are going to turn to a different class of operators. For a compact and connected metric graph $\mathcal{G}$ and $p \in (1, \infty)$ we let $W^{1,p}(\mathcal{G})$ denote the space of edgewise $W^{1,p}$-functions that are continuous across the vertices. The p-Laplacian on metric graphs can be generally introduced by considering the Fréchet differentiable energy functional

$$\mathfrak{E}_p : u \mapsto \int_{\mathcal{G}} |u'|^p \, \mathrm{d}x, \qquad u \in D(\mathfrak{E}_p) := W^{1,p}(\mathcal{G}), \tag{5.21}$$

and taking its Fréchet derivative in the real Hilbert space $L^2(\mathcal{G})$; this returns standard vertex conditions, i.e., continuity across the vertices along with a nonlinear analogue of Kirchhoff's condition. Unlike in the linear case of $p = 2$, different notions of eigenvalues for the p-Laplacian may *a priori* coexist, see §5.2.2, with *Carathéodory* eigenvalues being more general than *variational* ones. Given a general compact metric graph, it seems to be unknown how large the the set of Carathéodory eigenvalues of this operator is, but its subset that is most relevant for our purposes – the set of variational eigenvalues – is certainly countably infinite; such variational eigenvalues can be characterized by the Ljusternik–Schnirelmann principle, a nonlinear counterpart of the linear min-max principle.

Here we will denote by $(\lambda_{n,p}(\mathcal{G}))_{n\in\mathbb{N}}$ the sequence of variational eigenvalues, along with a sequence of associated (Carathéodory) eigenfunctions $(\psi_{n,p})_{n\in\mathbb{N}}$, which we fix throughout; each eigenfunction has $\nu_{n,p}$ corresponding nodal domains $\mathcal{G}_1, \ldots, \mathcal{G}_{\nu_{n,p}}$.

Actually, in view of the nonlinear versions of the Beurling–Dény conditions in [CG03], as in (5.2), different vertex conditions inducing (nonlinear) positive semigroups can be obtained upon considering the above energy on spaces of the form $W^{1,p}_w(\mathcal{G})$ and/or adding boundary terms; we expect our results to continue to hold for these. However, owing to a lack of background theory available for such nonlinear operators on metric graphs, we will not pursue such generalisations here.

In this section we will always impose the following

Assumption 5.5.1. *$\mathcal{G}$ is a compact, connected metric graph with underlying combinatorial graph $G = (V, E)$ and edge lengths ℓ_{e}, $\mathsf{e} \in E$; we set $\ell_{\min} := \min_{\mathsf{e}\in E} \ell_{\mathsf{e}}$. We also fix $p \in (1, \infty)$ and let $q = \frac{p}{p-1}$ be its Hölder conjugate.*

Our third main result of the chapter, a version of Pleijel's theorem for the p-Laplacian with standard vertex conditions, is a direct analogue of Theorem 5.3.3.

Theorem 5.5.2. *Under Assumption 5.5.1, and with the notation on the nodal count introduced above, we have*

$$\operatorname{acc}\left\{\tfrac{\nu_{n,p}}{n} : n \in \mathbb{N}\right\} \subset \left\{\frac{\sum_{\mathsf{e}\in E_0} \ell_{\mathsf{e}}}{|\mathcal{G}|} : E \supset E_0 \text{ is a nonempty set of edges}\right\}. \tag{5.22}$$

In particular, $\operatorname{acc}\left\{\frac{\nu_{n,p}}{n} : n \in \mathbb{N}\right\}$ *is a finite set, and*

$$0 < \frac{\ell_{\min}}{|\mathcal{G}|} \le \liminf_{n\to\infty} \frac{\nu_{n,p}}{n} \le \limsup_{n\to\infty} \frac{\nu_{n,p}}{n} \le 1,$$

where $\ell_{\min} := \min\{\ell_{\mathsf{e}} : \mathsf{e} \in E\}$.

We also observe that Proposition 5.3.4 holds verbatim with $\nu_{n,p}$ and $\psi_{n,p}$ in place of ν_n and ψ_n, respectively. The proof of Theorem 5.5.2 (and Proposition 5.3.4 in this case) follows exactly the same lines as above.

In this case, we give a short proof of the Weyl asymptotics for $\lambda_{n,p}(\mathcal{G})$ in the appendix (see Theorem 5.2.5), as it does not previously seem to have been established for the p-Laplacian on metric graphs. We next state p-versions of unique continuation (cf. Lemma 5.3.7), the fact that $\lambda_{n,p}$ is the first Dirichlet eigenvalue restricted to each nodal domain of $\psi_{n,j}$ (cf. Lemma 5.3.10) and a basic upper bound on the first Dirichlet eigenvalue (cf. Proposition 5.2.2), respectively.

The following lemma on unique continuation is actually valid for any vertex conditions enforced in the (real) Sobolev space $W^{1,p}(\mathcal{G})$, the domain of $\mathfrak{E}_p$, since they necessarily result in real eigenvalues and eigenfunctions.

Lemma 5.5.3 (Possible values of $|\operatorname{supp}\psi_{n,p}|$)**.** *Under Assumption 5.5.1,*

$$\left\{|\mathit{supp}\,\psi_{n,p}| : n \in \mathbb{N}\right\} \subset \left\{\sum_{\mathsf{e}\in E_0} \ell_{\mathsf{e}} : E \supset E_0 \text{ is a nonempty set of edges}\right\}.$$

Proof. This follows immediately from the assertion that if $\psi_{n,p}(x) = 0$ for some x in the interior of an edge e, then either $\psi_{n,p}$ changes sign in any open neighborhood of x, or $\psi_{n,p}$ vanishes identically on that edge. Suppose that $\psi_{n,p}(x) = 0$ at some interior point $x \in \mathsf{e}$, and that $\psi_{n,p}$

does *not* change sign at x. Then by the smoothness properties of $\psi_{n,p}$ stated in Lemma 5.2.3, we also have $\psi_{n,p}'(x) = 0$. That is, $\psi_{n,p}$ is a solution of

$$\begin{aligned} u' &= |v|^{\frac{1}{p-1}} \operatorname{sgn} v \\ v' &= -\lambda |u|^{p-1} \operatorname{sgn} u \end{aligned} \qquad \text{in a neighborhood of } x$$

with boundary conditions

$$u(x) = v(x) = 0.$$

By [LE11, Theorem 3.1], this equation has exactly one smooth solution, which in this case is clearly the zero function. Hence $\psi_{n,p}$ vanishes identically in a neighborhood of x and so, extending the argument, on the whole metric edge $\mathsf{e} \simeq (0, \ell_{\mathsf{e}})$. □

Lemma 5.5.4. *Under Assumption 5.5.1, for all $n \in \mathbb{N}$*

$$\lambda_{n,p}(\mathcal{G}) = \lambda_1(\mathcal{G}_j),$$

where the latter is the smallest variational eigenvalue of the p-Laplacian on $\mathcal{G}_j$ with Dirichlet conditions at all the boundary points of $\mathcal{G}_j$ corresponding to zeros of $\psi_{n,p}$ and standard conditions at all other vertices of $\mathcal{G}_j$.

Proof. In analogy with (5.3), denote by $W_0^{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)$ the domain of the functional associated with the eigenvalue problem on $\mathcal{G}_j$ as described in the assertion; then by choice of $\mathcal{G}_j$, $\psi_{n,p}|_{\mathcal{G}_j} \in W_0^{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)$. As usual, in a slight abuse of notation we will identify $W_0^{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)$ with a closed subspace of $W^{1,p}(\mathcal{G})$ and in particular simply write $\psi_{n,p} \in W_0^{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)$. We start by observing that $\psi_{n,p}$ is clearly an eigenfunction on $\mathcal{G}_j$, for the eigenvalue $\lambda_{n,p}(\mathcal{G})$, as follows from the fact that

$$\int_{\mathcal{G}} |\psi_{n,p}'(x)|^{p-2} \psi_{n,p}'(x) \varphi'(x) \, \mathrm{d}x = \lambda_{n,p}(\mathcal{G}) \int_{\mathcal{G}} |\psi_{n,p}(x)|^{p-2} \psi_{n,p}(x) \varphi(x) \, \mathrm{d}x$$

for all $\varphi \in W^{1,p}(\mathcal{G})$ and hence, in particular, for all $\varphi \in W_0^{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)$. Moreover, $\psi_{n,p}$ is either strictly positive or strictly negative in (the connected set) $\mathcal{G}_j \setminus \partial\mathcal{G}_j$, as is an immediate consequence of the definition of nodal domains. The proof of [KL06, Theorem 1.1] may now be repeated verbatim to show that $\lambda_{n,p}(\mathcal{G})$ is in fact the first eigenvalue of the p-Laplacian on $\mathcal{G}_j$ with the desired vertex conditions. □

The following upper bound was proved in [DR16, Theorem 3.8]. Again, this bound extends to the lowest variational eigenvalue of all realizations of the p-Laplacian induced by the functional $\mathfrak{E}_p$ defined on a superset of $W_0^{1,p}(\mathcal{G})$.

Lemma 5.5.5. *Under Assumption 5.5.1, let $\mathcal{V}^D$ be a (finite) non-empty set of points of $\mathcal{G}$, such that $\mathcal{G} \setminus \mathcal{V}^D$ is connected, and, for $p \in (1, \infty)$, let $\lambda_{1,p}(\mathcal{G}; V_0)$ be the first eigenvalue of the*

p-Laplacian with Dirichlet conditions at $\mathcal{V}^D$ and standard conditions at all other vertices. Then

$$\lambda_{1,p}(\mathcal{G}, \mathcal{V}^D) \leq \frac{p}{q}\left(\frac{\pi_p|E|}{|\mathcal{G}|}\right)^p.$$

Here, as usual, π_p is the constant defined via $\pi_p = \frac{2\pi}{p\sin(\frac{\pi}{p})}$.
The final auxiliary result we need is an analogue of Lemma 5.3.11, an estimate from above on the size of the nodal domains (equivalently, a lower bound on $\lambda_{n,p}$), which is itself a direct consequence of the preceding two lemmata. This establishes in particular (together with Lemma 5.5.3) that the number of nodal domains does in fact diverge to infinity as $n \to \infty$.

Lemma 5.5.6. *Fix $n \in \mathbb{N}$ and let $\mathcal{G}_1, \ldots, \mathcal{G}_{\nu_{n,p}}$ be the nodal domains of $\psi_{n,p}$. Then for all $j = 1, \ldots, \nu_{n,p}$ we have*

$$|\mathcal{G}_j| \leq \frac{2\pi_p|E|p^{1/p}}{(q\lambda_{n,p}(\mathcal{G}))^{1/p}}. \tag{5.23}$$

In particular, if $n \in \mathbb{N}$ is large enough, specifically, if $\lambda_{n,p}(\mathcal{G}) > \frac{p}{q}\left(\frac{2\pi_p|E|}{|\mathcal{G}_j|}\right)^p$, then no nodal domain can contain more than one vertex.

Proof. Fix a nodal domain $\mathcal{G}_j$, then since $\mathcal{G}_j$ cannot have more than $2|E|$ edges, by Lemma 5.5.4 and Lemma 5.5.5, the latter applied to $\mathcal{G}_j$, we have

$$\lambda_{n,p}(\mathcal{G}) = \lambda_{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j)[= \lambda_{1,p}^D(\mathcal{G}_j)] \leq \frac{p}{q}\left(\frac{\pi_p|E|}{|\mathcal{G}|}\right)^p.$$

Rearranging yields (5.23). The other assertion is clear. □

We can now formulate a version of the central Lemma 5.3.6 for the p-Laplacian.

Lemma 5.5.7. *For all sufficiently large $n \in \mathbb{N}$, we have*

$$\frac{|\mathit{supp}\ \psi_{n,p}|}{\pi_p}\cdot\left(\frac{q\lambda_{n,p}(\mathcal{G})}{p}\right)^{1/p} - (2|E|-1)|V| \leq \nu_{n,p} \leq \frac{|\mathit{supp}\ \psi_{n,p}|}{\pi_p}\cdot\left(\frac{q\lambda_{n,p}(\mathcal{G})}{p}\right)^{1/p} + |V| \tag{5.24}$$

Concretely, the condition on $\lambda_{n,p}(\mathcal{G})$ from Lemma 5.5.6 is enough to ensure that (5.24) holds.

