



Fluids, graphs and Fourier transform : three incarnations of the laplacian

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présentée par

Guillaume LÉVY

Fluides, graphes et transformée de Fourier : trois incarnations du laplacien

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Fluides, graphes et transformée de Fourier : trois incarnations du laplacien.

Guillaume Lévy

À ma famille, à mes amis.

Merci de vous être tenus à mes côtés.

Cet accomplissement est aussi le vôtre.

Fluides, graphes et transformée de Fourier : trois incarnations du laplacien.

Résumé. Cette thèse est consacrée à l'étude de propriétés du laplacien dans trois contextes bien distincts. Dans une première partie, celui-ci nous sera utile pour régulariser des solutions d'équations venues de la mécanique des fluides incompressibles. En application, on montrera un théorème dans la lignée des résultats de J. Serrin et de ses continuateurs. Dans une deuxième partie, le laplacien est vu comme le pendant stationnaire de l'opérateur des ondes sur un graphe, dont les modes et fréquences propres déterminent la propagation de perturbations sur le graphe. On y explore et démêle les liens entre la topologie du graphe, sa forme et sa première fréquence propre non nulle. Dans une dernière partie, le laplacien est pensé comme un opérateur linéaire à diagonaliser dans une base adaptée, objectif dont l'accomplissement est intimement lié à la transformée de Fourier. Deux difficultés majeures apparaissent ici : la non commutativité des groupes auxquels nous nous intéressons d'une part, l'apparition d'une limite singulière de la transformée de Fourier d'autre part.

Mots-clés. Fluides incompressibles, fonctions propres, graphes quantiques, groupes nilpotents, laplacien, Navier-Stokes, optimisation de formes, représentations unitaires irréductibles, théorème de Serrin, transformée de Fourier.

Fluids, graphs and the Fourier transform : three incarnations of the laplacian.

Abstract. This thesis is devoted to the study of the laplacian properties in three fully distinct contexts. In a first part, it will be used to smooth solutions of equations coming from incompressible fluid mechanics. As an application, we will show a result in the spirit of J. Serrin and his continuators' theorem. In a second part, the laplacien is seen as the stationary counterpart of the wave operator on a graph, whose eigenmodes and eigenfrequencies determine the propagation of perturbations on the graph. We explore and disentangle the ties between the graph's topology, its shape and its first nonzero eigenfrequency. In the last part, the laplacian is thought of as a linear operator which we wish to diagonalize in an appropriate basis, a goal which is intimately tied to the Fourier transform. Two major difficulties appear in our context : the noncommutativity of the groups of interest on the one hand, the appearance of a singular limit in the Fourier transform on the other hand.

Keywords. Eigenfunctions, Fourier transform, incompressible fluids, laplacian, Navier-Stokes, nilpotent groups, quantum graphs, Serrin theorem, shape optimization, unitary irreducible representations.

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1. Oui, je sais, il faut absolument que je rencontre ce 'Nico'. Un jour. :)

2. Six et deux font dix, scopa !

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Introduction générale

Cette thèse est composée de trois parties qui, bien que très différentes par les problèmes posés et les méthodes de résolutions employées, sont unies par un objet commun, un trait d'union entre plusieurs domaines distincts : le laplacien. L'ubiquité de cet opérateur et la multiplicité de ses visages ne sont plus à démontrer ; citons entre autres son lien avec la courbure d'une variété en géométrie (où il est connu sous le nom d'opérateur de Laplace-Beltrami), celui entre son spectre et le comportement en temps long de solutions d'équations emblématiques (ainsi en est-il de l'équation de la chaleur, des ondes ou de Schrödinger), son interprétation en tant qu'opérateur de diffusion en physique ou encore le rôle qu'il a joué, visible dans le nom, dans la définition des solutions de viscosité des équations d'Hamilton-Jacobi.

La première partie de ce manuscrit s'appuie sur la Note aux Comptes Rendus [27] publiée en 2016, son prolongement dans l'article accepté [28] ainsi que l'article [29], soumis. Le laplacien joue ici le rôle d'opérateur régularisant, dont la présence permet de gagner en intégrabilité dans un premier temps, puis en régularité. C'est par son truchement qu'une hypothèse de régularité modérée sur une solution faible de l'équation de Navier-Stokes est transformée, à la fin de la preuve, en la lissité de cette solution, en suivant en cela l'idée du théorème de Serrin.

La deuxième partie repose sur l'article soumis [41] en collaboration avec R. Band, du Technion. Elle est consacrée à l'étude de la première valeur propre du laplacien sur un graphe continu et à son extrémisation sous une contrainte de volume analogue à celle imposée dans les inégalités de Faber-Krahn ou de Szegő-Weinberger. Dans ce cadre, en raison de la compacité de l'ensemble des formes admissibles, le problème admet à la fois un minimum et un maximum, là où l'inégalité de Faber-Krahn fait apparaître un minimum sans maximum et inversement pour l'inégalité de Szegő-Weinberger.

Dans la troisième et dernière partie, non encore soumise, nous reprenons les travaux de H. Bahouri, J.-Y. Chemin et R. Danchin [86] sur les groupes de Heisenberg et les généralisons à une famille de groupes de Lie dont ceux de Heisenberg forment un cas particulier. La motivation principale de ces deux travaux est de disposer d'une théorie de Fourier sur ces groupes aussi analogue que possible à celle que l'on connaît sur les groupes commutatifs localement compacts, dont font partie le tore et l'espace euclidien usuel. Il existe déjà une théorie de Fourier générale sur des groupes non nécessairement commutatifs, nettement plus complexe que son homologue commutative. Il est possible, à titre d'exemple, de prouver des inégalités de Hardy ou de Strichartz sur de tels groupes, au prix toutefois de méthodes sensiblement plus élaborées que dans le cas de l'espace entier. Disposer d'une réécriture plus familière de la théorie de Fourier permettrait de reprouver ces inégalités nettement plus aisément en adaptant les preuves connues dans le cas de l'espace. L'analyse harmonique et l'étude des équations aux dérivées partielles sur de tels groupes s'en trouverait grandement facilitée.

1 Mécanique des fluides incompressibles

Cette partie de la thèse se décompose en deux sous-parties, la première servant d'appui à la seconde. On commence par démontrer des résultats d'unicité pour des équations de transport-diffusion proches, dans leur écriture, de l'équation sur la vorticité de Navier-Stokes. On s'inspire pour cela des idées de la théorie de R. J. DiPerna et J.-L. Lions, en étendant leurs résultats à des équations dans lesquelles apparaît un laplacien. On se sert ensuite de ces résultats pour prouver des théorèmes dans l'esprit du résultat de J. Serrin [32], qui assurent la lissité d'une solution faible de Navier-Stokes sous des hypothèses de régularité critique.

1.1 Équations de Navier-Stokes-Euler homogènes incompressibles

1.1.1 Les équations

On s'intéresse dans cette partie de la thèse aux équations régissant le mouvement d'un fluide incompressible homogène, possiblement visqueux et « emplissant l'espace », pour reprendre l'expression de J. Leray dans son célèbre article de 1934 [25]. L'espace dont il est question sera, selon le cas, l'espace physique $\mathbb{R}^3$ ou son analogue compact, le tore $\mathbb{T}^3$. Lorsqu'on voudra parler indifféremment des deux possibilités, nous emploierons la notation $\mathbb{X}$ ou $\mathbb{X}^3$. Certains de nos résultats s'appliquant aussi bien aux équations de Navier-Stokes et d'Euler homogènes incompressibles, nous faisons le choix de confondre en un unique nom les deux équations en laissant libre le paramètre de viscosité, qui sera noté ν . En notant $u = (u^1, u^2, u^3)$ le champ de vitesses du fluide, u_0 un champ de vitesses initial et p le champ de pression, l'équation de Navier-Stokes-Euler s'écrit

$$(NSE) \begin{cases} \partial_t u(t, x) + \nabla \cdot (u \otimes u)(t, x) - \nu \Delta u(t, x) = -\nabla p(t, x), & t \geq 0, x \in \mathbb{X}^3, \\ \operatorname{div} u \equiv 0, \\ u(0, x) = u_0(x). \end{cases}$$

On a noté ici

$$\operatorname{div} u(t, x) := \sum_{j=1}^3 \partial_j u^j(t, x)$$

la divergence du champ u ,

$$\nabla \cdot (u \otimes u)(t, x) := \sum_{j=1}^3 \partial_j (u u^j)(t, x)$$

le terme d'advection et

$$\Delta u(t, x) := \sum_{j=1}^3 \partial_j^2 u(t, x)$$

le laplacien du champ u . Le terme d'advection rend compte de transport du champ de vitesses par lui-même au cours du temps; si l'on suit une particule fictive portée par le champ u au cours du temps et que l'on note $x(t)$ sa position dans l'espace au temps $t \geq 0$, son accélération à $t > 0$ vaut

$$\frac{d}{dt}(u(t, x(t))) = \partial_t u(t, x(t)) + \frac{dx}{dt}(t) \cdot \nabla u(t, x(t)) = \partial_t u(t, x(t)) + u(t, x(t)) \cdot \nabla u(t, x(t)).$$

On établit alors l'équation de Navier-Stokes-Euler en appliquant la seconde loi de Newton à cette particule fictive en supposant qu'elle ne subit que deux types de forces : celles dues à la viscosité, modélisées par le laplacien et dont l'intensité est proportionnelle au coefficient de viscosité du fluide ν et les forces de pression, qui sont créées par la contrainte d'incompressibilité et apparaissent

mathématiquement comme un multiplicateur de Lagrange associé à la contrainte d'incompressibilité (ou de préservation du volume), qui se traduit par la nullité de la divergence du champ de vitesses.

On retrouve bien entendu les équations de Navier-Stokes si ν est strictement positive et d'Euler si ν est nulle. La présence de deux inconnues (u et p), de deux équations indépendantes (l'équation principale et la contrainte d'incompressibilité), d'une donnée initiale (u_0) et l'absence de bord (que $\mathbb{X}$ soit $\mathbb{R}$ ou $\mathbb{T}$) permet d'espérer, au moins heuristiquement, que la résolution du système (NSE) soit une question qui ait un sens. On peut également éliminer la pression en appliquant le projecteur de Leray $\mathbb{P}$ sur les champs de vecteurs à divergence nulle à la première équation. On obtient ainsi une version alternative de (NSE) , que l'on notera $(\mathbb{P}NSE)$.

$$(\mathbb{P}NSE) \begin{cases} \partial_t u(t, x) + \mathbb{P} \nabla \cdot (u \otimes u)(t, x) - \nu \Delta u(t, x) = 0, & t \geq 0, x \in \mathbb{X}^3, \\ \operatorname{div} u \equiv 0, \\ u(0, x) = u_0(x). \end{cases}$$

On rappelle que le projecteur de Leray est défini par la formule

$$\mathbb{P} := \operatorname{Id} - \nabla \operatorname{div} \Delta^{-1}.$$

De manière équivalente, le symbole de $\mathbb{P}$ est

$$\widehat{\mathbb{P}}(\xi) = 1 - \frac{\xi \otimes \xi}{|\xi|^2} \quad \text{pour } \xi \in \mathbb{R}^3 \setminus \{0\} \text{ ou } \mathbb{Z}^3 \setminus \{0\}.$$

Dans l'heuristique précédente, on a volontairement omis les (nombreuses) discussions entourant les espaces dans lesquels on peut choisir u_0 , dans lesquels on peut résoudre le système (NSE) ou quel(s) type(s) de solution(s) seront considéré(s) comme admissibles.

1.1.2 Invariances

Il est fréquent que des équations venues de la physique possèdent des propriétés algébriques particulières, dont l'invariance d'échelle fait partie. Étant donnée une fonction u dépendant de l'espace et du temps et un réel λ strictement positif, on définit u_λ par

$$u_\lambda(t, x) := \lambda^a u(\lambda^b t, \lambda^c x),$$

où a, b, c sont trois paramètres réels. Une équation est dite posséder une invariance d'échelle (pour les paramètres réels a, b, c) si l'affirmation

$$u \text{ est solution de l'équation} \implies \forall \lambda > 0, u_\lambda \text{ est aussi solution de l'équation}$$

est vraie. Notons que cette définition est homogène en le triplet (a, b, c) ; en effet, pour tout réel α , le changement de paramètre $\lambda \leftarrow \lambda^\alpha$ montre que l'équation possède aussi une invariance d'échelle pour le triplet $(\alpha a, \alpha b, \alpha c)$. Dans le cas de l'équation de Navier-Stokes-Euler, l'équilibre entre le terme de dérivée en temps et le terme d'advection implique la relation $b = a + c$. Si de plus la viscosité ν est non nulle, l'équilibre entre le terme de dérivée en temps et le laplacien livre la deuxième relation $b = 2c$. Ainsi, l'équation de Navier-Stokes ne possède qu'une seule invariance d'échelle à homogénéité près, représentée par le triplet $(1, 2, 1)$. À l'inverse, l'équation d'Euler possède une multitude d'invariances d'échelle, dont celle représentée par le triplet $(0, 1, 1)$.

D'autre part, l'équation d'Euler-Navier-Stokes est invariante par translation : si x_0 appartient à $\mathbb{X}^3$, pour toute solution d'Euler-Navier-Stokes u , la translatée

$$\tau_{x_0} u := u(\cdot, \cdot - x_0)$$

est aussi une solution. La sous-section suivante explique l'intérêt et l'influence de telles invariances sur le choix des espaces fonctionnels dans lesquels résoudre l'équation.

1.2 Notions de solutions

1.2.1 Solution fortes

L'équation principale du système (*NSE*) étant une équation d'évolution, il est naturel de vouloir appliquer un théorème de point fixe de type Cauchy-Lipschitz. À cette fin, on commence par réécrire cette équation sous la forme de Duhamel, en voyant les termes non-linéaires comme une perturbation de l'équation de la chaleur. Pour la compacité de l'écriture, on préférera la forme projetée de (*PNSE*) à la forme originale de (*NSE*). On obtient ainsi la nouvelle équation

$$u(t) = e^{\nu t \Delta} u_0 + \int_0^t e^{\nu(t-s)\Delta} \mathbb{P} \nabla \cdot (u(s) \otimes u(s)) ds \quad \text{pour } t \geq 0,$$

dont la forme, du type

$$u = a + B(u, u)$$

en notant

$$a(t) := e^{\nu t \Delta} u_0$$

la solution libre et

$$B(u, u)(t) := \int_0^t e^{\nu(t-s)\Delta} \mathbb{P} \nabla \cdot (u(s) \otimes u(s)) ds$$

le terme bilinéaire, est plus adaptée à l'application d'un théorème de point fixe, à condition toutefois que la viscosité ν soit strictement positive. Dans le cas où celle-ci est nulle, deux preuves distinctes, l'une due à H. Swann [36] et l'autre de T. Kato [22] utilisent une suite de solutions pour ν strictement positif et font tendre ν vers 0. Les deux stratégies reposent de manière cruciale sur l'existence d'un temps de vie de la solution uniforme en ν . Revenons maintenant au cas de l'équation de Navier-Stokes. Pour pouvoir appliquer le théorème de point fixe au membre de droite de la forme du Duhamel, il est nécessaire de trouver un espace fonctionnel X tel que B envoie continûment $X \times X$ dans X . Or, en raison de l'invariance d'échelle de l'équation, un tel espace X doit lui-même être invariant d'échelle, au sens où sa norme $\|\cdot\|_X$ doit satisfaire, pour tout u dans X et tout λ strictement positif,

$$\|u_\lambda\|_X = \|u\|_X.$$

En dimension 3, tout espace X continûment inclus dans $\mathcal{S}'$, invariant sous le changement d'échelle de Navier-Stokes et par translation s'injecte dans l'espace de Besov homogène $\dot{B}_{\infty,\infty}^{-1}$. Nous ne rentrerons pas ici dans les détails techniques de cet espace, nous bornant simplement à rappeler la définition d'une de ses normes ; si une distribution tempérée u appartient à $\dot{B}_{\infty,\infty}^{-1}$, alors

$$\|u\|_{\dot{B}_{\infty,\infty}^{-1}} := \sup_{t>0} \|\sqrt{t} e^{t\Delta} u\|_{L^\infty} < \infty.$$

La liste des espaces fonctionnels classiques satisfaisant les deux invariances sus-citées est longue, nous n'en rappellerons donc que quelques uns. On trouve, parmi d'autres exemples, les espaces

$$L^4(\mathbb{R}_+, \dot{H}^1(\mathbb{X}^3)) \text{ et } L^p(\mathbb{R}_+, L^q(\mathbb{X}^3)) \text{ pour } \frac{2}{p} + \frac{3}{q} = 1 \text{ avec } p < \infty.$$

À l'heure actuelle, bien que le caractère bien posé de l'équation de Navier-Stokes localement en temps soit connu pour une pléthore d'espaces (à l'exception notable de l'espace final $\dot{B}_{\infty,\infty}^{-1}$, sur lequel l'opérateur B est discontinu), son pendant global reste largement ouvert, quoique plusieurs sous-cas soient connus. Classiquement, toute donnée initiale u_0 suffisamment petite dans un espace

invariant d'échelle engendre une solution globale. La preuve de ce fait remonte à l'article fondateur de J. Leray [25]. C'est également le cas si u_0 est supposée « presque bidimensionnelle », au sens où elle peut s'écrire, pour (x_1, x_2, x_3) dans $\mathbb{X}^3$, sous la forme

$$u_0(x_1, x_2, x_3) = (u_0^h(x_1, x_2, \varepsilon x_3), 0)$$

avec ε un paramètre réel positif suffisamment petit et la contrainte de divergence nulle devient ici

$$\partial_1 u_0^1 + \partial_2 u_0^2 = 0.$$

Ce résultat est prouvé dans [11]. De façon plus surprenante, des oscillations de grande amplitude et de fréquence très élevée dans la donnée initiale sont une aide - et non un obstacle, comme on pourrait le penser - à l'existence de solutions globales. Pour éclairer le propos, fixons

$$\varphi : \mathbb{R}^3 \longrightarrow \mathbb{R}^3$$

lisse, à support compact et de moyenne nulle en sa troisième variable. Pour (x_1, x_2, x_3) dans $\mathbb{R}^3$, on définit $\Phi(x_1, x_2, x_3)$ par

$$\Phi(x_1, x_2, x_3) := \int_{-\infty}^{x_3} \varphi(x_1, x_2, y_3) dy_3.$$

Fixons α dans $]0, 1[$, un réel strictement positif ε et définissons pour x dans $\mathbb{R}^3$ la donnée initiale $u_{0,\varepsilon,\alpha}$ par

$$u_{0,\varepsilon,\alpha}(x_1, x_2, x_3) := \varepsilon^{-\alpha} \left(\varphi(x) \cos \frac{x_2}{\varepsilon}, \varphi(x) \cos \frac{x_1}{\varepsilon}, -\partial_1 \Phi(x) \cos \frac{x_2}{\varepsilon} - \partial_2 \Phi(x) \cos \frac{x_1}{\varepsilon} \right).$$

Le paramètre α quantifie l'amplitude des oscillations, qui sont de l'ordre de $\varepsilon^{-\alpha}$, tandis que leur fréquence est de l'ordre de ε^{-1} , donc bien plus élevée. Une conséquence du résultat de M. Cannone, Y. Meyer et F. Planchon dans [9] est que de telles données initiales engendrent une solution globale, pourvu que ε soit suffisamment petit.