Proof. We suppose n is large enough that there are in fact $|V|$ nodal domains containing exactly one vertex of $\mathcal{G}$, while the rest contain no vertices; that this is possible is guaranteed by Lemma 5.5.6. Let $\mathcal{G}_1, \ldots, \mathcal{G}_{\nu_{n,p}}$ be the nodal domains of $\psi_{n,p}$. We assume that $\mathcal{G}_1, \ldots, \mathcal{G}_{|V|}$ each contain a vertex, while the rest do not; then each $\mathcal{G}_j$ is an interval with Dirichlet conditions at its endpoints if $j > |V|$, and in this case

$$\lambda_{n,p}(\mathcal{G}) = \lambda_{1,p}(\mathcal{G}_j; \partial\mathcal{G}_j) = \frac{p}{q}\left(\frac{\pi_p}{|\mathcal{G}_j|}\right)^p,$$

i.e., $|\mathcal{G}_j| = \pi_p \left(\frac{p}{q\lambda_{n,p}(\mathcal{G})}\right)^{1/p}$. Hence, as in the proof of Lemma 5.3.6, using the definition of the nodal domains,

$$|\operatorname{supp}\psi_{n,p}| = \sum_{j=1}^{\nu_{n,p}} |\mathcal{G}_j| = \sum_{j=1}^{|V|} |\mathcal{G}_j| + (\nu_{n,p} - |V|)\pi_p \left(\frac{p}{q\lambda_{n,p}(\mathcal{G})}\right)^{1/p}.$$

The sum on the right-hand side is non-negative and may be controlled from above using Lemma 5.5.6; this yields

$$\begin{aligned}(\nu_{n,p} - |V|)\pi_p \left(\frac{p}{q\lambda_{n,p}(\mathcal{G})}\right)^{1/p} \le |\operatorname{supp}\psi_{n,p}| &\le (\nu_{n,p} - |V|)\pi_p \left(\frac{p}{q\lambda_{n,p}(\mathcal{G})}\right)^{1/p} \\ &\quad + 2\pi_p |V||E| \left(\frac{p}{q\lambda_{n,p}(\mathcal{G})}\right)^{1/p}.\end{aligned}$$

Rearranging yields (5.24). □

Proof of Theorem 5.5.2 and of Proposition 5.3.4 for the p-Laplacian. Upon combining the result of Lemma 5.5.7 with the Weyl asymptotics of Theorem 5.2.5, we obtain

$$\nu_{n,p} = \frac{|\operatorname{supp}\psi_{n,p}|}{|\mathcal{G}|} n + o(n) \qquad \text{as } n \to \infty,$$

which in particular proves Proposition 5.3.4 for the p-Laplacian. Lemma 5.5.3 now yields (5.22); the other assertions of Theorem 5.5.2 follow immediately. □

Chapter 6

Numerical methods

In this chapter we introduce a method to approximate eigenvalues of the Laplacian with standard conditions at the vertices via approximation of graphs. In §6.1 we fix the setting and show some preliminary results. In §6.2 we introduce the combinatorial Laplacian and recall our main result in context from §1.3.4. In §6.3 we show a-priori and a-priori bounds for the relative error of the eigenvalues of the Laplacian with standard conditions at the vertices for approximations of graphs. In §6.4 we discuss in depth von Below's theorem and extend the results to rational graphs. In §6.5 we present an approximation technique and put our results into context with known approximation theorems. We conclude the chapter with a summary of algorithms and a few applications in §6.6. This chapter corresponds to the joint work [HST] in preparation.

6.1 Notation and preliminaries

In this chapter we consider the eigenvalue problem associated to the free Laplacian with natural vertex conditions and show in this context extensions of von Below's theorems and approximation estimates as summarized in §1.3.4. This involves partitioning each edge into a suitable number of subintervals of similar length.

In fact, as shown in §2.1.2 two metric graphs are isometrically isomorphic if the metric graphs obtained after removal of dummy vertices are the same up to relabelling the vertices and the edges, as well as the corresponding lengths. Isometrically isomorphic graphs form an equivalence class and we will use the term *representative* to denote elements of each of these classes. The *canonical representative* of each class is the metric graph obtained by removing all the dummy vertices. This operation is called *cleaning* and the resulting graph can also be called *clean graph* [KS01; Now08]. The clean graph representative is unique, up to relabelling. It is important to note that, from the spectral point of view, the underlying combinatorial graph G of a metric graph $\mathcal{G}$ does not uniquely determine the metric graph. In fact, introducing dummy vertices, i.e. effectively replacing one interval by two intervals whose corresponding lengths sum to the length of the original interval, one can always find a representative $\widetilde{\mathcal{G}}$ in the same equivalence class of $\mathcal{G}$ having a different underlying combinatorial graph $\widetilde{G}$. However, isometric isomorphic graphs are isospectral, i.e. the corresponding eigenvalue problems do not depend on the choice of the explicit representative.

A type of metric graph that is of particular interest is a graph that admit an equilateral or a rational representative, i.e. a representative whose edges have all the same *basic length* u or are integer multiple of u, respectively.

Definition 6.1.1. Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ be a metric graph with edge lengths $\boldsymbol{\ell} = \{\ell_\mathsf{e}\}$ and total length $\mathrm{sum}(\boldsymbol{\ell}) := \sum_{\mathsf{e}\in E} \ell_\mathsf{e}$. If all edges of $\mathcal{G}$ have the same length, then $\mathcal{G}$ is called *equilateral*. If instead $\boldsymbol{\ell}/\mathrm{sum}(\boldsymbol{\ell})$ is a vector of rational numbers, then $\mathcal{G}$ is called *rational*.

It is important to notice that one can always construct equilateral representatives of rational graphs. More precisely:

Remark 6.1.2. Suppose $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ is a rational metric graph, then for every $\mathsf{e} \in E$, there exist two coprime natural numbers $p_\mathsf{e}, q_\mathsf{e} \in \mathbb{N}$, $\gcd(p_\mathsf{e}, q_\mathsf{e}) = 1$ such that

$$\frac{\ell_\mathsf{e}}{\mathrm{sum}(\boldsymbol{\ell})} = \frac{p_\mathsf{e}}{q_\mathsf{e}}.$$

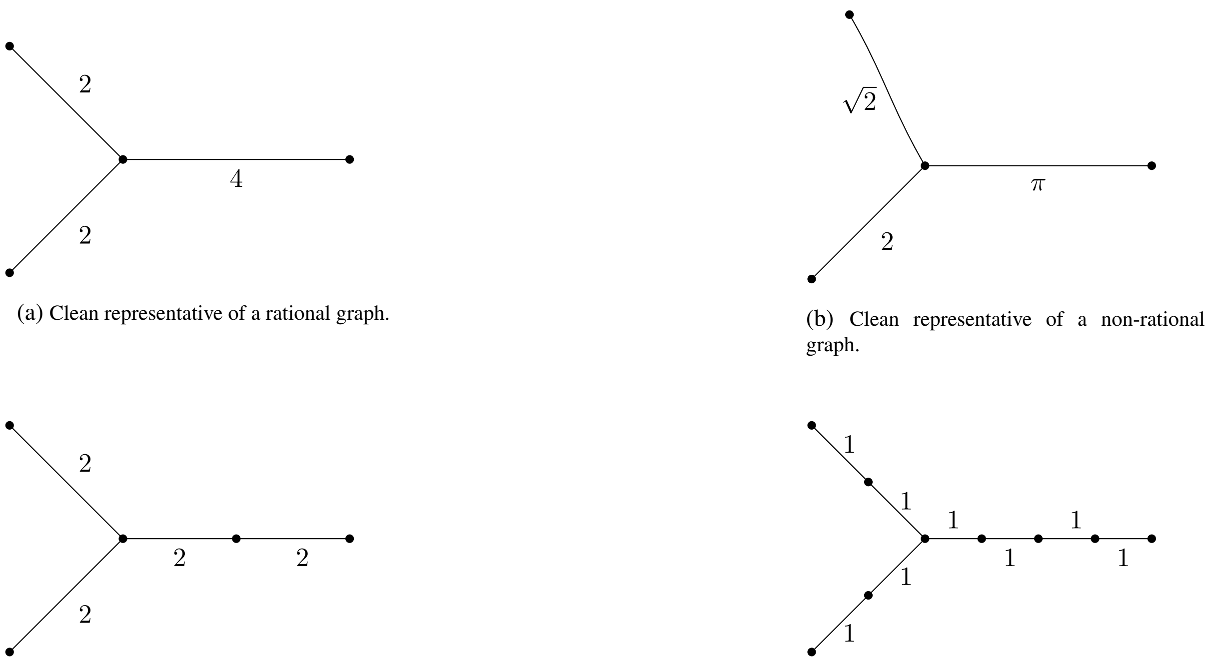
Thus, by letting $q = \mathrm{lcm}(\boldsymbol{q})$ with $\boldsymbol{q} = (q_\mathsf{e})_{\mathsf{e}\in E}$ and by splitting each edge $\mathsf{e} \in E$ in $(q/q_\mathsf{e})p_\mathsf{e}$ subintervals, each of length $\mathrm{sum}(\boldsymbol{\ell})/q$, we obtain an equilateral graph.

This action of splitting the edges of a metric graph is what we call a *subdivision of* $\mathcal{G}$.

Definition 6.1.3. Given a metric graph $\mathcal{G}(G, \boldsymbol{\ell})$ with m edges and a vector $\boldsymbol{p} = (p_\mathsf{e})_{\mathsf{e}\in E} \in \mathbb{N}^m$, let $\mathcal{G}_{\boldsymbol{p}}$ be the graph obtained from $\mathcal{G}$ by replacing each edge e with an equilateral path graph of p_e edges, each of length $\ell_\mathsf{e}/p_\mathsf{e}$. The graph $\mathcal{G}_{\boldsymbol{p}}$ is called subdivision of $\mathcal{G}$ by $\boldsymbol{p}$. If $\gcd(\boldsymbol{p}) = 1$ then the subdivision $\mathcal{G}_{\boldsymbol{p}}$ is called irreducible.

Example 6.1.4. Consider the three-star G as in Figure 6.1. Then, in fact, if we allow restrict ourselves to lengths in $\mathbb{Q}$ the graphs are obviously rational. However, if we have any irrational lengths the graph may be not rational and there does not exist a splitting of edges into an equilateral graph as in Remark 6.1.2 (e.g. in Subfigure 6.1b). In Figure 6.1 we give examples of equilateral representatives that are irreducible or reducible for a given rational graph.

In general, given a rational graph $\mathcal{G}$, there is no unique equilateral representative as for any $k \in \mathbb{N}$ and any equilateral graph, obtained from G as in Remark 6.1.2, we can further partition each edge in k more subintervals all of equal length to obtain arbitrarily many equilateral representatives. In other terms, for any $\boldsymbol{p} = (p_\mathsf{e})$, if $\mathcal{G}_{\boldsymbol{p}}$ is a equilateral subdivision, then $\mathcal{G}_{k\boldsymbol{p}}$ is also equilateral, for any $k \in \mathbb{N}$. However, the construction of Remark 6.1.2 yields a irreducible and equilateral subdivision, which is in some sense canonical. We show below that such representative is unique:



(a) Clean representative of a rational graph.

(b) Clean representative of a non-rational graph.

(c) Irreducible equilateral graph.

(d) Reducible equilateral graph.

Figure 6.1: Topologically equivalent graphs. Some examples of topologically equivalent graphs with different properties.