1.2.2 Dissipation de l'énergie

Une autre caractéristique de l'équation de Navier-Stokes, partagée avec d'autres équations venues de la physique (on peut citer l'équation de Schrödinger, celle de Maxwell ou de Boltzmann, entre autres), est de posséder une quantité soit décroissante au cours du temps, soit conservée. Cette quantité n'est autre que l'énergie cinétique globale du fluide ici. En effet, si u est une solution de l'équation de Navier-Stokes avec donnée initiale u_0 dans $L^2(\mathbb{X}^3)$, des calculs formels montrent que

$$\frac{1}{2} \frac{d}{dt} \|u(t)\|_{L^2(\mathbb{X}^3)}^2 = -\nu \|\nabla u(t)\|_{L^2(\mathbb{X}^3)}^2 \quad \text{pour } t \geq 0.$$

En intégrant en temps cette égalité, on obtient ainsi

$$\frac{1}{2} \|u(t)\|_{L^2(\mathbb{X}^3)}^2 + \nu \int_0^t \|\nabla u(s)\|_{L^2(\mathbb{X}^3)}^2 ds = \frac{1}{2} \|u_0\|_{L^2(\mathbb{X}^3)}^2 \quad \text{pour } t \geq 0.$$

On interprète cette égalité (formelle à ce stade, rappelons-le) de la manière suivante : un fluide possédant une énergie cinétique totale finie à un instant donné dissipe progressivement cette énergie à cause des forces de viscosité internes au fluide, le taux de dissipation étant proportionnel au coefficient de viscosité du fluide et au carré de son accélération. Ainsi, plus un fluide est loin de la famille des écoulements uniformes et plus il va dissiper son énergie rapidement. Or, le seul écoulement

uniforme d'énergie finie est l'état de repos, pour lequel la vitesse du fluide est identiquement nulle. L'équation sur l'énergie contient donc, à première vue, une information cruciale (et physiquement raisonnable) : tout fluide visqueux, incompressible et homogène sur lequel aucune force extérieure n'est appliquée tend à revenir à l'état de repos en dissipant son énergie par frottements (on omet ici de parler d'éventuels bords, que l'on néglige). L'article de M. Wiegner [39] apporte une preuve de cette affirmation pour toute solution dite « de Leray » de l'équation de Navier-Stokes avec donnée initiale d'énergie finie, solutions que nous définissons ci-dessous.

1.2.3 Solutions faibles

Toujours dans son article de 1934, en plus de montrer l'existence de solutions fortes (globalement en temps en dimension 2, localement en dimension supérieure) et de donner des conditions d'explosion en temps fini, J. Leray a défini un type de solution entièrement nouveau à l'époque, qu'il a qualifiées de « *solutions turbulentes* ». Ces solutions sont construites en approximant l'équation originale par une suite d'autres, plus simples à traiter et pour lesquelles l'équation sur l'énergie est aisée à établir. J. Leray se sert alors de l'équation sur l'énergie pour borner les solutions de ces équations approchées dans un espace de fonctions plus régulières qu'un simple espace L^2 , plus spécifiquement de la dissipation d'énergie. Un théorème de compacité lui permet alors de passer à la limite dans les termes non-linéaires, lui livrant ainsi une « solution turbulente » (on parle aujourd'hui de solution faible) de l'équation originale. À la limite, l'équation sur l'énergie devient une *inéquation*, laissant ouverte la possibilité de discontinuités dans l'énergie à condition qu'elles soient décroissantes. En d'autres termes, le procédé d'approximation ne permet pas d'exclure la possibilité de dissipations brutales et instantanées de l'énergie, mais toute augmentation subite de celle-ci est proscrite pour de telles solutions. Explicitons quelque peu les idées que nous venons d'énoncer. Donnons-nous u_0 dans $L^2(\mathbb{X}^3)$ une donnée initiale à divergence nulle, un coefficient ν strictement positif et $(\rho_n)_{n \in \mathbb{N}}$ une suite régularisante. On considère alors le problème suivant : pour chaque entier n , résoudre

$$(NS)_n \begin{cases} \partial_t u_n(t, x) + \nabla \cdot (u_n \otimes (\rho_n * u_n))(t, x) - \nu \Delta u_n(t, x) = -\nabla p_n(t, x), & t \geq 0, x \in \mathbb{X}^3, \\ \operatorname{div} u_n \equiv 0, \\ u_n(0, x) = \rho_n * u_0(x). \end{cases}$$

Grâce aux propriétés régularisantes de ρ_n , l'existence d'une solution lisse u_n à l'équation $(NS)_n$ ne pose aucune difficulté. Cette existence légitime les calculs qui vont suivre, qui n'étaient que formels dans la section précédente. En multipliant l'équation principale par u_n et en intégrant en espace, on obtient

$$\frac{1}{2} \frac{d}{dt} \int_{\mathbb{X}^3} |u_n(x, t)|^2 dx + \nu \int_{\mathbb{X}^3} |\nabla u_n(x, t)|^2 dx = 0 \quad \text{pour } t \geq 0.$$

En effet, un examen de chaque terme de l'équation nous apprend que

$$\begin{aligned} \int_{\mathbb{X}^3} u_n(x, t) \cdot \partial_t u_n(x, t) dx &= \frac{1}{2} \int_{\mathbb{X}^3} \partial_t (|u_n(x, t)|^2) dx = \frac{1}{2} \frac{d}{dt} \int_{\mathbb{X}^3} |u_n(x, t)|^2 dx; \\ \int_{\mathbb{X}^3} u_n(x, t) \cdot (\nabla \cdot (u_n \otimes (\rho_n * u_n)))(x, t) dx &= \frac{1}{2} \int_{\mathbb{X}^3} \nabla \cdot (|u_n|^2 \otimes (\rho_n * u_n))(x, t) dx = 0; \\ -\nu \int_{\mathbb{X}^3} u_n(x, t) \cdot \Delta u_n(x, t) dx &= \nu \int_{\mathbb{X}^3} |\nabla u_n(x, t)|^2 dx; \\ -\int_{\mathbb{X}^3} u_n(x, t) \cdot \nabla p_n(x, t) dx &= \int_{\mathbb{X}^3} p_n(x, t) \operatorname{div} u_n(x, t) dx = 0. \end{aligned}$$

Nous insistons sur le fait que toutes les interversions dérivée-intégrale et intégrations par parties sont licites pour chaque entier n et non pas uniquement formelles. Le traitement du deuxième et du quatrième terme utilise de manière cruciale l'incompressibilité de u_n . En intégrant l'équation sur l'énergie en temps, on trouve alors, pour chaque entier n ,

$$\frac{1}{2}\|u_n(t)\|_{L^2(\mathbb{X}^3)}^2 + \nu \int_0^t \|\nabla u_n(s)\|_{L^2(\mathbb{X}^3)}^2 ds = \frac{1}{2}\|\rho_n * u_0\|_{L^2(\mathbb{X}^3)}^2 \quad \text{pour } t \geq 0.$$

Le membre de droite étant borné uniformément en n par l'énergie cinétique initiale, que l'on a supposé finie, l'équation sur l'énergie nous livre alors une borne sur u_n dans l'espace dit *espace d'énergie*

$$L^\infty(\mathbb{R}_+, L^2(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, \dot{H}^1(\mathbb{X}^3)),$$

cette borne étant uniforme en n . En combinant cette information avec le théorème de Rellich, on déduit que $(u_n)_{n \in \mathbb{N}}$ est localement fortement compacte en espace. L'équation $(NS)_n$ nous permet alors d'affirmer que $(\partial_t u_n)_{n \in \mathbb{N}}$ est bornée dans $L_{\text{loc}}^1(\mathbb{R}_+, \dot{H}_{\text{loc}}^{-2}(\mathbb{X}^3))$. Le lemme d'Aubin-Lions nous assure qu'avec les deux bornes établies ci-dessus, la suite $(u_n)_{n \in \mathbb{N}}$ est *fortement* compacte dans, disons, $L^2(\mathbb{R}_+ \times \mathbb{X}^3)$. Notons alors u une valeur d'adhérence de $(u_n)_{n \in \mathbb{N}}$ dans $L^2(\mathbb{R}_+ \times \mathbb{X}^3)$. Il est aisé de montrer que u est une solution faible de l'équation de Navier-Stokes. Le lemme de Fatou appliqué à l'équation d'énergie implique l'appartenance de u à

$$L^\infty(\mathbb{R}_+, L^2(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, \dot{H}^1(\mathbb{X}^3)).$$