Proposition 6.1.5. *Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ be a rational metric graph. Then there exists unique irreducible equilateral subdivision of $\mathcal{G}$.*

Proof. By Remark 6.1.2 there exists an irreducible representative. Let $\mathcal{G}_{p^{(1)}}, \mathcal{G}_{p^{(2)}}$ be two irreducible equilateral subdivision of $\mathcal{G}$ with basic length u_1, u_2 respectively which we assume to be distinct. Then

$$u_1 \boldsymbol{p}^{(1)} = \boldsymbol{\ell} = u_2 \boldsymbol{p}^{(2)}.$$

Assume $u_1 > u_2$, then $u_1/u_2 \in \mathbb{N}_{>1}$ and so $(u_1/u_2)\boldsymbol{p}^{(1)} = \boldsymbol{p}^{(2)}$ contradicts the irreducibility of $\boldsymbol{p}^{(2)}$.

$\square$

We use the unique equilateral irreducible subdivision of the clean representative of a rational graph in order to design an algorithm that approximates the eigenvalues of the Laplacian on an arbitrary metric graph $\mathcal{G}$. To this end, we will assume in this chapter that a given metric graph $\mathcal{G}$ is a clean graph. As already observed, this can be done without loss of generality as one can always remove dummy vertices from the input graph without altering its spectrum.

6.2 Graph Laplacians and summary of main results

Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ be a metric graph with underlying combinatorial graph G and length vector $\boldsymbol{\ell}$. Then we consider

Similarly, for a discrete graph $G = (V, E)$ we consider the combinatorial normalized Laplacian, defined as

$$(Lu)_{\mathsf{v}} = \sum_{\tilde{\mathsf{v}}:(\tilde{\mathsf{v}},\mathsf{v})\in E} \frac{u_{\mathsf{v}} - u_{\tilde{\mathsf{v}}}}{d_{\mathsf{v}}}$$

for a vector $u \in \mathbb{R}^n$. If A is the adjacency matrix matrix of G defined via

$$A_{\mathsf{v}_1,\mathsf{v}_2} = \begin{cases} \#\{(\mathsf{v}_1, \mathsf{v}_2) \in E\}, & \mathsf{v}_1 \neq \mathsf{v}_2 \\ 2\#\{(\mathsf{v}_1, \mathsf{v}_2) \in E\}, & \mathsf{v}_1 = \mathsf{v}_2. \end{cases}$$

and D is the diagonal matrix of the degrees $D_{ii} = \sum_j A_{ij}$, then the matrix representation of L is given by

$$L = I - D^{-1}A\,.$$

As for the Laplacian operator on $\mathcal{G}$, L is a positive semi-definite matrix with eigenvalues

$$0 = \mu_1(G) \leq \mu_2(G) \leq \mu_3(G) \cdots \leq \mu_{|V|}(G) = 2 \tag{6.1}$$

Consider an equilateral metric graph $\mathcal{G}(G, \boldsymbol{\ell})$, $\boldsymbol{\ell} = \ell\mathbf{1}$. It is well known that the eigenvalues $\lambda_k = \lambda_k(\mathcal{G})$ of the Laplacian $-\Delta$ on $\mathcal{G}$ with $D(-\Delta) = H^2(\mathcal{G})$ as defined in §2.2.2 and the eigenvalues $\mu_k = \mu_k(G)$ of the normalized Laplacian on G are closely related by Theorem 1.2.2 (von Below's theorem) and we have the correspondence betweeen eigenvalues λ and μ via

$$1 - \cos \ell\sqrt{\lambda} = \mu. \tag{6.2}$$

Moreover if $\mu \neq 0, 2$ and $\lambda \neq u\sqrt{\lambda}/\pi \notin \mathbb{Z}$ then the multiplicities of μ and λ realizing (6.2) coincide. We review the statement and proof of this result in Theorem 6.4.1.

The von Below formula (6.2) lies at the foundation of our proposed method of approximating the eigenvalues of a generic compact metric graph. In fact, we will see in §6.4 that we can compute eigenvalues via eigenvalue functions for rational graphs using the eigenvalues of the combinatorial Laplacian on a suitable equilateral representative.

Before we are able to provide more details we need to introduce a notion of distance between graphs having the same underlying combinatorial graph. Essentially, the distance is induced by the max-norm over the space of the edge lengths.

Recall from Definition 2.1.2:

Definition 6.2.1. Given two metric graphs $\mathcal{G}_1 = \mathcal{G}(G, \boldsymbol{\ell}^{(1)})$ and $\mathcal{G}_2 = \mathcal{G}(G, \boldsymbol{\ell}^{(2)})$ with the same underlying combinatorial graph, let

$$d_G\mathcal{G}_1, \mathcal{G}_2) = \|\boldsymbol{\ell}^{(1)} - \boldsymbol{\ell}^{(2)}\|_\infty = \max_{\mathsf{e}\in E} |\ell_{\mathsf{e}}^{(1)} - \ell_{\mathsf{e}}^{(2)}|\,.$$

Thus, for a sequence $\mathcal{G}^{(n)} = (G, \boldsymbol{\ell}^{(n)})$, we say that $\mathcal{G}^{(n)} = (G, \boldsymbol{\ell}^{(n)})$ converges to $\mathcal{G} = (G, \boldsymbol{\ell})$ if

$$\operatorname{dist}(\mathcal{G}^{(n)}, \mathcal{G}) \to 0 \qquad (n \to \infty).$$

In Section 6.5 we show that approximating the graphs by perturbing its lengths while preserving its total length in a way that

$$\operatorname{dist}(\mathcal{G}^{(n)}, \mathcal{G}) \to 0 \qquad \text{as } n \to \infty,$$

then

$$\sup_{k\in\mathbb{N}} \left| \frac{\lambda_k(\mathcal{G}) - \lambda_k(\mathcal{G}^{(n)})}{k^2} \right| \to 0 \qquad \text{as } n \to \infty.$$

More precisely, we show the following:

Theorem 6.2.2. *Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ and $\widetilde{\mathcal{G}} = \mathcal{G}(G, \widetilde{\boldsymbol{\ell}})$ be metric graphs with $\operatorname{sum}(\boldsymbol{\ell}) = \operatorname{sum}(\widetilde{\boldsymbol{\ell}})$, then*

$$\operatorname{rel\,err}(\lambda_k) := \left| \frac{\lambda_k(\mathcal{G}) - \lambda_k(\widetilde{\mathcal{G}})}{\lambda_k(\mathcal{G})} \right| \le C_k \max_{e\in E} \frac{|\ell_e - \widetilde{\ell}_e|}{\min\{\ell_e, \widetilde{\ell}_e\}}$$

where β is the Betti number of G, $|N|$ is the number of leafs, i.e. vertices of degree 1, and

$$C_k := \left(\frac{k - 2 + \frac{3\beta+|N|}{2}}{\min\{k - \frac{\beta+|N|}{2}, 2k\}} \right)^2 \le \max\{8, 2(3\beta + |N| - 2)^2\}$$

Moreover, we have the following asymptotic estimate:

Corollary 6.2.3. *Suppose $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ and $\mathcal{G}^{(n)} = \mathcal{G}^{(n)}(G, \boldsymbol{\ell}^{(n)})$ with $\operatorname{sum}(\boldsymbol{\ell}) = \operatorname{sum}(\boldsymbol{\ell}^{(n)})$, and $\mathcal{G}^{(n)} \to \mathcal{G}$ as $n \to \infty$, then for sufficiently large n, there exists $C > 0$ independent of k such that*

$$\operatorname{rel\,err}(\lambda_k) \le C \operatorname{dist}(\mathcal{G}^{(n)}, \mathcal{G}).$$

The following result guarantees the existence of graphs that approximate $\mathcal{G}$ arbitrarily exactly and algorithms to achieve this can be found in Section 6.5:

Theorem 6.2.4. *Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ be a metric graph with $\langle \boldsymbol{\ell}, \mathbf{1} \rangle = 1$, then for all $q \in \mathbb{N}$ there exists a metric graph $\mathcal{G}_q = \mathcal{G}_q(G, \boldsymbol{n}_q/q)$ with $\boldsymbol{n}_q \in \mathbb{N}^{|E|}$ such that*

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_q) \le \frac{C_1}{q}$$

for some $C_1 > 0$. Furthermore, for every $q \in \mathbb{N}$ there exists $Q > q$, such that

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_Q) \le \frac{C_2}{Q^{\frac{N}{N-1}}}$$

for some $C_2 > 0$.

Remark 6.2.5. The proof of this theorem is constructive and can be found in Section 6.5. In fact, suppose $q \in \mathbb{N}$ and $\mathcal{G}_q$ as in Theorem 6.2.4 by Corollary 6.2.3 we have

$$\operatorname{rel\,err}(\lambda_n(\mathcal{G}), \lambda_n(\mathcal{G}_q)) \to 0 \qquad (q \to \infty).$$

Furthermore,

$$\liminf_{q\to\infty} \ q^{\frac{N}{N-1}} \operatorname{rel\,err}(\lambda_n(\mathcal{G}), \lambda_n(\mathcal{G}_q)) < \infty.$$

The principal strategy can than be than summarized as follows, which we will develop fully in Algorithm 5 and Algorithm 6:

Algorithm 1: Computation of eigenvalues for equilateral graphs.

Input: Metric graph $\mathcal{G}$, i.e. the underlying combinatorial graph G and the edge lengths vector $\boldsymbol{\ell}$ and the prescribed relative error ϵ for the computation of the eigenvalues.

Output: A list of eigenvalues of the discrete Laplacian.

1 Compute q and $\boldsymbol{n} \in \mathbb{N}^{|E|}$ such that the RHS of (6.2.2) is smaller of ϵ where $\widetilde{\boldsymbol{\ell}} = \boldsymbol{n}/q$

2 Compute the spectrum of $\mathcal{G}_q = \mathcal{G}(G, \widetilde{\boldsymbol{\ell}})$ via Algorithm 2

6.3 A-priori and A-posteriori estimates for the relative error of eigenvalues

In this section we will show Theorem 6.3.1. Our main result will be the following a-posteriori estimate on the eigenvalues of metric graphs with same underlying combinatorial graph and total length.

Theorem 6.3.1 (a-posteriori estimate)**.** *Let $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell}), \widetilde{\mathcal{G}} = \mathcal{G}(G, \widetilde{\boldsymbol{\ell}})$ be a metric graph with*

$$\mathcal{L} = \langle \boldsymbol{\ell}, \mathbf{1} \rangle = \langle \widetilde{\boldsymbol{\ell}}, \mathbf{1} \rangle$$

and $n \in \mathbb{N}$, then

$$|\lambda_n(\mathcal{G}(G, \widetilde{\boldsymbol{\ell}})) - \lambda_n(\mathcal{G}(G, \boldsymbol{\ell}))| \le 2\Lambda_n(\mathcal{L}, P, \beta) \max_{\mathsf{e}\in E} \frac{|\widetilde{\ell}_{\mathsf{e}} - \ell_{\mathsf{e}}|}{\min\{\ell_{\mathsf{e}}, \widetilde{\ell}_{\mathsf{e}}\}}, \tag{6.3}$$

where

$$\Lambda_n(\mathcal{L}, |N|, \beta) = \left(\frac{\pi}{\mathcal{L}}\right)^2 \left(n - 2 + \frac{|N|}{2} + \frac{3}{2}\beta\right)^2.$$

The bound in the estimate can be achieved without dependence of the particular choice of $\widetilde{\boldsymbol{\ell}}$ under the assumption of an a-priori bound:

Corollary 6.3.2 (a-priori estimate)**.** *Under the same assumptions as Proposition 6.3.1, if $\|\widetilde{\boldsymbol{\ell}} - \boldsymbol{\ell}\|_\infty \le \epsilon$ we have*

$$|\lambda_n(\boldsymbol{\ell}) - \lambda_n(\widetilde{\boldsymbol{\ell}})| \le 2\Lambda_n(\mathcal{L}, |N|, \beta) \frac{\epsilon}{\min_{\mathsf{e}} \ell_{\mathsf{e}} - \epsilon}.$$

Proof. It is an immediate consequence of Proposition 6.3.1 since

$$|\lambda_n(\boldsymbol{\ell}) - \lambda_n\widetilde{(\boldsymbol{\ell})}| \leq 2\Lambda_n(\mathcal{L}, |N|, \beta) \max_{\mathsf{e}\in E} \frac{|\widetilde{\ell}_{\mathsf{e}} - \ell_{\ e}|}{\min\{\ell_{\mathsf{e}}, \widetilde{\ell}_{\mathsf{e}}\}} \leq 2\Lambda_n(\mathcal{L}, |N|, \beta) \frac{\epsilon}{\min_{\mathsf{e}} \ell_{\mathsf{e}} - \epsilon}$$

□

In the following lemma, we show the Hadamard type formula for computing the derivative of eigenvalues with respect the length of the edges, which is a known result when the considered eigenvalues are simple and the proof will be in fact following [BL17a, Lemma 5.2] closely. Suppose $u \in \mathcal{F}$ is an eigenfunction of λ. Consider along an edge $\mathsf{e} \in E$ the quantity

$$\mathcal{E}_{\mathsf{e}}(x) := \frac{1}{\ell_e^2}(u_{\mathsf{e}}')^2 + \lambda(u_{\mathsf{e}})^2. \tag{6.4}$$

Then

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}x}\mathcal{E}_{\mathsf{e}}(x) &= u'(x)u''(x) + \lambda u(x)u'(x) + \lambda u'(x) + u(x) \\
&= 2(u''(x) + \lambda u(x))u'(x) = 0
\end{aligned}$$

and $\mathcal{E}_{\mathsf{e}}$ is constant along edges. In particular, we have the following:

Lemma 6.3.3. *Let $\mathcal{G}$ be a metric graph and $\boldsymbol{\mathcal{E}} = (\mathcal{E}_{\mathsf{e}})_{\mathsf{e}\in E}$ defined as in* (6.4). *Then*

$$\boldsymbol{\mathcal{E}} \cdot \boldsymbol{\ell} = 2\lambda.$$

Proof. Let us consider the integral of the energy on the whole graph, on one hand we have

$$\int_{\mathcal{G}} \mathcal{E}(x)\, dx = \sum_{e_i\in E} \int_{e_i} \mathcal{E}(x)\, dx = \sum_{e_i\in E} \mathcal{E}_i \ell_i.$$

By integration by parts one gets the other side of the equality

$$\begin{aligned}
\int_{\mathcal{G}} \mathcal{E}(x)\, dx &= \int_{\mathcal{G}} |\psi'(x)|^2 + \lambda|\psi(x)|^2\, dx, \\
&= \sum_{e_i\in E} \left[\psi'\bar{\psi}\right]_{x_{2i-1}}^{x_{2i}} + \left(\int_{\mathcal{G}} -\psi''(x)\bar{\psi}(x)\, dx\right) + \int_{\mathcal{G}} \lambda|\psi(x)|^2\, dx, \\
&= \sum_{v\in V} \bar{\psi}(v) \sum_{x_i\in v} \partial\psi(x_i) + 2\lambda \int_{\mathcal{G}} |\psi(x)|^2\, dx = 2\lambda.
\end{aligned}$$

□

We need an adaptation of the Hadamard formula from [BL17a, Lemma 5.2] here:

Lemma 6.3.4. *Suppose $\boldsymbol{\ell}_0, \boldsymbol{\ell}_1 \in \mathbb{R}^{|E|}_{>0}$ and $v \in \mathbb{R}^{|E|}$. Suppose $\gamma(t) := \boldsymbol{\ell}_0 + t(\boldsymbol{\ell}_1 - \boldsymbol{\ell}_0)$. Let $\lambda(t)$ be a locally analytic eigenvalue curve and $f(s;\cdot)$ be a locally analytic curve of eigenfunctions associated to $\lambda(t)$ as in Theorem 2.6.1, then*

$$\frac{\mathrm{d}}{\mathrm{d}t}\lambda(t)\bigg|_{t=0} = -\boldsymbol{\mathcal{E}} \cdot \mathbf{v}. \tag{6.5}$$

Proof. Let $s \in \mathbb{R}$ and let $\widetilde{e}$ be an edge of $\mathcal{G}(\mathcal{G}.\boldsymbol{\ell})$. Denote $\boldsymbol{\ell}(s) := \boldsymbol{\ell} + s\boldsymbol{v}$ and $\mathcal{G}(s) := \mathcal{G}(\mathcal{G}; \boldsymbol{\ell}(s))$. Then by Theorem 2.6.1 there exists a corresponding set of eigenfunctions denoted by $f(s;\cdot)$ analytically depending on s and we may proceed as in [BL17a, Lemma 5.2] to prove the Hadamard formula in the form of (6.5).

□

Corollary 6.3.5. *Suppose $\boldsymbol{\ell}_0, \boldsymbol{\ell}_1 \in \mathbb{R}^{|E|}_{>0}$ and $v \in \mathbb{R}^{|E|}$. Suppose $\gamma(t) := \boldsymbol{\ell}_0 + t(\boldsymbol{\ell}_1 - \boldsymbol{\ell}_0)$. Let $\lambda(t)$ be a locally analytic eigenvalue curve and $f(s;\cdot)$ be a locally analytic curve of eigenfunctions associated to $\lambda(t)$ as in Theorem 2.6.1, then $\boldsymbol{\mathcal{E}}(t)$ is analytic in t.*

Proof. Since the pair of eigenvalue and eigenfunction are locally analytic functions in the lengths of the edges of the graph (c.f. §2.6), the same property holds for the function $\boldsymbol{\mathcal{E}}$ as defined in (6.4). □

In order to be able to provide a good estimate of the error on the computation of the eigenvalues we need some type of upper bound on the eigenvalues which is independent on the lengths of the edges of the graph. The following result is shown in [BKKM17, Theorem 4.9]:

Proposition 6.3.6. *Let $\Gamma = (G, \boldsymbol{\ell})$ be a metric graph with total length $\mathcal{L} = \langle \boldsymbol{\ell}, \mathbf{1} \rangle$, first Betti number $\beta = |E| - |V| + 1$ and let $|N|$ be the number of vertices of degree 1. Then the eigenvalues λ_n of* (1.15) *satisfy the following upper and lower estimates*

$$\mu_n(\mathcal{L}, |N|, \beta) \leq \lambda_n \leq \Lambda_n(\mathcal{L}, |N|, \beta),$$

where

$$\mu_n(\mathcal{L}, |N|, \beta) = \left(\frac{\pi}{\mathcal{L}}\right)^2 \max\left\{\left(n - \frac{|N| + \beta}{2}\right)^2, \frac{n^2}{4}\right\},$$
$$\Lambda_n(\mathcal{L}, |N|, \beta) = \left(\frac{\pi}{\mathcal{L}}\right)^2 \left(n - 2 + \frac{|N|}{2} + \frac{3}{2}\beta\right)^2.$$

Proof of Theorem 6.3.1. Let $\boldsymbol{\ell}(t) := \boldsymbol{\ell} + t\left(\widetilde{\boldsymbol{\ell}} - \boldsymbol{\ell}\right)$, then $\lambda_n(\mathcal{G}(G, \boldsymbol{\ell}(t))$ is differentiable up to a discrete set of exceptional points by Theorem 2.6.1. Suppose

$$0 = t_0 < t_1 < \cdots < t_{N-1} < t_N = 1$$

such that the exceptional points are contained in $\{t_0, \ldots, t_N\}$, then with Lemma 6.3.4 and Corollary 6.3.5 we compute

$$
\begin{aligned}
|\lambda_n(\mathcal{G}(G,\widetilde{\boldsymbol{\ell}})) - \lambda_n(\mathcal{G}(G,\boldsymbol{\ell}))| &\leq \sum_{i=0}^{N-1} \int_{t_i}^{t_{i+1}} \left| \frac{\mathrm{d}}{\mathrm{d}t} \lambda_n\left(\mathcal{G}(G,\boldsymbol{\ell}(t))\right) \right| \mathrm{d}t \\
&\leq \max_{t\in[0,1]} |\boldsymbol{\mathcal{E}}\left(\boldsymbol{\ell}(t)\right) \cdot \left(\widetilde{\boldsymbol{\ell}} - \boldsymbol{\ell}\right)| \leq \max_{t\in[0,1]} |\sum_{\mathsf{e}\in E} \mathcal{E}_{\mathsf{e}}\left(\boldsymbol{\ell}(t)\right) \ell_{\mathsf{e}}(t) \frac{\widetilde{\ell}_{\mathsf{e}} - \ell_{\mathsf{e}}}{\ell_{\mathsf{e}}(t)}| \\
&= \max_{t\in[0,1]} |\boldsymbol{\mathcal{E}}\left(\boldsymbol{\ell}(t)\right) \cdot \boldsymbol{\ell}(t)| \max_{\mathsf{e}} \frac{|\widetilde{\ell}_{\mathsf{e}} - \ell_{\mathsf{e}}|}{\ell_{\mathsf{e}}(t)} = \max_{t\in[0,1]} 2\lambda_n(\boldsymbol{\ell}(t)) \max_{\mathsf{e}} \frac{|\widetilde{\ell}_{\mathsf{e}} - \ell_{\mathsf{e}}|}{\min\{\ell_{\mathsf{e}}, \widetilde{\ell}_{\mathsf{e}}\}},
\end{aligned}
$$

where we used Lemma 6.3.4 in the first and Lemma 6.3.3 in the last step. Using Proposition 6.3.6 we conclude (6.3). □

Theorem 6.2.2 is then a direct consequence of Theorem 6.3.1 and Proposition 6.3.6.

Proof of Theorem 6.2.2. By Theorem 6.3.1 and Proposition 6.3.6 we have

$$
\mathrm{rel\ err}(\lambda_k) := \left| \frac{\lambda_k(\mathcal{G}) - \lambda_k(\widetilde{\mathcal{G}})}{\lambda_k(\mathcal{G})} \right| \leq C_k \max_{\mathsf{e}\in E} \frac{|\ell_e - \widetilde{\ell}_e|}{\min\{\ell_e, \widetilde{\ell}_e\}}.
$$

with

$$
C_k = 2 \left(\frac{k - 2 + \frac{3\beta + |N|}{2}}{\max\{k - \frac{\beta+|N|}{2}, k/2\}} \right)^2.
$$

Let us conclude the proof by showing

$$
C_k(\mathcal{G}) \leq \max\{8, 2(3\beta + P - 1)^2\},
$$

- If $k \geq \beta + P$ then

$$
\begin{aligned}
C_k(\mathcal{G}) &= 2 \left(\frac{k - 2 + \frac{3\beta+P}{2}}{k - \frac{\beta+P}{2}} \right)^2 \\
&= 2 \left(1 + \frac{2\beta + P - 2}{k - \frac{\beta+P}{2}} \right)^2
\end{aligned}
$$

  and because $k - (\beta + P)/2 \geq (\beta + P)/2 \geq 1$ then

$$
C_k(\mathcal{G}) \leq 2\left(2\beta + P - 1\right)^2.
$$

- If $k \leq \beta + P$ then

$$C_k(\mathcal{G}) = 2\left(\frac{k-2+\frac{3\beta+P}{2}}{k/2}\right)^2$$
$$= 2\left(2+\frac{3\beta+P-4}{k}\right)^2$$

if $3\beta + P - 4 \geq 0$ then $k = 1$ provides an upper bound

$$C_k(\mathcal{G}) \leq 2\,(3\beta + P - 2)^2$$

if instead $3\beta + P - 4 < 0$ then $C_k(\mathcal{G}) \leq 8$ then all together

$$C_k(\mathcal{G}) \leq \max\{8, 2\,(3\beta + P - 2)^2\} =: C(\mathcal{G}).$$

□

6.4 On the spectrum of rational metric graphs

Let $\mathcal{G}(G, \boldsymbol{\ell})$ be an equilateral graph with base length ℓ, i.e. with $\ell_{\mathsf{e}} = u$ for all $e \in E$ and let $L = L(G)$ be the averaged Laplacian of G.