En outre, u vérifie l'inégalité d'énergie

$$\frac{1}{2}\|u(t)\|_{L^2(\mathbb{X}^3)}^2 + \nu \int_0^t \|\nabla u(s)\|_{L^2(\mathbb{X}^3)}^2 ds \leq \liminf_{n \rightarrow \infty} \frac{1}{2}\|\rho_n * u_0\|_{L^2(\mathbb{X}^3)}^2 = \frac{1}{2}\|u_0\|_{L^2(\mathbb{X}^3)}^2 \quad \text{pour } t \geq 0.$$

1.2.4 Entre le fort et le faible

Deux types de solutions ont été définis jusqu'à présent, l'un plus restrictif a priori que l'autre. Dans l'optique d'énoncer un jour un résultat d'unicité de grande portée, il serait bon de pouvoir décider si ces deux types de solutions ne font qu'un. Le plus simple des liens unissant ces deux notions de solution est le suivant : toute solution forte des équations de Navier-Stokes satisfait l'égalité d'énergie aussi longtemps qu'elle est définie. Une contrainte plus profonde s'incarne dans le théorème *d'unicité fort-faible*. Supposons disposer de deux données initiales $u_{0,F}$ et $u_{0,f}$ pour lesquelles on puisse définir respectivement une solution forte u_F et une solution faible u_f . Fixons un intervalle temporel $]t_1, t_2[$ sur lequel les deux solutions existent. Dans son article [25], J. Leray parvient à montrer l'estimation de stabilité

$$\begin{aligned} \frac{1}{2}\|u_F(t) - u_f(t)\|_{L^2(\mathbb{X}^3)}^2 + \nu \int_0^t \|\nabla u_F(s) - \nabla u_f(s)\|_{L^2(\mathbb{X}^3)}^2 ds \\ \leq \frac{1}{2}\|u_{0,F} - u_{0,f}\|_{L^2(\mathbb{X}^3)}^2 \exp\left(\frac{1}{2\nu} \int_0^t \|u_F(s)\|_{L^\infty(\mathbb{X}^3)}^2 ds\right). \end{aligned}$$

sur l'énergie de la différence $u_F - u_f$. En particulier, pour toute donnée initiale u_0 engendrant à la fois une solution forte et une solution faible (supposer $u_0 \in (L^2 \cap L^3)(\mathbb{X}^3)$ suffit), les deux solutions coïncident aussi longtemps que la solution forte est définie. Pour cette raison, on appelle ce résultat le théorème d'unicité fort-faible ; il y a unicité faible dès lors qu'il y a existence forte.

Un résultat plus fin, car local en espace, est celui de J. Serrin [32], repris puis amélioré par une quantité considérable d'auteurs (voir [3], [8], [17], [18], [19], [21], [35], [38] et les références

auxquelles ces articles renvoient). L'esprit de ces théorèmes est de supposer qu'une solution de Leray de l'équation de Navier-Stokes satisfait une certaine hypothèse de régularité critique, au sens où l'on suppose que la restriction de cette solution faible à un certain domaine d'espace-temps appartient à un espace critique. La conclusion de ce type de théorème est la lissité de la solution faible là où l'hypothèse de régularité a été faite. C'est dans cette lignée que nos résultats se situent, avec le soutien notable de la théorie de R. J. DiPerna et P.-L. Lions, théorie dont nous rappelons les grandes lignes ci-après.

1.3 Théorie de DiPerna-Lions

1.3.1 Motivations et stratégie

Dans leur article de 1989 [15], R. J. DiPerna et J.-L. Lions constatent que le théorème de Cauchy-Lipschitz est inopérant dès lors que le champ de vecteurs de l'équation différentielle n'est plus lipschitzien, en rappelant que plusieurs branches des mathématiques bénéficieraient d'une extension de ce célèbre théorème. En étudiant non plus l'équation différentielle mais l'équations aux dérivées partielles de transport associée, ils parviennent à établir une nouvelle série de résultats d'existence et d'unicité de solutions pour cette équation de transport. En retour, ils en déduisent un résultat d'existence et d'unicité beaucoup plus général que le théorème de Cauchy-Lipschitz, permettant de choisir des champs de vecteurs seulement $W^{1,1}$ et à divergence bornée. Le prix à payer est l'affaiblissement de la notion de solution ; on ne résout ainsi plus l'équation de transport au sens des distributions pour la solution elle-même mais seulement pour des fonctions non-linéaires de celles-ci, fonctions sur lesquelles on impose une condition de croissance modérée (logarithmique) à l'infini. Ces solutions très faibles sont appelées, tant dans l'article que dans la terminologie moderne, des solutions *renormalisées*, la renormalisation étant le changement non-linéaire d'inconnue. Notons que les mêmes idées ont mené à la découverte des solutions renormalisées (dites de DiPerna-Lions) de l'équation de Boltzmann ainsi que d'autres équations centrales en théorie cinétique (voir l'article original [16] pour une liste exhaustive des équations considérées).

1.3.2 Idées et techniques

Nous n'exposerons pas, dans ces quelques lignes, l'intégralité des idées de l'article original, préférant mettre l'accent sur celles qui nous seront le plus utiles par la suite. Pour fixer les notations, donnons-nous une équation différentielle (autonome pour simplifier l'exposition du propos)

$$(E) \begin{cases} \dot{x}(t) = v(x(t)), & t \geq 0, \\ x(0) = x_0 \in \mathbb{R}^n. \end{cases}$$

Si l'on suppose que le champ

$$v : \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

est continu, le théorème de Peano assure l'existence d'au moins une solution au problème ci-dessus. Si l'on suppose de plus que v est lipschitzien ou, à peine plus généralement, que le module de continuité de v satisfait la condition d'Osgood, il y a unicité de la solution. Sans nous étendre exagérément sur cette condition, nous signalons que toute fonction lipschitzienne satisfait automatiquement la condition d'Osgood mais que la réciproque est fautive, la fonction

$$x \mapsto x \ln x$$

fournissant un contre-exemple en dimension 1. A contrario, une fonction puissance

$$x \mapsto x^a, \quad 0 < a < 1$$

ne satisfait pas cette condition (et pour une telle fonction, il est aisé de construire une infinité de solutions si $x_0 = 0$). Nous renvoyons le lecteur intéressé à l'article original de W. F. Osgood [30].

La première idée-clé de l'article de R. J. DiPerna et J.-L. Lions est de s'appuyer sur la formulation transport de l'équation différentielle. Si l'on note X le flot de l'équation et

$$a : \mathbb{R}_+ \times \mathbb{R}^n \longrightarrow \mathbb{R}$$

une fonction constante le long des caractéristiques, la fonction

$$t \mapsto a(t, X(t, x))$$

est par définition constante pour chaque point x de $\mathbb{R}^n$ fixé et a résout, au moins formellement,

$$(T) \quad \partial_t a + v \cdot \nabla a = 0 \quad t \geq 0, x \in \mathbb{R}^n.$$

En considérant le flot plutôt qu'une trajectoire particulière, une équation non-linéaire en dimension finie est remplacée par une équation linéaire en dimension infinie. Il devient éminemment plus simple de prouver l'existence de solutions à cette nouvelle équation sous des hypothèses de régularité très modérées sur la donnée initiale $a(0)$ et le champ de transport v , grâce à des techniques d'approximation standard. Ainsi, on peut se contenter de faire une hypothèse d'intégrabilité sur a et les dérivées de v . En particulier, dès que la dimension d'espace est au moins égale à 2, on est capables de montrer un résultat d'existence alors même que v n'est pas forcément continu. D'autre part, la prise en compte de données initiales sur lesquelles seule une hypothèse d'intégrabilité est faite a des motivations physiques; en effet, si l'équation est censée modéliser le transport d'un composé dans un milieu fluide, il est naturel dans les applications de supposer que la masse totale (la norme L^1 de la densité) du composé est finie à l'instant initial. La preuve de l'unicité des solutions repose sur un lemme de base de la théorie des distributions.

Lemma. *Soit u dans $L^1_{loc}(\mathbb{R}^n)$. Si pour toute fonction test φ de $\mathcal{C}^\infty(\mathbb{R}^n)$ on a*

$$\int_{\mathbb{R}^n} u(x)\varphi(x)dx = 0,$$

alors u est identiquement nulle.