The following Theorem is due to Von Below [Bel85] and it establishes a correspondence between the eigenvalues $\{\mu\}$ of L and the eigenvalues $\{\lambda\}$ of $-\Delta$, the Laplacian operator on the metric graph $\mathcal{G}(G,\ \ell)$. We provide a formulation which is an adaptation for our purposes from [Kur08]. Here we provide a possible proof for the sake of completeness (c.f. [Bel85], [Kur08], [Kur]).

Theorem 6.4.1 (von Below's formula)**.** *Let $\mathcal{G} = \mathcal{G}(G, u\mathbf{1})$ be an equilateral metric graph with basic length $\ell > 0$. For any $\mu \neq 0, 2$ eigenvalue of the normalized Laplacian L of the underlying discrete graph G, there exists λ solution to the Kirchoff–Neumann eigenvalue problem* (1.15) *for the Laplacian of the metric graph $\mathcal{G}$, such that $\ell\sqrt{\lambda}/\pi \notin \mathbb{Z}$ and*

$$1 - \cos \ell\sqrt{\lambda} = \mu. \tag{6.6}$$

Furthermore, the multiplicities of the two eigenvalues λ and μ coincide and the values of the associated eigenvectors and eigenfunctions can be chosen such that their values coincide at the corresponding vertices.

Proof. Let $\mu \neq 0, 2$ be associated to the eigenvector $\boldsymbol{\psi} \in \mathbb{R}^{|V|}$ and $k > 0$ such that $\sin k\ell \neq 0$, we are going to construct an eigenfunction φ on the equilateral metric graph $\mathcal{G}(G, \boldsymbol{\ell})$ such that its associated eigenvalue satisfies (6.6).

Consider φ defined edgewise, i.e. for each edge $e \in E$ connecting two vertices v_1, v_2 we define $\varphi_e \in C^2([0,\ell])$ via

$$\varphi_e(x) := \psi_{v_1}\left(\cos kx - \frac{\cos k\ell}{\sin k\ell}\sin kx\right) + \psi_{v_2}\left(\cos k(\ell - x) - \frac{\cos ku}{\sin k\ell}\sin k(\ell - x)\right)$$

such that 0 corresponds to v_1 and 1 corresponds to v_2. By construction, $\varphi \in C(\mathcal{G}, \mathbf{1})$ and for all $v \in V$ we compute

$$\begin{aligned}
\sum_{\substack{(x,e)\in v\\ \mathsf{e}=(\mathsf{v}_e,\mathsf{v})}} \partial\varphi_e(\mathsf{v}) &= \sum_{\substack{(x,e)\in v\\ \mathsf{e}=(\mathsf{v}_e,\mathsf{v})}} -\psi_{\mathsf{v}} k \frac{\cos k\ell}{\sin k\ell} + \psi_{\mathsf{v}_\mathsf{e}} k \left(\sin k\ell + \frac{\cos^2 k\ell}{\sin k\ell}\right) \\
&= \frac{k}{\sin k\ell} \sum_{\substack{(x,\mathsf{e})\in \mathsf{v}\\ \mathsf{e}=(\mathsf{v}_e,\mathsf{v})}} -\psi_{\mathsf{v}} \cos k\ell + \psi_{\mathsf{v}} \\
&= \frac{k}{\sin k\ell}\left(-\deg(\mathsf{v})\psi_{\mathsf{v}}\cos k\ell + \sum_{\substack{(x,\mathsf{e})\in \mathsf{v}\\ \mathsf{e},(\mathsf{v}_e,v)}} \psi_{\mathsf{v}_\mathsf{e}}\right) \\
&= \frac{k\deg(v)}{\sin k\ell}\left(\psi_{\mathsf{v}}(1-\cos k\ell) - \psi_{\mathsf{v}} + \frac{1}{\deg(v)} \sum_{\substack{(x,\mathsf{e})\in \mathsf{v}\\ \mathsf{e},(\mathsf{v}_e,v)}} \psi_{\mathsf{v}_\mathsf{e}}\right)
\end{aligned}$$

and $\varphi \in \mathfrak{D}(-\Delta)$ if and only if

$$\psi_{\mathsf{v}}(1-\cos k\ell) = \psi_{\mathsf{v}} - \frac{1}{\deg(\mathsf{v})} \sum_{\substack{(x,\mathsf{e})\in \mathsf{v}\\ \mathsf{e},(\mathsf{v}_e,v)}} \psi_{\mathsf{v}_\mathsf{e}}$$

or equivalently $(1-\cos k\ell)\psi = L\psi$. By construction $\varphi_\mathsf{e}'' = k^2\varphi_\mathsf{e}$ and we deduce $k^2 \in \sigma(\Delta)$ if and only if $(1-\cos k\ell)\psi = L\psi$. Since $\sin k\ell = 0$ if and only if $1-\cos k\ell \neq 0, 2$ we infer the statement.

□

The remaining two cases $\mu = 0$ or $\mu = 2$, which are not covered by Theorem 6.4.1 can be considered by following Propositions (see also [Kur08], [Kur]). For the proofs of the following proposition we refer to [Kur08, Theorem 2].

Proposition 6.4.2. *Let $\mathcal{G} = \mathcal{G}(G, \ell\mathbf{1})$ be an equilateral metric tree graph with basic length $\ell > 0$ and let $n \in \mathbb{N}_0$. Then $\lambda = k^2 \in \sigma(-\Delta)$ with $k = \frac{2n\pi}{\ell}$ is a simple eigenvalue. Furthermore, $k = \frac{(2n+1)\pi}{\ell}$ is a (simple) eigenvalue if and only if G is bipartite.*

Proposition 6.4.3. *Let $\mathcal{G} = \mathcal{G}(G, \ell\mathbf{1})$ be an equilateral metric graph with basic length $\ell > 0$, Betti number $\beta \geq 1$. Then $\lambda = k^2 \in \sigma(-\Delta)$ with $k = \frac{n\pi}{\ell}$ for all $n \in \mathbb{N}_0$ with multiplicities $\beta + 1$*

if G is bipartite. On the other hand, if G is not bipartite, then the eigenvalues corresponding to n even have algebraic multiplicity $m_{even} = \beta + 1$ and the eigenvalues corresponding to n odd have algebraic multiplicity $m_{odd} = \beta - 1$.

The following algorithm can then be used to compute the eigenvalues of an equilateral graph, which we summarize in Theorem 6.4.4:

Algorithm 2: Computation of eigenvalues for equilateral graphs.

Input: Combinatorial graph $G = (V, E)$ with combinatorial Laplacian $L \in \mathbb{R}^{n\times n}$,
basic length $\ell > 0$, $j \in \mathbb{N}$

Output: $k_j = \sqrt{\lambda_j}$ the j-th eigenfrequency of the Laplacian $-\Delta$

$[\mu_1, \dots, \mu_n] = \texttt{eig}(L)$ `# Compute eigenvalues of` L

$\beta := |V| - |E| - 1$ `# Compute the Betti number`

$m_\mu := \#\{\mu_i, \mu_i \notin \{0, 2\}\}$ `# Quantities regarding number of eigenvalues`

if *G is bipartite* **then**

  $m_{\text{odd}} = m_{\text{even}} = \beta + 1$

else

  $m_{\text{odd}} = \beta - 1, \qquad m_{\text{even}} = \beta + 1$

$m_p = 2m_\mu + m_{\text{odd}} + m_{\text{even}}$ `# Then the spectrum admits a periodic structure and within each period the number of eigenvalues is`

$a = \texttt{floor}(j/m_p), \qquad r = j - a m_p$ `# Division with remainder`

`# eigenfrequency function`

$$K(r) := \begin{cases} 0 & r = 0; \\ \arccos(1 - \mu_r) & 0 < r \le m_\mu; \\ \pi & m_\mu < r \le m_\mu + m_{\text{odd}}; \\ 2\pi - \arccos(1 - \mu_{(2m_\mu + m_{\text{odd}} - r)}) & m_\mu + m_{\text{odd}} < r \le 2m_\mu + m_{\text{odd}}; \\ 2\pi & m_p - m_{\text{even}} < r < m_p. \end{cases}$$

$k_j = \frac{1}{\ell}(2\pi a + K(r))$

Algorithm 2 is based on the following result:

Theorem 6.4.4. *Let $\mathcal{G} = \mathcal{G}(G, \ell\mathbf{1})$ be an equilateral metric graph with basic length ℓ with Betti number $\beta \in \mathbb{N}_0$. Let $m_\mu := \#\{\mu_i \neq 0, 2\}$, $m_{even} := \beta + 1$*

$$m_{odd} := \begin{cases} \beta + 1, & G \text{ is bipartite;} \\ max\{\beta - 1, 0\}, & \text{otherwise.} \end{cases}$$

then the spectrum of $-\Delta_\Gamma$ is given as $\lambda_j = k_j^2$ with

$$k_j = \frac{1}{\ell}\Big(2\pi\Big\lfloor\frac{j-1}{m_p}\Big\rfloor + K\Big((j-1) \mod m_p\Big)\Big);$$

where

$$K(j) := \begin{cases} 0 & j = 0; \\ \arccos(1 - \mu_j) & 0 < j \le m_\mu; \\ \pi & m_\mu < j \le m_\mu + m_{odd}; \\ 2\pi - \arccos(1 - \mu_{(2m_\mu + m_{odd} - j)}) & m_\mu + m_{odd} < j \le 2m_\mu + m_{odd}; \\ 2\pi & m_p - m_{even} < j < m_p. \end{cases}$$

In order to motivate the next section consider an example of a rational metric graph where the corresponding equilateral graph has a very large number of edges (for the graph $\mathcal{G}$ in Example 6.4.5 this number would be 300). Intuition should suggest that the equilateral graph $\mathcal{G}'$ is a good approximation of $\mathcal{G}$ with just three edges and therefore it is much easier to compute the spectrum of $\mathcal{G}'$ rather than $\mathcal{G}$. The purpose of §6.5 is to find approximations that allow us to compute the spectrum using Theorem 6.4.4.

Example 6.4.5. Consider the the three-star G as in Figure 6.2, The length of the metric graph $\mathcal{G}$ in subfigure 6.2a can be perturbed slightly to achieve an equilateral metric graph $\mathcal{G}'$ with basic length 1 and by construction

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}') = 0.01.$$

In fact, by Algorithm 5 and Algorithm 6 one can achieve arbitrary good perturbation such that the Hausdorff distance between these graphs can be controlled. By Corollary 6.2.3 in particular Algorithm 5 and Algorithm 6 terminate after a finite numbers of steps.

(a) Graph $\mathcal{G}$. An equilateral subdivision requires a large amount of subdivisions here.

(b) Graph $\mathcal{G}'$. The equilateral 3-star $\mathcal{G}'$ with same underlying combinatorial graph as $\mathcal{G}$ is a "good" approximation for the graph in subfigure 6.2a.

Figure 6.2: Three-stars with similar lengths. Comparison between graphs with similar length parameter and their equilateral representatives.

6.5 Approximation techniques

Given a metric graph $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ with total length $\operatorname{sum}(\boldsymbol{\ell})$ we construct rational graphs $\mathcal{G}^{(n)}$ such that

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}^{(n)}) \to 0 \qquad (n \to \infty).$$

In particular by Proposition 6.3.1 we infer

$$\lambda_k(\Gamma^{(n)}) \to \lambda_k(\Gamma) \qquad (n \to \infty)$$

and (6.3) offers an estimate to the error of such a approximation with respect to the Hausdorff-distance. Therefore, we construct minimizers to the minimization problem

$$\min_{1 \le q \le Q} \min_{\langle \boldsymbol{n}, \boldsymbol{1} \rangle = q} \left\| \boldsymbol{\ell} - \frac{\boldsymbol{n}}{\langle \boldsymbol{n}, \boldsymbol{1} \rangle} \right\|. \tag{6.7}$$

in this section.

Our main result in this section is the following:

Theorem 6.5.1. *Let $\mathcal{G} = (G, \boldsymbol{\ell})$ be a metric graph with edge set E. Then for every $Q \in \mathbb{N}$ there exists $1 \le q \le Q$ and $\boldsymbol{n} \in \mathbb{N}_0^{|E|}$ with $\langle \boldsymbol{n}, \boldsymbol{1} \rangle = q$ that minimizes*

$$\min_{1 \le q \le Q} \min_{\langle \boldsymbol{n}, \boldsymbol{1} \rangle = q} \left\| \boldsymbol{\ell} - \frac{\boldsymbol{n}}{\langle \boldsymbol{n}, \boldsymbol{1} \rangle} \right\|.$$

Furthermore, for sufficiently large Q we have $\boldsymbol{n} \in \mathbb{N}^{|E|}$ and if we define $\widetilde{G}(G, \frac{\boldsymbol{n}}{\langle \boldsymbol{n}, \boldsymbol{1} \rangle})$, then

$$\operatorname{dist}(\mathcal{G}, \widetilde{\mathcal{G}}) \le \min \left\{ \frac{3}{2Q}, \frac{1}{q} \left(\frac{\sqrt{N} A_N}{Q} \right)^{\frac{1}{N-1}} \right\}.$$

An immediate consequence of this result is Theorem 6.2.4:

Proof of Theorem 6.2.4. For sufficiently large $q \in \mathbb{N}$ by Theorem 6.5.1 there exist graphs $\mathcal{G}_q$ with same underlying graph as $\mathcal{G}$ such that

$$\operatorname{dist}(\mathcal{G}, \widetilde{\mathcal{G}}) \le \min \left\{ \frac{3}{2Q}, \frac{1}{q} \left(\frac{\sqrt{N} A_N}{Q} \right)^{\frac{1}{N-1}} \right\}.$$

In particular,

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_q) \le \frac{C_1}{q} \tag{6.8}$$

for some $C_1 > 0$. Furthermore, since due to (6.8)

$$\operatorname{dist}(\mathcal{G}, \mathcal{G}_q) \to 0 \qquad (q \to \infty)$$

there exists $Q > q$ such that

$$Q = \mathrm{argmin}_{1 \le q \le Q} \min_{\langle \boldsymbol{n}, \boldsymbol{1} \rangle = q} \left\| \boldsymbol{\ell} - \frac{\boldsymbol{n}}{\langle \boldsymbol{n}, \boldsymbol{1} \rangle} \right\|$$

and by Theorem 6.5.1 we infer

$$\mathrm{dist}(\mathcal{G}, \mathcal{G}_Q) \le \frac{1}{Q} \left(\frac{\sqrt{N} A_N}{Q} \right)^{\frac{1}{N-1}}.$$

$\square$

It turns out that (6.7) is an adaptation of the so called *Simultaneous Dirichlet Approximation* or *Simultaneous Diophantine Approximation* (SDAP).

The SDAP consists in finding the vector of rational numbers which best approximate a given vector of real numbers in the maximum norm under the condition of having the least common multiple of the denominators bounded by a given $Q \in \mathbb{N}$. Notice that the SDAP already made appearance in quantum graphs in [ET17].

Problem 6.5.2 (Classic SDAP [Sch80])**.** Given $\boldsymbol{\alpha} \in \mathbb{R}^N$ and $Q \in \mathbb{N}$ find $\boldsymbol{n} \in \mathbb{Z}^N$ and $q \in \mathbb{N}$ such that $q \le Q$ which minimize $\|\boldsymbol{\alpha} - \boldsymbol{n}/q\|_\infty$.

It is known that the minimum exists with the following general estimate, see [Sch80]

Proposition 6.5.3. *There exists a solution to Problem 6.5.2, such that*

$$\|\boldsymbol{\alpha} - \frac{\boldsymbol{n}}{q}\|_\infty \le \frac{1}{q\, Q^{1/N}}. \tag{6.9}$$

Finding a rational graph $\widetilde{\Gamma}$ with same underlying discrete graph Γ and with the same total length $\widetilde{\mathcal{L}} = \mathcal{L}$ is equivalent to solving a modified version of problem 6.5.2 where $\boldsymbol{\alpha} = \boldsymbol{\ell}/\mathcal{L}$ and in addition we require $q = \langle \boldsymbol{n}, \boldsymbol{1} \rangle$.

Problem 6.5.4 (Constrained SDAP)**.** Given $\boldsymbol{\alpha} \in \mathbb{R}^N$ such that $\boldsymbol{\alpha} \cdot \boldsymbol{1} = 1$ and $Q \in \mathbb{N}$ find $\boldsymbol{n} \in \mathbb{Z}^N$ such that $\sum_{i=1}^N n_i \le Q$ which minimizes $\|\boldsymbol{\alpha} - \boldsymbol{n}/\langle \boldsymbol{n}, \boldsymbol{1} \rangle\|_\infty$.

We show that we can still have an estimate just slightly worse than (6.9).

Theorem 6.5.5. *There exists a solution to Problem 6.5.4, $\boldsymbol{n} \in \mathbb{Z}^N \setminus \{\boldsymbol{0}\}$, $q = \boldsymbol{n} \cdot \boldsymbol{1}$, such that*

$$\|\boldsymbol{\alpha} - \frac{\boldsymbol{n}}{q}\|_\infty \le \frac{1}{q} \left(\frac{\sqrt{N} A_N}{Q} \right)^{\frac{1}{N-1}}. \tag{6.10}$$

where A_N is the $N-1$ volume of the central section of the unit N-cube orthogonal to the main diagonal

$$A_N = \mathit{Vol}_{N-1} \left(\left[-\frac{1}{2}, +\frac{1}{2} \right]^N \cap \boldsymbol{1}^\perp \right).$$

with $\mathbf{1}$ *being the vector* $1_i = 1, i = 1, \ldots, N$.

We are going to prove this result using a similar idea of the proof of Proposition 6.5.3 using Minkovski's convex body Theorem.

Proposition 6.5.6 (Minkovski's convex body Theorem [Sch80]). *Let* $\Omega \subset \mathbb{R}^N$ *be convex, symmetric about the origin, bounded and with volume* $Vol_N(\Omega)$. *Assume either that* $Vol_N(\Omega) > 2^N$ *or that* Ω *is compact and* $Vol_N(\Omega) \geq 2^N$. *Then* Ω *contains an integer point different from the origin.*

Proof of Theorem 6.5.5. Let $s = \left(\sqrt{N} Q A_N\right)^{-\frac{1}{N-1}}$ and consider the following set

$$\Omega_N := \left\{ \boldsymbol{x} \in \mathbb{R}^N : |\boldsymbol{x} \cdot \mathbf{1}| \leq Q,\ \|\boldsymbol{x} - (\boldsymbol{x} \cdot \mathbf{1})\boldsymbol{\alpha}\|_\infty \leq s \right\}. \tag{6.11}$$

We claim that Ω_N satisfies the requirements of Minkovski's Theorem and in particular that Ω_N is compact and $\mathrm{Vol}_N(\Omega_N) = 2^N$.The fact the Ω_N is convex, compact and symmetric with respect to the origin is clear by construction, hence we only need to compute the volume of Ω_N.

We start by analysing the construction of Ω_N.

- The first condition in (6.11), $\boldsymbol{x} \cdot \mathbf{1} = a \in [-Q, +Q]$, describes the union of the hyperplanes $H_{N-1}(a) := \frac{a}{N}\mathbf{1} + \mathbf{1}^\perp = a\boldsymbol{\alpha} + \mathbf{1}^\perp$ for $|a| \leq Q$.

- The second condition in (6.11) alone with $(\boldsymbol{x} \cdot \mathbf{1})$ replaced by a reads as $\|\boldsymbol{x} - a\boldsymbol{\alpha}\|_\infty \leq s$ and describes the points of the cube $C_N(a) = a\boldsymbol{\alpha} + [-s, +s]^N$.

For any fixed $a \in [-Q, +Q]$ these two conditions together describe the central section of the cube $C_N(a)$ orthogonal to the main diagonal of direction $\mathbf{1}$. Hence Ω_N can be seen as the union of the sections $C_N(a) \cap H_{N-1}(a)$ for $a \in [-Q, +Q]$ and

$$\begin{aligned}
\Omega_N &= \{\boldsymbol{x} \in \mathbb{R}^N : \|\boldsymbol{x} - (\boldsymbol{x} \cdot a\mathbf{1})\boldsymbol{\alpha}\| \leq s\} \cap \bigcup_{a \in [-Q, +Q]} C_N(a) \\
&= \bigcup_{a \in [-Q, +Q]} C_N(a) \cap H_{N-1}(a) \\
&= \bigcup_{a \in [-Q, +Q]} a\boldsymbol{\alpha} + \left([-s, +s]^N \cap \mathbf{1}^\perp\right).
\end{aligned}$$

Namely Ω_N is a prism of bases $\left([-s, +s]^N \cap \mathbf{1}^\perp\right) \pm Q\boldsymbol{\alpha}$ and height given by the distance between the two planes $\boldsymbol{x} \cdot \mathbf{1} = \pm Q$, i.e. $\|Q\mathbf{1} - (-Q\mathbf{1})\|_2 = 2Q\sqrt{N}$. Thus, the $N-$dimensional volume of Ω_N is

$$\mathrm{Vol}_N \Omega_N = 2Q\sqrt{N} \cdot \mathrm{Vol}_{N-1}\left([-s, +s]^N \cap \mathbf{1}^\perp\right).$$

Since $\left([-s, +s]^N \cap \mathbf{1}^\perp\right) = 2s([-1/2, +1/2]^N \cap \mathbf{1}^\perp)$ the $N - 1$ volume of the section is A_N

scaled by $(2s)^{N-1}$

$$\begin{aligned}\mathrm{Vol}_{N-1}\left([-s,+s]^N \cap \mathbf{1}^\perp\right) &= (2s)^{N-1}A_N \\ &= \frac{2^{N-1}}{\sqrt{N}Q}.\end{aligned}$$

and finally

$$\mathrm{Vol}_N\Omega_N = 2Q\sqrt{N}\cdot\frac{2^{N-1}}{\sqrt{N}Q} = 2^N.$$

By Minkovski's Thereom there exists an integer point $\boldsymbol{n} \in \Omega_N \setminus \{\mathbf{0}\}$. Notice that by symmetry of Ω_N we can choose $\boldsymbol{n}$ such that $\boldsymbol{n}\cdot\mathbf{1} = q > 0$. The second inequality in (6.11) with $\boldsymbol{x} = \boldsymbol{n}$ reads then as (6.10). □

Remark 6.5.7. Calculating and estimating the volumes of sections, slabs and slices of the N dimensional cube are well studied problems, we refer the interested reader to [CL91; Zon06; Ber10; FR12] and references therein. The $N-1$ volume of the central section of the N-dimensional cube with respect to the main diagonal can be computed by either of the following (see [CL91])

$$\begin{aligned}A_N &= \frac{\sqrt{N}}{(N-1)!}\sum_{j=0}^{\lfloor N/2\rfloor}(-1)^j\binom{N}{j}\left(\frac{N}{2}-j\right)^{N-1} \\ &= \frac{\sqrt{N}}{\pi}\int_{-\infty}^{+\infty}\left(\frac{\sin t}{t}\right)^N dt.\end{aligned}$$

It is known that in general the volume of sections of the unit cube with respect to subspaces are bounded from below by 1 with equality given by coordinate subspaces (for the hyperplane see Hadwinger [Had72] and Hensley [Hen79], and for the generic subspace case see Vaaler [Vaa79]), moreover it was conjectured in [Hen79] and proved by Ball [Bal86] that the upper bound for the hyperplane case is $\sqrt{2}$ with equality holding for the so called suspension of the diagonal section, c.f. [Ber10]. Thus $1 < A_N \leq \sqrt{2}$, with the latter equality holding only for $N = 2$. In [CL91] it is reported that both Laplace [Lap95] and Polya [Pol13] proved the following limit

$$\lim_{N\to\infty} A_N = \sqrt{\frac{6}{\pi}}.$$

We present an algorithm for finding $\boldsymbol{n}$ satisfying (6.10) and consequently a vector of lengths $\widetilde{\boldsymbol{\ell}}$ with the properties claimed by the previous corollary. In the rest of the section let $[\cdot] : \mathbb{R} \to \mathbb{Z}$ denote the rounding function to the nearest integer,

$$[x] = \begin{cases} \lceil x\rceil & \text{if } |x| - \lfloor x\rfloor \geq 1/2 \\ \lfloor x\rfloor & \text{if } |x| - \lfloor x\rfloor < 1/2. \end{cases}$$

The extension $[\cdot] : \mathbb{R}^N \to \mathbb{Z}^N$ is element-wise, i.e. $[\boldsymbol{v}]_i = [v_i]$.