L'enjeu est d'arriver à utiliser l'équation de transport sur a afin de prouver la nullité de ces intégrales pour toute fonction test. À cette fin, multiplions l'équation sur a par une fonction lisse ψ dépendant cette fois de l'espace et du temps et réalisons quelques intégrations par parties formelles. On obtient ainsi, pour tout $T > 0$,

$$\int_{\mathbb{R}^n} a(T, x)\psi(T, x)dx - \int_{\mathbb{R}^n} a(0, x)\psi(0, x)dx = \int_0^T \int_{\mathbb{R}^n} a(t, x) (\partial_t \psi(t, x) + \nabla \cdot (v(x)\psi(t, x))) dx dt.$$

Si l'on suppose que la donnée initiale $a(0, \cdot)$ est nulle et que l'on est capables, pour toute fonction test φ de prouver l'existence d'une solution ψ au problème adjoint

$$(T^{\text{adj}}) \quad \begin{cases} \partial_t \psi + \nabla \cdot (v\psi) = 0 & t \geq 0, x \in \mathbb{R}^n \\ \psi(T) = \varphi, \end{cases}$$

l'équation intégrale sur a se réduira alors, pour tout $T > 0$, à

$$\int_{\mathbb{R}^n} a(T, x)\varphi(x)dx = 0.$$

En vertu du lemme énoncé ci-dessus, on en déduira alors que a est identiquement nulle au temps T , ce qui terminera la preuve puisque T est quelconque. On remarque que l'équation adjointe est d'une écriture très proche de celle du problème initial, à ceci près que v apparaît cette fois dans la dérivée et non plus devant. La différence entre les deux termes n'est autre que

$$\nabla \cdot (av) - v \cdot \nabla a = a \operatorname{div} v.$$

On comprend dès lors l'importance que peuvent avoir les diverses hypothèses faites sur la divergence de v , la plus simple étant sa nullité. Sous cette hypothèse d'incompressibilité de v , l'équation de (T) est identique à celle de (T^{adj}) . Le renversement du temps entre les deux problèmes incarné par le passage d'une donnée initiale à une donnée finale ne pose aucune difficulté conceptuelle ou technique ; cela revient simplement à changer le signe du champ v . Dans le cas de la divergence nulle, le problème initial et son adjoint sont donc entièrement équivalents. L'article original de R. J. DiPerna et J.-L. Lions [15] généralise cette résolution au cas d'une divergence bornée, hypothèse essentiellement optimale si l'on souhaite disposer de bornes d'intégrabilité sur a .

1.4 Résultats

Dans une première sous-partie, on démontre un résultat d'unicité faible pour des équations de transport-diffusion (Théorème 1.1.2 page 26) sous des hypothèses de même nature que celles du théorème de DiPerna-Lions. Ce résultat d'unicité faible est très versatile et susceptible d'adaptations à d'autres problèmes où les phénomènes de transport et de diffusion jouent un rôle prédominant.

Dans une seconde sous-partie, on démontre un analogue du théorème de J. Serrin (Théorèmes 2.5.1 page 45 pour le cas du tore et 2.6.1 page 47 pour celui d'un domaine de l'espace) dans lequel l'hypothèse de régularité critique est faite sur une seule composante du champ de vitesses. Le prix à payer pour cette hypothèse anisotrope est double. D'une part, l'intégrabilité critique est remplacée par une hypothèse sur les dérivées de la composante du champ de vitesses, nettement plus forte. D'autre part, les techniques de preuve sont plus élaborées en ce que celle-ci fait inévitablement intervenir des opérateurs pseudodifférentiels anisotropes.

2 Graphes quantiques

Cette partie de la thèse est consacrée à l'étude du spectre du laplacien de Neumann sur des graphes métriques et plus spécifiquement à sa première valeur propre non triviale. On pose un problème d'optimisation de forme visant à minimiser (resp. maximiser) cette valeur propre en ne pouvant que changer les longueurs des arêtes, en préservant la longueur totale du graphe. On aimerait trouver les valeurs extrémales atteignables sous ces contraintes ainsi que les formes de graphes obtenues à la limite. On répond entièrement aux deux questions dans le cas du minimum et apporte des réponses partielles dans le cas du maximum. Ce travail a été réalisé en collaboration avec R. Band, du Technion Institute.

2.1 Bref historique

Les graphes quantiques sont des objets dont on fait remonter la première apparition, quoiqu'implicitement, dans un article de chimie des années 30 par J. Pauling [74]. Dans cet article, la motivation principale de l'auteur est de calculer les susceptibilités diamagnétiques de certaines molécules organiques, dont le naphthalène. La finesse des dites molécules conduit à l'assimiler à un graphe, ou à un petit voisinage d'un graphe. Afin de comprendre la délocalisation des électrons sur une telle molécule, il est nécessaire de résoudre l'équation de Schrödinger sur (un petit voisinage de) ce graphe.

Un développement systématique de la méthode, toujours en vue d'applications en chimie organique, remonte aux années 50 avec l'article de K. Ruedenberg et C. W. Scherr [80]. L'appellation moderne de « graphes quantiques » a gardé la trace de cette origine. Le développement moderne de nanocircuits électriques, de structures en graphène ou de cristaux photoniques, pour ne citer que quelques exemples marquants, renouvelle l'intérêt porté à ces objets mathématiques. Dans ces applications, les graphes sont vus comme des limites de leurs voisinages tubulaires lorsque le diamètre transverse du voisinage tend vers zéro.

Du côté mathématique, divers résultats de convergence ont été établis, montrant que le spectre du laplacien sur le graphe donne, sous des conditions favorables, le comportement asymptotique du spectre du laplacien usuel sur un voisinage tubulaire du graphe dans la limite de diamètre transverse nul. Le Théorème 7.5.1 de [43], lui-même résumé des travaux de P. Kuchment et H. Zeng ([65], [66]), de J. Rubinstein et M. Schatzman ([77], [78], [79]) et de M. Schatzman [83], en est un exemple emblématique. On peut citer également les travaux de Y. Saito ([81], [82]). Le lecteur intéressé par le sujet trouvera des informations historiques plus précises dans la revue de littérature [64].

2.2 Définitions essentielles

2.2.1 Graphes discrets

On rappelle qu'un graphe (on précise parfois en parlant de graphe *combinatoire* ou *discret*) est un couple (V, E) où V est un ensemble de sommets et E un ensemble d'arêtes reliant les sommets de V . On insiste ici sur le fait que cette définition autorise a priori la présence de plusieurs arêtes reliant la même paire de sommets, ainsi que l'existence de boucles reliant un sommet à lui-même. Le graphe est dit *simple* si E est un sous-ensemble de $\mathcal{P}_2(V)$, où $\mathcal{P}_2(V)$ est l'ensemble des parties à deux éléments de V , autrement dit si toute paire de sommets est reliée par au plus une arête et que le graphe ne contient aucune boucle. Contrairement à un usage répandu en théorie des graphes, nous ne supposons jamais que nos graphes sont simples. Au contraire, nous autorisons explicitement les graphes que nous considérons à avoir des arêtes multiples et/ou des boucles. Le graphe est dit fini si V et E sont des ensembles finis. Le *degré* d'un sommet est le nombre d'extrémités d'arêtes connectées à ce sommet. En particulier, une boucle augmente le degré d'un sommet de deux, tandis que toute autre arête ne l'augmente que de un.

2.2.2 Graphes métriques

Un graphe *métrique* (ou *continu*, selon la littérature choisie) est un triplet $\Gamma = (V, E, \mathcal{L})$ où (V, E) est un graphe discret et $\mathcal{L} : E \rightarrow \mathbb{R}_+$ est une fonction associant une longueur réelle positive à chaque arête. Le lecteur remarquera que la définition de $\mathcal{L}$ autorise une ou plusieurs arêtes à posséder une longueur nulle. Si $v_1, v_2 \in V$ sont deux sommets reliés par une arête $e \in E$ telle que $\mathcal{L}(e) = 0$, on convient alors de confondre v_1 et v_2 en un seul sommet v , de supprimer e et de relier toute autre arête liée à v_1 ou v_2 au nouveau sommet v . Ce choix est cohérent avec l'intuition selon laquelle deux sommets infiniment proches sont indistinguables et ne font qu'un.

On peut ainsi voir un graphe métrique comme une union disjointe d'intervalles $\bigsqcup_{e \in E} [0, \mathcal{L}(e)]$ dont certaines extrémités sont identifiées par une relation d'équivalence rendant compte de la topologie du graphe discret (V, E) . Il pourra être utile, selon le contexte, d'assimiler les arêtes à des intervalles ouverts ou fermés. Un tel graphe est muni d'une distance naturelle héritée de la distance euclidienne sur $\mathbb{R}_+$, appelée la distance géodésique du graphe. Le graphe est dit *compact* si (V, E) est un graphe discret fini. On remarque que la terminologie est cohérente en ce qu'un graphe métrique compact au sens précédent est un espace métrique compact pour la distance géodésique.

2.2.3 Paramétrisation d'une arête

Une arête d'un graphe n'étant pas naturellement orientée, au contraire d'un intervalle de la droite réelle, il y a un choix de paramétrisation à effectuer. Si e est une arête d'un graphe métrique $(V, E, \mathcal{L})$ reliant les sommets v_1 et v_2 , que l'on assimile à l'intervalle $[0, \mathcal{L}(e)]$, on peut définir une première coordonnée x_e en associant au sommet v_1 le point 0 et au sommet v_2 le point $\mathcal{L}(e)$. On peut également définir $\tilde{x}_e$ en choisissant l'association inverse. Les deux coordonnées sont liées par la relation $x_e + \tilde{x}_e = \mathcal{L}(e)$. Dans le problème qui nous occupera, le choix de l'une ou l'autre paramétrisation n'aura aucune influence et l'on choisira à chaque instant celle des deux qui nous semblera la plus appropriée, facilitant au mieux l'écriture.