Algorithm 3: Search by adjustments.

Data: $\boldsymbol{\alpha} \in \mathbb{R}^N : \boldsymbol{\alpha} \cdot 1 = 1, Q \in \mathbb{N}$

Result: $\boldsymbol{n} \in \mathbb{Z}^N$: estimate (6.10) holds

$N_{\min} := 1$
for $1 \leq q \leq Q$**do**
  $\widetilde{\boldsymbol{n}} := [q\,\boldsymbol{\alpha}]$
  while $\widetilde{\boldsymbol{n}} \cdot \mathbf{1} > q$ **do**
    $M := \arg\max_i(\widetilde{n}_i - q\alpha_i)$
    $\widetilde{n}_M := \widetilde{n}_M - 1$
  end
  while $\widetilde{\boldsymbol{n}} \cdot \mathbf{1} < q$ **do**
    $m := \arg\min_i(\widetilde{n}_i - q\alpha_i)$
    $\widetilde{n}_m := \widetilde{n}_m + 1$
  end
  if $\|\widetilde{\boldsymbol{n}} - q\boldsymbol{\alpha}\|_\infty < N_{\min}$ **then**
    $\mathrm{N}_{\min} := \|\widetilde{\boldsymbol{n}} - q\boldsymbol{\alpha}\|_\infty$
    $\boldsymbol{n} := \widetilde{\boldsymbol{n}}$
  end
end

We make some general observation regarding Algorithm 3. The Algorithm 3 computes for each q a unique integer point $\widetilde{\boldsymbol{n}}(q)$. The point $\boldsymbol{n}$ is then chosen to be the $\widetilde{\boldsymbol{n}}(q)$ which minimizes $\|\widetilde{\boldsymbol{n}}(q) - q\boldsymbol{\alpha}\|$ over all positive integers $q \leq Q$.

Assume that for a certain q we have $[q\boldsymbol{\alpha}] \cdot \mathbf{1} > q$. Because $|\,[q\alpha_i] - q\alpha_i| \leq 1/2$ hence $|\,[q\boldsymbol{\alpha}] \cdot \mathbf{1} - q| \leq N/2$, then the first while cycle is computed up to $\lfloor N/2 \rfloor$ times and generates just as many indices M_is. It easy to see that the M_is are all distinct since $|\widetilde{n}_{M_i} - q\alpha_{M_i}| \geq 1/2$, while for any other index $j \notin \{M_i\}$ —which exist because $\sharp\{M_i\} \leq N/2$— we have $|\widetilde{n}_j - q\alpha_j| \leq 1/2$. At the end of the day, if $[q\boldsymbol{\alpha}] \cdot \mathbf{1} > q$ then $1/2 \leq \|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}(q)\|_\infty \leq 3/2$, and a similar argument can be carried out for the opposite inequality leading to the same conclusion. Thus the outcomes of Algorithm 3 can be divided into the following two cases:

1. $\exists q \leq Q$ such that $[q\boldsymbol{\alpha}] \cdot \mathbf{1} = q$, then $\boldsymbol{n} = [q\boldsymbol{\alpha}]$ and $\|q\boldsymbol{\alpha} - \boldsymbol{n}\|_\infty \leq 1/2$.

2. $\forall q \leq Q$ we have $[q\boldsymbol{\alpha}] \cdot \mathbf{1} \neq q$, then for $q = \boldsymbol{n} \cdot \mathbf{1}$, $3/2 \geq \|q\boldsymbol{\alpha} - \boldsymbol{n}\|_\infty \geq 1/2$.

It is clear that in the first case the resulting $\boldsymbol{n}$ is optimal. This is less obvious for case 2. and it needs to be proved. We anticipate that Case 2. may occur if Q is chosen relatively small with respect to N, but we discuss this in more details after the proof.

Theorem 6.5.8. *Under the assumptions of the constrained SDAP (Problem 6.5.4) the result of Algorithm 3 provides a solution $\boldsymbol{n}$ which consequently satisfies the estimate* (6.10). *Moreover $\boldsymbol{n}$ minimizes $q = \boldsymbol{n} \cdot \mathbf{1}$.*

Proof. Let q be fixed and such that $[q\boldsymbol{\alpha}] \cdot \mathbf{1} \neq q$. Let $\widetilde{\boldsymbol{n}} = \widetilde{\boldsymbol{n}}(q)$ and assume $\widetilde{\boldsymbol{n}}'$ is an integer point $\widetilde{\boldsymbol{n}}' \neq \widetilde{\boldsymbol{n}}$ such that $\widetilde{\boldsymbol{n}}' \cdot \mathbf{1} = q$ and

$$\|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}'\|_\infty < \|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}\|_\infty. \tag{6.12}$$

Without loss of generality assume $[q\boldsymbol{\alpha}] \cdot \mathbf{1} > q$ (the argument works similarly for the opposite inequality). Let $\{M_i\}_{i=1}^k$ with $k \leq \lfloor N/2 \rfloor$ as in the above discussion. We already know

$\widetilde{n}_{M_i} = [q\alpha_{M_i}] - 1$ for all M_i, while $\widetilde{n}_j = [q\alpha_j]$ for $j \notin \{M_i\}$, moreover

$$\begin{aligned}\|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}\|_\infty &= \max_i (q\alpha_i - \widetilde{n}_i) \\ &= q\alpha_{M_k} - \widetilde{n}_{M_k} \leq q\alpha_i - (\widetilde{n}_i - 1) \qquad \forall i.\end{aligned}$$

Since $\widetilde{\boldsymbol{n}} - \widetilde{\boldsymbol{n}}' \neq \mathbf{0}$ is a zero sum vector in $\mathbb{Z}^N$, then $\exists i, \widetilde{n}_i - \widetilde{n}'_i \geq 1$ and therefore

$$\begin{aligned}\|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}\|_\infty &= q\alpha_{M_k} - \widetilde{n}_{M_k} \\ &\leq q\alpha_i - (\widetilde{n}_i - 1) \\ &\leq q\alpha_i - \widetilde{n}'_i \\ &\leq \|q\boldsymbol{\alpha} - \widetilde{\boldsymbol{n}}'\|_\infty,\end{aligned}$$

which leads to a contradiction with (6.12). □

Let us proceed now with the proof of Theorem 6.5.1:

Proof of Theorem 6.5.1. Apply Theorem 6.5.5 to $\boldsymbol{\alpha} = \boldsymbol{\ell}/\mathcal{L}$. Then together with the discussion after Algorithm 3 we infer the existence of $\boldsymbol{n} \in \mathbb{Z}^{|E|}$ such that

$$\min_{1 \leq q \leq Q} \min_{\langle \boldsymbol{n}, \mathbf{1}\rangle = q} \left\| \boldsymbol{\ell} - \frac{\boldsymbol{n}}{\langle \boldsymbol{n}, \mathbf{1}\rangle} \right\|.$$

Moreover, the graph $\widetilde{\mathcal{G}}(G, \boldsymbol{n}\langle \boldsymbol{n}, \mathbf{1}\rangle)$ corresponding minimizer necessarily satisfies

$$\operatorname{dist}(\mathcal{G}, \widetilde{\mathcal{G}}) \leq \min\left\{ \frac{3}{2Q}, \frac{1}{q}\left(\frac{\sqrt{N}A_N}{Q}\right)^{\frac{1}{N-1}} \right\}.$$

□

Remark 6.5.9. If the coefficient of right hand side of (6.10) is strictly smaller than $1/2$, then we can speed up the algorithm by discarding to check all q such that $[q\,\boldsymbol{\alpha}] \cdot \mathbf{1} \neq q$ because according to the discussion following Algorithm 3 they would lead to $\widetilde{\boldsymbol{n}}(q)$ which fail to be a candidate for $\boldsymbol{n}$. This condition is satisfied if Q is chosen sufficiently large, namely $Q \geq (\sqrt{N}/A_N)2^{N-1}$ or in alternative, using the same estimates as in Corollary 6.5.1, if

$$Q \geq 2^{3(N-1)/2}. \tag{6.13}$$

Therefore, under condition (6.13) Algorithm 4 finds the same solution $\boldsymbol{n}$ as Algorithm 3.

Algorithm 4: Lazy search.

Data: $\boldsymbol{\alpha} \in \mathbb{R}^N : \boldsymbol{\alpha} \cdot \mathbf{1} = 1, Q \in \mathbb{N} :$ (6.13) is satisfied
Result: $\boldsymbol{n} \in \mathbb{Z}^N :$ estimate (6.10) holds

$N_{\min} := 1$
for $1 \leq q \leq Q$**do**
  $\widetilde{\boldsymbol{n}} := [q\,\boldsymbol{\alpha}]$
  if ($\widetilde{\boldsymbol{n}} \cdot \mathbf{1} = q$ **and** $\|\widetilde{\boldsymbol{n}} - q\boldsymbol{\alpha}\|_\infty < N_{\min}$) **then**
    $\boldsymbol{n} := \widetilde{\boldsymbol{n}}$
    $\mathrm{N}_{\min} := \|\boldsymbol{n} - q\boldsymbol{\alpha}\|_\infty$
  end
end

6.6 Algorithm and Applications

Recall that by Theorem 6.2.2 given two graphs $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ and $\widetilde{\mathcal{G}} = \mathcal{G}(G, \widetilde{\boldsymbol{\ell}})$ with $\mathrm{sum}(\boldsymbol{\ell}) = \mathrm{sum}(\widetilde{\boldsymbol{\ell}})$, then

$$\text{rel err}(\lambda_k) := \left| \frac{\lambda_k(\mathcal{G}) - \lambda_k(\widetilde{\mathcal{G}})}{\lambda_k(\mathcal{G})} \right| \leq \max\{8, 2(2\beta + |N| - 1)^2\} \max_{e \in E} \frac{|\ell_e - \widetilde{\ell}_e|}{\min\{\ell_e, \widetilde{\ell}_e\}} \tag{6.14}$$

where β is the Betti number of G, $|N|$ is the number of pendants, i.e. vertices of degree 1.

Algorithm 5: Approximation of metric graphs by adjustments.

Data: $\boldsymbol{\ell} \in \mathbb{R}^{|E|}_{>0} : \langle \boldsymbol{\ell}, \mathbf{1} \rangle = 1, \epsilon_{\text{tol}} > 0, |N|$ the number of vertices of degree 1 and Betti number $\beta > 0$
Result: $n \in \mathbb{N}^{|E|}, q = \sum_{i=1}^{|E|} n_i$ satisfying (6.14) with $\widetilde{\ell}_i = n_i/q$

$N_{\min} := 1$
$\boldsymbol{n} := \mathbf{1}$
$Q = |E|$
$\widetilde{\boldsymbol{\ell}} = 1/Q \cdot \mathbf{1}$
while (6.14) *is not satisfied* **do**
  $\widetilde{\boldsymbol{n}} = \mathtt{round}.(Q\boldsymbol{\ell})$
  while $\langle \widetilde{n}, \mathbf{1} \rangle > Q$ **do**
    $M := \arg\max_i(\widetilde{n}_i - Q\ell_i)$
    $\widetilde{n}_M := \widetilde{n}_M - 1$
  end
  while $\langle \widetilde{n}, \mathbf{1} \rangle < Q$ **do**
    $m := \arg\min_i(\widetilde{n}_i - Q\ell_i)$
    $\widetilde{n}_m := \widetilde{n}_m + 1$
  end
  if $\|\widetilde{\boldsymbol{n}} - Q\widetilde{\boldsymbol{\ell}}\|_\infty < N_{min}$ **then**
    $N_{\min} := \|\widetilde{\boldsymbol{n}} - Q\widetilde{\boldsymbol{\ell}}\|_\infty$
    $\boldsymbol{n} := \widetilde{\boldsymbol{n}}$
    $q = Q$
  end
  Q:=Q+1
end

By Remark 6.5.9 if the problems requires a very large number of splittings we do not need to check the condition that the corresponding lengths of the rounding procedure preserve the total length and we suggest the following algorithm that in that case uses a simplified procedure analogue as in Algorithm 4.