2.2.4 Fonctions sur un graphe métrique

Étant donné un graphe métrique $\Gamma = (V, E, \mathcal{L})$, on peut définir une fonction f sur Γ par l'ensemble de ses restrictions $(f|_e)_{e \in E}$ aux arêtes de Γ . En choisissant pour chaque $e \in E$ une paramétrisation, la restriction $f|_e$ devient une fonction d'une variable réelle sur un intervalle $]0, \mathcal{L}(e)[$. On peut donc parler sans ambiguïté de l'intégrabilité ou de la dérivabilité de $f|_e$, pour ne citer que quelques propriétés naturelles. Ces notions sont bien sûr indépendantes de la paramétrisation choisie pour chaque arête. Les espaces fonctionnels sur Γ sont définis par leurs restrictions à chacune de ses arêtes. Ainsi, on a par exemple

$$L^2(\Gamma) := \bigoplus_{e \in E} L^2(e) \sim \bigoplus_{e \in E} L^2(]0, \mathcal{L}(e)[),$$

$$\tilde{H}^1(\Gamma) := \bigoplus_{e \in E} H^1(e) \sim \bigoplus_{e \in E} H^1(]0, \mathcal{L}(e)[) \quad \text{et} \quad \tilde{H}^2(\Gamma) := \bigoplus_{e \in E} H^2(e) \sim \bigoplus_{e \in E} H^2(]0, \mathcal{L}(e)[).$$

On notera $\mathcal{C}(\Gamma)$ l'espace des fonctions continues sur l'espace métrique (Γ, d) , où d est la distance géodésique sur Γ .

2.2.5 Graphes quantiques

Un graphe *quantique* est la donnée d'un graphe métrique Γ , d'un opérateur différentiel D agissant sur un espace fonctionnel du graphe (le domaine de l'opérateur) et de conditions aux sommets, ces dernières étant les analogues des conditions au bord pour les domaines ou les variétés. Dans ce manuscrit, le seul opérateur considéré sera le laplacien unidimensionnel $D = \Delta$, qui n'est autre que la dérivée seconde. La dérivée étant d'ordre pair, elle est indépendante du choix de la paramétrisation choisie sur l'arête, au contraire d'une dérivée d'ordre impair. Le domaine du laplacien sur Γ est l'espace $\tilde{H}^2(\Gamma)$.

2.2.6 Conditions aux sommets

Il reste à choisir des conditions aux sommets pour compléter la description. Dans leur forme leur plus générale, les conditions aux sommets linéaires homogènes en l'inconnue prennent la forme suivante. Pour chaque sommet v d'un graphe métrique Γ de degré d_v , on choisit deux matrices (A_v, B_v) dans $\mathcal{M}_{d_v}(\mathbb{C})$. Soit $e_1, \dots, e_{d_v}$ les arêtes dont v est une extrémité, paramétrées de telle sorte que v soit l'origine de la paramétrisation. (On appelle souvent cette paramétrisation l'orientation sortante pour v .)

Si $f : \Gamma \rightarrow \mathbb{C}$ est une fonction définie sur le graphe appartenant à $\tilde{H}^2(\Gamma)$, la théorie usuelle des espaces de Sobolev en dimension un nous permet d'affirmer que chacune des restrictions de f

aux arêtes $e_1, \dots, e_{d_v}$ admet une trace en v , ainsi que les dérivées premières de ces restrictions. Ces limites sont notées $f|_{e_1}(v), \dots, f|_{e_{d_v}}(v)$ et $f'|_{e_1}(v), \dots, f'|_{e_{d_v}}(v)$ respectivement. En définissant les vecteurs des valeurs de f et f' en v par

$$F(v) := \begin{pmatrix} f|_{e_1}(v) \\ \vdots \\ f|_{e_{d_v}}(v) \end{pmatrix} \quad \text{et} \quad F'(v) := \begin{pmatrix} f'|_{e_1}(v) \\ \vdots \\ f'|_{e_{d_v}}(v) \end{pmatrix},$$

les conditions recherchées s'écrivent sous la forme

$$A_v \cdot F(v) + B_v \cdot F'(v) = 0.$$

Afin d'obtenir le bon nombre d'équations indépendantes, il est impératif d'imposer que le rang de la matrice concaténée $(A_v \ B_v) \in \mathcal{M}_{d_v \times 2d_v}(\mathbb{C})$ soit maximal, i.e. égal à d_v . Pour des raisons physiques (conservation du courant de probabilité quantique), il est raisonnable d'imposer qu'une telle condition au sommet rende l'opérateur étudié autoadjoint. On montre alors (se reporter à la référence [43], Théorème 1.4.4) que dans le cas du laplacien (ainsi que de tout opérateur de Schrödinger), cette contrainte est équivalente, en sus de la condition de rang maximal mentionnée précédemment, au caractère hermitien de la matrice $A_v B_v^*$, où B_v^* est la transconjuguée (ou adjointe hermitienne) de B_v . On notera que chaque sommet peut porter une condition différente, aussi longtemps que chacune de ces conditions permet au laplacien d'être autoadjoint. On peut, à titre d'exemple, imposer une condition de Neumann sur un sous-ensemble quelconque de sommets et une condition de Dirichlet sur tous les sommets restants (voir ci-après pour une définition de ces conditions).

2.2.7 Conditions δ

Un sous-ensemble particulièrement étudié de conditions est celui des conditions δ , qui prennent la forme suivante. On dit qu'une fonction $f \in \tilde{H}^2(\Gamma, \mathbb{C})$ satisfait la condition δ au sommet v avec le paramètre (réel ou infini) α_v si f est continue en v , i.e. si toutes les traces au bord $f|_{e_1}(v), \dots, f|_{e_{d_v}}(v)$ sont égales et si

$$\sum_{i=1}^{d_v} f'|_{e_i}(v) = \alpha_v f(v),$$

où l'on a noté $f(v)$ la valeur $f|_{e_1}(v)$. Dans le cas α_v est infini, cette dernière condition est remplacée par la nullité de f au sommet v . On appelle *condition de Neumann en v* la condition δ avec paramètre α_v nul et *condition de Dirichlet en v* la condition δ avec paramètre α_v infini. Ces deux conditions sont de loin les plus fréquentes dans la littérature des graphes quantiques, particulièrement la condition de Neumann. Elles sont, comme on s'en doute, les analogues dans ce contexte des conditions de Dirichlet et Neumann pour les domaines et les variétés. On imposera par la suite la seule condition de Neumann à tous les sommets, à l'exception notable du Théorème 3.2.6 dont la formulation requiert une brève mention de la condition de Dirichlet.

2.3 Formulation du problème

2.3.1 Éléments de théorie spectrale

La théorie spectrale d'un graphe quantique dont l'opérateur est le laplacien (ou plus généralement un opérateur de Schrödinger) muni de conditions aux sommets rendant cet opérateur autoadjoint est très simple ; en effet, les théorèmes usuels pour le laplacien (ou les opérateurs de Schrödinger)

sur les domaines compacts s'appliquent *mutadis mutandis* au cas des graphes quantiques compacts. Nous citons ci-dessous une version affaiblie du Théorème 3.1.1 de [43], suffisante pour servir nos objectifs.

Theorem 2.1. *Soit Γ un graphe métrique compact muni du laplacien $-\Delta$ agissant sur les fonctions définies sur les arêtes et de conditions δ aux sommets. Alors le spectre de $-\Delta$ est l'union d'une suite de valeurs propres $(\lambda_n)_{n \in \mathbb{N}}$ (comptées avec multiplicité) de multiplicités finies avec*

$$\lambda_n \rightarrow +\infty \text{ lorsque } n \rightarrow +\infty.$$

De plus, il existe une base hilbertienne $(f_n)_{n \in \mathbb{N}}$ de $L^2(\Gamma)$ telle que pour tout entier n

$$-\Delta f_n = \lambda_n f_n$$

et f_n satisfait les conditions aux sommets prescrites. Enfin, en notant

$$h(f, f) := \langle -\Delta f, f \rangle_{L^2(\Gamma)}$$

la forme quadratique associée à l'opérateur $-\Delta$, de domaine $\text{Dom}(h) \subset \tilde{H}^1(\Gamma)$, les valeurs propres satisfont pour tout $n \in \mathbb{N}$ les égalités variationnelles

$$\lambda_n = \min_{\substack{f \in \text{Dom}(h); \\ f \perp f_0, \dots, f_{n-1}}} \frac{h(f, f)}{\|f\|_{L^2(\Gamma)}^2}.$$

La quantité minimisée dans le membre de droite s'appelle le quotient de Rayleigh de f et est notée plus simplement $\mathcal{R}(f)$. Pour de petits numéros de valeurs propres (typiquement 0, 1 ou 2), il est possible de choisir des fonctions tests sur Γ dans $\text{Dom}(h)$ dont le quotient de Rayleigh sera facile à calculer, permettant ainsi une majoration aisée de la valeur propre qui nous préoccupe.

2.3.2 Trou spectral

La quantité $\lambda_1 - \lambda_0$ porte souvent le nom de *trou spectral* et est d'une grande importance dans les applications. Lors de l'étude d'un phénomène diffusif sur le graphe, c'est elle qui donne la constante de temps générique du retour à l'équilibre après une perturbation. Ainsi, si l'on chauffe une zone du graphe au temps $t_0 = 0$ et que l'on étudie l'écart entre la température sur le graphe et sa moyenne spatiale à un instant t donné, cet écart est de l'ordre de $e^{-(\lambda_1 - \lambda_0)t}$ en norme L^2 . Disposer de méthodes efficaces pour calculer (ou *a minima* estimer) ce trou spectral apparaît donc comme un objectif aux retombées pratiques indéniables. Dans le cas des domaines, ce rôle est joué par les inégalités de Faber-Krahn ([52], [62], [63]) pour la condition de Dirichlet et de Szegő-Weinberger ([84], [85]) pour la condition de Neumann. Ces inégalités prouvent que la boule est, à mesure fixée, l'unique domaine connexe réalisant le minimum (pour la condition de Dirichlet) ou le maximum (pour la condition de Neumann) de la première valeur propre non nulle. Cette valeur propre est égale à λ_0 dans le cas Dirichlet et à λ_1 dans le cas Neumann; en effet, on observe trivialement que pour la condition de Neumann, $\lambda_0 = 0$ avec les constantes pour fonctions propres et que cette valeur propre a pour multiplicité le nombre de composantes connexes du domaine. Nous imposerons dans la suite la condition de Neumann à tous les sommets du graphe, nous plaçant ainsi dans la lignée du théorème de G. Szegő et H. F. Weinberger. Par commodité, on appelle ces graphes des *graphes de Neumann*. L'observation précédente faite pour les domaines s'applique de manière identique aux graphes de Neumann compacts connexes, dont le trou spectral est alors égal à la première valeur propre non

nulle λ_1 . Pour ce choix de conditions, la forme quadratique h n'est autre que le carré de la norme $\dot{H}^1$ sur le graphe :

$$h(f, f) = \int_{\Gamma} |f'(x)|^2 dx.$$

Le domaine de h est alors $\tilde{H}^1(\Gamma) \cap \mathcal{C}(\Gamma)$, que l'on note habituellement $H^1(\Gamma)$.

2.3.3 Contrainte d'échelle

Tout comme dans le cas des domaines, il est nécessaire d'imposer une restriction sur le volume des graphes considérés si l'on veut que notre recherche d'extrema ait un sens. En effet, si $\Gamma = (V, E, \mathcal{L})$ est un graphe métrique et L est un paramètre strictement positif fixé, on définit le graphe

$$L \cdot \Gamma := (V, E, L \cdot \mathcal{L}).$$

Autrement dit, on a simplement dilaté toutes les arêtes de Γ d'un facteur L en conservant sa topologie. On vérifie alors aisément que le spectre de $L \cdot \Gamma$ est dilaté d'un facteur L^{-2} et que les multiplicités sont conservées. Enfin, les fonctions propres de $L \cdot \Gamma$ sont, à une dilatation de la variable d'un facteur L^{-1} près, les mêmes que celles de Γ . Ainsi, en choisissant L arbitrairement petit (resp. grand), il est possible de rendre les valeurs propres aussi grandes (resp. petites) que l'on veut. Dans l'optique de comprendre les formes optimales de graphes, celles pour lesquelles une certaine valeur propre sera maximale ou minimale, nous choisissons de travailler sous la contrainte

$$\mathcal{L}_{\text{tot}} := \sum_{e \in E} \mathcal{L}(e) = 1.$$

Le volume du graphe, qui n'est autre que sa longueur totale, sera fixé égal à une unité.

2.3.4 Énoncé du problème

Étant donné un graphe discret $G = (V, E)$, on considère la famille des graphes métriques

$$\{\Gamma = (V, E, \mathcal{L}) \text{ t.q. } \mathcal{L}_{\text{tot}} = 1\},$$

tous munis des conditions de Neumann à leurs sommets. On rappelle à toutes fins utiles la convention adoptée lorsqu'une longueur nulle est attribuée à une arête, consistant en la fusion des sommets aux extrémités en un seul. On considérera dans la suite

$$\mathfrak{L} := \{\mathcal{L} : E \rightarrow \mathbb{R}_+ \text{ t.q. } \mathcal{L}_{\text{tot}} = 1\}$$

l'ensemble des $\mathcal{L}$ admissibles comme un sous-ensemble du cône positif de $\mathbb{R}^{|E|}$ muni de la topologie euclidienne. L'ensemble $\mathfrak{L}$ est évidemment compact pour cette topologie. Si Γ est un graphe de cette famille, on voit la première valeur propre non nulle de Γ comme une fonction de la variable $\mathcal{L}$ et on note $\lambda_1(\mathcal{L})$ pour insister sur la dépendance de cette valeur propre en les longueurs des arêtes. En admettant pour le moment que λ_1 est une fonction continue sur $\mathfrak{L}$ et en fixant dans la suite un graphe G , on souhaite répondre aux questions suivantes.

1. Quel est la valeur du minimum/du maximum sur $\mathfrak{L}$ de λ_1 ?
2. Quels sont les graphes réalisant ce minimum/maximum ?

Pour bien comprendre la deuxième question il faut se rappeler, une fois de plus, que l'on autorise certaines arêtes à avoir une longueur nulle. Ce faisant, on autorise une dégénérescence continue de la topologie du graphe, en interdisant cependant toute coupure ou ajout d'arête. En particulier, une fois que G est fixé, tous les graphes métriques admissibles sont homotopes en tant qu'espaces topologiques. On peut reformuler la deuxième question comme suit.

(2)' Quels sont les graphes discrets pour lesquels il existe un choix de $\mathcal{L}$ dans $\mathfrak{L}$ à coordonnées *toutes strictement positives* réalisant le minimum/maximum de λ_1 sur $\mathfrak{L}$?

La condition supplémentaire a pour but de prévenir toute dégénérescence, en s'assurant que la topologie prescrite par G est strictement conservée.

2.4 Résultats

Concernant le problème du minimum, les deux questions ont reçu une réponse complète, en s'appuyant partiellement sur la littérature préexistante (Théorème 3.2.1 page 60). Selon que le graphe possède ou non un pont, le minimiseur est l'intervalle unité ou un collier symétrique (voir l'exemple 3.1.7 page 60 pour une définition de ceux-ci) et le trou spectral correspondant vaut respectivement π^2 ou $(2\pi)^2$. Mieux encore, on est capables de caractériser topologiquement les colliers symétriques accessibles à un graphe sans pont donné (voir la fin de la section 3.3). Le cas du maximum est partiellement résolu mais reste encore ouvert. Il est toutefois possible d'apporter une réponse complète dans le cas où G est un arbre (Théorème 3.2.2 page 61). On fournit de plus des critères pratiques permettant de se réduire à des sous-graphes (Théorème 3.2.6) ainsi que d'exclure certains graphes de la famille des maxima (Théorème 3.2.4). On conclut en énonçant deux conjectures sur ce problème du maximum (voir la section 3.9). La première affirme qu'en dehors de quelques cas exceptionnels les flétoiles équilatérales, recollement d'étoiles et de fleurs, forme l'unique famille de graphes maximisant le trou spectral à longueur totale fixée, les cas exceptionnels étant couverts par les mandarines équilatérales. La deuxième conjecture, qui se décline en deux versions, relie la maximisation du trou spectral à la maximisation des symétries du graphe en deux sens distincts selon que l'on préfère considérer le groupe d'automorphismes du graphe ou la dégénérescence de son trou spectral.

3 Groupes de Lie et transformée de Fourier

Dans cette dernière partie, nous reprenons les travaux de H. Bahouri, J.-Y. Chemin et R. Danchin sur les groupes de Heisenberg [86] et les généralisons au cas des groupes de Lie nilpotents simplement connexes d'indice 2, dont les groupes de Heisenberg forment un sous-ensemble.

3.1 Groupes et algèbres de Lie.

Commençons par quelques rappels et donnons-nous un groupe $(G, \cdot)$. On dit que $(G, \cdot)$ est un groupe de Lie si il est de plus muni d'une structure de variété différentielle $\mathcal{C}^\infty$ compatible avec la structure de groupe, au sens où la multiplication

$$\cdot : G \times G \rightarrow G$$

et l'inversion

$$^{-1} : G \rightarrow G$$

sont des applications $\mathcal{C}^\infty$. On supposera toujours dans la suite que G est connexe. L'algèbre de Lie du groupe, notée, $\mathfrak{g}$, est définie comme étant l'espace vectoriel des champs de vecteurs invariants à

gauche sur G . On montre (voir par exemple [92]) que cet espace est isomorphe à l'espace tangent de G en l'élément neutre. Un groupe de Lie est dit nilpotent si son algèbre de Lie est nilpotente, i.e. s'il existe un entier $n \in \mathbb{N}$ tel que toute chaîne de commutateurs de longueur $n + 1$ s'annule. Précisément, on demande que pour tout $(g_1, \dots, g_{n+1})$ de $\mathfrak{g}^{n+1}$ l'on ait

$$[\dots[[g_1, g_2], g_3] \dots, g_{n+1}] = 0.$$

L'indice de nilpotence de $\mathfrak{g}$ - et partant, de G - est par définition le plus petit entier n tel que l'égalité précédente ait lieu pour tout $(n + 1)$ -uplet d'éléments de $\mathfrak{g}$. Une conséquence immédiate de cette définition est la caractérisation de la commutativité de $(G, \cdot)$ par un indice de nilpotence égal à 1. Dans ce cas, le groupe est isomorphe, en tant que groupe de Lie, à $(\mathbb{R}^{\dim G}, +)$. Le cas où cet indice est égal à 2 peut être vu comme un « exemple minimal non commutatif » ; en particulier, il devrait être le plus simple à traiter parmi les groupes de Lie nilpotents.