Algorithm 6: Optimized Adjustments

Data: $\boldsymbol{\ell} \in \mathbb{R}^{|E|}_{>0} : \langle \boldsymbol{\ell}, \mathbf{1} \rangle = 1, \epsilon_{\text{tol}} > 0$, $|N|$ the number of vertices of degree 1 and Betti number $\beta > 0$

Result: $n \in \mathbb{N}^{|E|}, q = \sum_{i=1}^{|E|} n_i$ satisfying (6.14) with $\widetilde{\ell}_i = n_i/q$

$C = 2\beta + |N| - 1$

$Q := \left\lceil \frac{3}{2 \min_e \ell_e} \left(\frac{C+\epsilon_{\text{tol}}}{\epsilon_{\text{tol}}} \right) \right\rceil$

if $Q < 2^{3(|E|-1)/2}$ **then**

  Proceed to Algorithm 5.

end

else

  $N_{\min} := 1$

  $\boldsymbol{n} := \mathbf{1}$

  $Q = |E|$

  $\widetilde{\boldsymbol{\ell}} = 1/Q \cdot \mathbf{1}$

  while (6.14) *is not satisfied* **do**

    $\widetilde{\boldsymbol{n}} := \texttt{round.}(Q\boldsymbol{\ell})$

    if ($\langle \widetilde{\boldsymbol{n}}, \mathbf{1} \rangle = Q$ **and** $\|\widetilde{\boldsymbol{n}} - Q\boldsymbol{\ell}\|_\infty < N_{\min}$) **then**

      $q = Q$

      $\boldsymbol{n} := \widetilde{\boldsymbol{n}}$

      $\mathrm{N}_{\min} := \|\boldsymbol{n} - q\boldsymbol{\ell}\|_\infty$

    end

    Q:=Q+1

  end

end

6.6.1 Star graph

Given an integer number d, suppose $\mathcal{S}^d$ is a d-star with edge lengths $\boldsymbol{\ell} = (\ell_1, \ldots, \ell_d)$ (c.f. Figure 6.3 with $d = 3$).

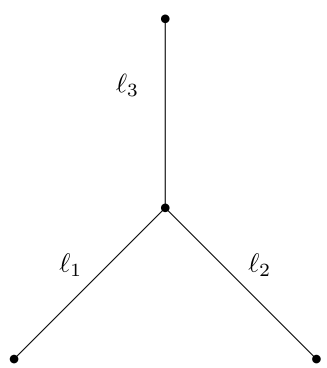


Figure 6.3: Three star with different lengths.

The set of eigenvalues of $\mathcal{S}^d$ counted with their multiplicities is given by the zeros of the following secular equation.

$$\left(\sum_{i=1}^{d} \tan(k\ell_i) \right) \prod_{i=1}^{d} \cos(k\ell_i) = 0,$$

see for instance [BK13, Example 2.1.12].

Consider the following example:

Example 6.6.1. Consider the three-star $\mathcal{S}^3$ with length vector

$$\boldsymbol{\ell} = (1.2, 2.399, 2.401),$$

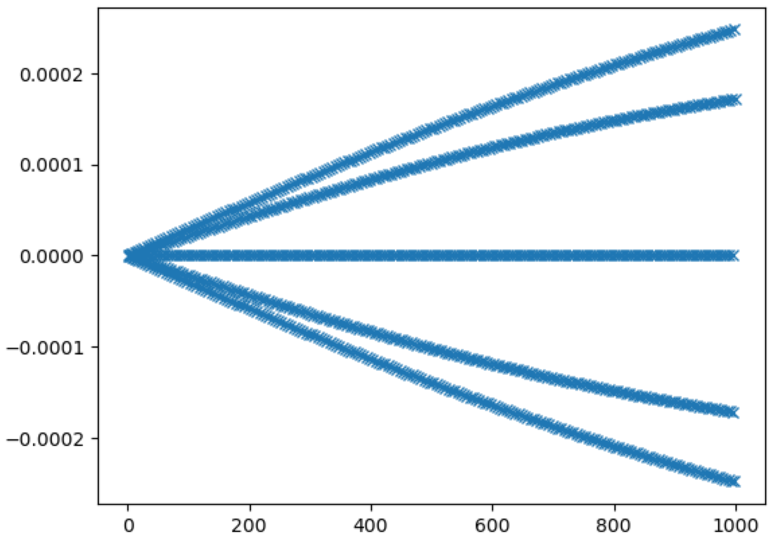


Figure 6.4: Plot of relative error for the three-star. An exemplary computation of the eigenvalues of the three star using Algorithm 5 (which coincides with Algorithm 6) in this case. Given an error tolerance of `0.01` we have the plot associated to the relative error for the first 1000 eigenvalues.

then applying Algorithm 6 (after norming the vector) with error tolerance of $\epsilon_{\text{tol}} = 0.01$, we can assert that the graph with length vector

$$\widetilde{\boldsymbol{\ell}} = (1.2, 2.4, 2.4)$$

satisfies

$$\text{rel err}(\lambda_n) \leq 8\frac{\|\boldsymbol{\ell} - \widetilde{\boldsymbol{\ell}}\|}{\ell_{\min}} \approx 0.0067 \leq \epsilon_{\text{tol}}$$

for all $n \in \mathbb{N}$. As one can see in Figure 6.4 the relative error is in this case much better in reality. The plots in Figure 6.4 show also how accurate the approximation is in this particular case. The advantage of computing the eigenvalues via approximation is that the equilateral representative of the graph associated with the length vector $\widetilde{\boldsymbol{\ell}}$ consists of only five edges whereas the equilateral representative of the original graph requires 6000 edges. This simplifies the computations significantly.

6.6.2 Lasso graph

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be the lasso graph (c.f. Figure 6.5) with

$$e_1 = [x_1, x_2] = [0, \ell_1], \qquad e_2 = [x_3, x_4] = [-\ell_2/2, +\ell_2/2]$$
$$x_2 \sim x_3 \sim x_4$$
$$\mathcal{G} = e_1 \oplus e_2 / \sim$$
$$V = \{v_1 = \{x_1\}, v_2 = \{x_2, x_3, x_4\}\}$$

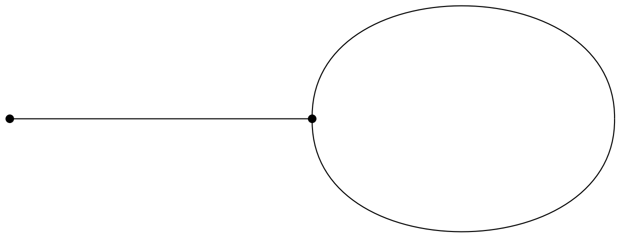


Figure 6.5: Lasso graph.

Using a decomposition in symmetric and antisymmetric eigenfunctions we have

$$\begin{aligned} u_1 &= u_1^a + u_1^s = a_1 \sin(kx) + b_1 \cos(kx) \\ u_2 &= u_2^a + u_2^s = a_2 \sin(kx) + b_2 \cos(kx) \,. \end{aligned}$$

Then due to symmetry in the graph it suffices to study the eigenvalues corresponding to the symmetric and antisymmetric projections:

$$\begin{aligned} u_1^a &= 0 \\ u_2^a &= a_2 \sin(kx) \end{aligned}$$

the latter of which satisfies the continuity condition at the vertex v_2 if and only if $u_2(-\ell_2/2) = u_2(+\ell_2/2) = 0$ i.e. $k = 2\pi m/\ell_2,\ m \in \mathbb{N}$.

Concerning the symmetric component u^s, after taking into account the conditions at v_1, we have

$$\begin{aligned} u_1^s &= b_1 \cos(kx) \\ u_2^s &= b_2 \cos(kx) \end{aligned}$$

the standard vertex conditions at v_2 for the function u^s read as follow

$$b_1 \cos(k\ell_1) = b_2 \cos\left(\pm k\frac{\ell_2}{2}\right)$$

and

$$kb_1 \sin(k\ell_1) + 2kb_2 \sin\left(k\frac{\ell_2}{2}\right) = 0$$

which can be combined together to obtain the following secular equation for eigenvalues associated to symmetric eigenfunctions

$$\sin(k\ell_1)\cos\left(k\frac{\ell_2}{2}\right) + 2\sin\left(k\frac{\ell_2}{2}\right)\cos(k\ell_1) = 0,$$

which is a trascendental equation.

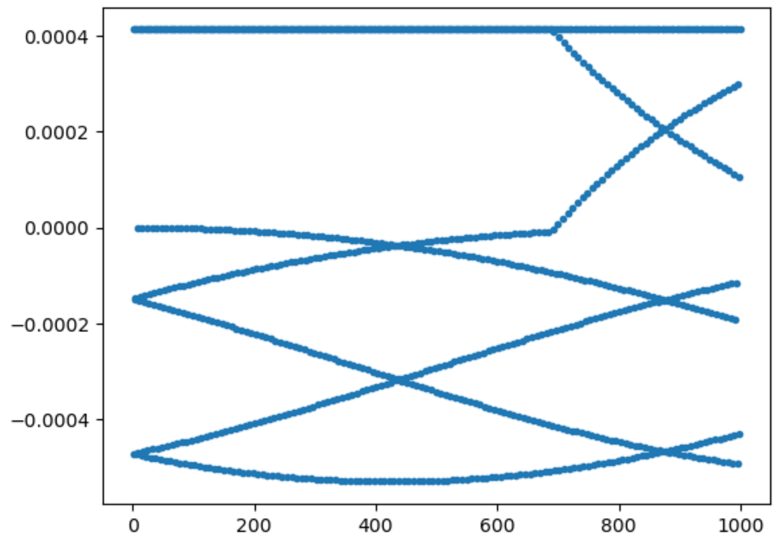


Figure 6.6: Plot for relative error for a lasso graph. An exemplary computation of the eigenvalues of the lasso graph using Algorithm 5 (which coincides with Algorithm 6) in this case. Given an error tolerance of `0.01` we present the relative error for the first 1000 eigenvalues.

Consider the following example:

Example 6.6.2. Consider the lasso graph $\mathcal{G} = \mathcal{G}(G, \boldsymbol{\ell})$ with length vector

$$\boldsymbol{\ell} = (1.199, 3.601),$$

then applying Algorithm 6 (after norming the vector) with error tolerance of $\epsilon_{\text{tol}} = 0.01$, we can assert that the graph with length vector

$$\widetilde{\boldsymbol{\ell}} = (1.2, 3.6)$$

after normalization satisfies

$$\text{rel err}(\lambda_n) \leq 8 \frac{\|\boldsymbol{\ell} - \widetilde{\boldsymbol{\ell}}\|}{\ell_{\text{min}}} \approx 0.0067 \leq \epsilon_{\text{tol}}$$

for all $n \in \mathbb{N}$. As in Example 6.6.1 one can see in Figure 6.6 the relative error is in this case much better in reality. The plots in Figure 6.6 show also how accurate the approximation is in this particular case. The advantage of computing the eigenvalues via approximation is that the equilateral representative of the graph associated with the length vector $\widetilde{\boldsymbol{\ell}}$ consists of only 4 edges whereas the equilateral representative of the original graph requires 4800 edges. This simplifies the computations significantly.

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