3.2 Groupes de Lie nilpotents

Cette sous-section a pour objectif de justifier brièvement l'identification que l'on fera par la suite entre un groupe de Lie (supposé nilpotent et simplement connexe), son algèbre de Lie et une certaine application bilinéaire antisymétrique. On renvoie le lecteur intéressé à la référence [91] pour de plus amples informations. On aura besoin pour cela d'un objet courant en théorie de Lie : l'application exponentielle

$$\exp : \mathfrak{g} \longrightarrow G.$$

Il existe plusieurs définitions équivalentes de l'application exponentielle en algèbre de Lie ; nous retiendrons la plus générale. Soit X un champ de vecteurs invariant à gauche sur $(G, \cdot)$ et notons 1_G le neutre de $(G, \cdot)$. Considérons l'équation différentielle sur G

$$\begin{cases} \dot{\gamma}(t) = X(\gamma(t)), t \in \mathbb{R} \\ \gamma(0) = 1_G. \end{cases}$$

Le théorème de Cauchy-Lipschitz assure que cette équation différentielle possède une solution locale en temps. L'invariance à gauche de X permet d'affirmer que cette solution est en fait globale en temps. On définit alors

$$\exp X := \gamma(1) \in G.$$

Dans le cas où $(G, \cdot)$ est un sous-groupe de $(GL_n(\mathbb{R}), \cdot)$, l'application exponentielle coïncide avec l'exponentielle usuelle de matrices, définie par sa série entière.

On rappelle que pour tout groupe de Lie $(G, \cdot)$, l'application exponentielle définit, par restriction, un difféomorphisme d'un voisinage de l'élément neutre de $(\mathfrak{g}, +)$ sur un voisinage de l'élément neutre de $(G, \cdot)$. De plus, si X, Y sont suffisamment proches de 0 dans $\mathfrak{g}$, on dispose de la formule de Baker-Campbell-Hausdorff (ou formule BCH en forme courte)

$$\exp X \exp Y = \exp Z$$

où Z est défini par une série absolument convergente de commutateurs itérés entre X et Y . Les premiers termes de cette série sont donnés par

$$Z = BCH(X, Y) := X + Y + \frac{1}{2}[X, Y] + \frac{1}{12}([X, [X, Y]] + [Y, [Y, X]]) + (\text{ordre supérieur}).$$

Supposons à partir de maintenant et dans toute la suite de cette partie que $(G, \cdot)$ est nilpotent et simplement connexe. Alors $\exp$ est elle-même un difféomorphisme global entre $\mathfrak{g}$ et G . De plus, la

fonction BCH ne comporte plus qu'un nombre fini de termes et devient dans ce cas une fonction polynomiale en X et Y . Enfin, si l'on munit $\mathfrak{g}$ de la loi de groupe de Lie $\odot$ donnée par cette même formule, autrement dit si l'on pose pour $X, Y \in \mathfrak{g}$

$$X \odot Y := BCH(X, Y),$$

alors l'application $\exp$ est un isomorphisme de Lie entre les groupes $(G, \cdot)$ et $(\mathfrak{g}, \odot)$. On peut alors, sous les conditions ci-dessus, légitimement identifier le groupe de Lie original $(G, \cdot)$ avec son algèbre de Lie $(\mathfrak{g}, +, \odot)$. Nous restreindrons encore une fois notre propos pour ne nous préoccuper que de groupes de Lie nilpotents, simplement connexes et d'indice 2. Cette famille particulière est nettement mieux connue que les groupes de Lie nilpotents généraux, ou même seulement que les groupes d'indice 3. En particulier, on connaît des formules explicites donnant les représentations unitaires irréductibles de ces groupes (voir par exemple la sous-section 3.3 et l'équation 4.2). On s'est donc, pour le moment, ramenés à l'étude de l'algèbre de Lie du groupe, qui possède en particulier une structure d'espace vectoriel. Ainsi, tout groupe de Lie nilpotent d'indice 2 simplement connexe est isomorphe à un groupe du type $(\mathbb{R}^{\dim G}, \odot)$, avec $\odot$ une loi à préciser. Avec ce qui précède, connaître $\odot$ est équivalent à connaître le crochet de Lie de $\mathfrak{g}$. Ce crochet est en particulier une application bilinéaire antisymétrique de $\mathfrak{g} \times \mathfrak{g}$ dans $\mathfrak{g}$, qui est de plus nilpotente au sens où si Z est un élément de $[\mathfrak{g}, \mathfrak{g}]$, alors $[Z, \mathfrak{g}] = \{0\}$. Réciproquement, choisissons un entier n et une application bilinéaire antisymétrique

$$\sigma : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}^n$$

telle que pour tout X dans $\mathbb{R}^n$ et tout Z dans $\sigma(\mathbb{R}^n, \mathbb{R}^n)$, la quantité $\sigma(Z, X)$ est nulle. Alors, si l'on définit sur l'ensemble $\mathbb{R}^n$ la loi $\odot$ par

$$\forall X, Y \in \mathbb{R}^n, \quad X \odot Y := X + Y + \frac{1}{2}\sigma(X, Y),$$

la structure $(\mathbb{R}^n, \odot)$ est un groupe de Lie nilpotent simplement connexe d'indice 2. Ceci justifie que l'on ne considère dans la suite que des groupes de Lie dont l'ensemble sous-jacent est $\mathbb{R}^n$ pour un certain entier $n \in \mathbb{N}$, par simple commodité d'écriture. Il est possible de raffiner encore un peu cette caractérisation. Notons p la dimension du centre $\mathfrak{z}$ de $(\mathbb{R}^n, \odot)$ et choisissons une décomposition en somme directe

$$\mathbb{R}^n = \mathfrak{z} \oplus \mathbb{R}^{n-p}.$$

L'application σ se restreint alors en une application bilinéaire antisymétrique de $\mathbb{R}^{n-p} \times \mathbb{R}^{n-p}$ dans $\mathfrak{z}$, que l'on continue de noter σ . On caractérise entièrement les groupes de Lie nilpotents simplement connexes d'indice 2 par le choix d'un entier p supérieur à 1, d'un entier n plus grand que p et d'une application σ vérifiant les conditions énoncées ci-dessus.

Terminons cette sous-section sur une note historique. Parmi les groupes de Lie nilpotents simplement connexes d'indice 2, on trouve la famille des groupes d'Heisenberg $((\mathbb{H}^d, \cdot))_{d \geq 1}$. Dans cette famille, le d -ème groupe a pour dimension totale $2d + 1$ et son centre est toujours de dimension 1. L'application σ s'identifie ici à la forme symplectique canonique σ_c sur $\mathbb{R}^d \times \mathbb{R}^d$ définie à partir du produit scalaire canonique $\langle \cdot, \cdot \rangle$ sur $\mathbb{R}^d$ par

$$\forall (x, y), (x', y') \in \mathbb{R}^d \times \mathbb{R}^d, \quad \sigma_c((x, y), (x', y')) := \langle x, y' \rangle - \langle x', y \rangle.$$

Le premier de ces groupes, $(\mathbb{H}^1, \cdot)$, parfois noté $(H_3(\mathbb{R}), \cdot)$, a permis à W. Heisenberg de montrer l'équivalence entre deux visions de la mécanique quantique : la représentation dite de Schrödinger et celle dite de Heisenberg. On se référera au livre [89] pour plus de détails historiques sur ce sujet.

3.3 Représentations unitaires irréductibles.

Passons maintenant à une famille d'objets qui nous intéressera plus particulièrement dans la suite : les représentations unitaires irréductibles. On rappelle qu'étant donné un groupe $(G, \cdot)$, une représentation de $(G, \cdot)$ est un couple $(\rho, \mathcal{H}_\rho)$ où $\mathcal{H}_\rho$ est un espace vectoriel et

$$\rho : G \longrightarrow GL(\mathcal{H}_\rho)$$

est un morphisme de groupes. La représentation $(\rho, \mathcal{H}_\rho)$ est dite *unitaire* si $\mathcal{H}_\rho$ est un espace de Hilbert (systématiquement supposé séparable) et que pour tout $g \in G$, $\rho(g)$ est un opérateur unitaire sur $\mathcal{H}_\rho$. si $\mathcal{H}_\rho$ et $\{0\}$ sont les seuls sous-espaces *fermés* stables par tous les $\rho(g)$ pour g de G , on dit que ρ est *irréductible*. Deux représentations $(\rho, \mathcal{H}_\rho)$ et $(\rho', \mathcal{H}_{\rho'})$ d'un même groupe $(G, \cdot)$ sont dites *équivalentes* si il existe un isomorphisme

$$\mathcal{I} : \mathcal{H}_\rho \longrightarrow \mathcal{H}_{\rho'}$$

tel que pour tout g de G , le diagramme

$$\begin{array}{ccc} \mathcal{H}_\rho & \xrightarrow{\rho(g)} & \mathcal{H}_\rho \\ \mathcal{I} \downarrow & & \downarrow \mathcal{I} \\ \mathcal{H}_{\rho'} & \xrightarrow{\rho'(g)} & \mathcal{H}_{\rho'} \end{array}$$

soit commutatif. Si de plus on peut choisir $\mathcal{I}$ unitaire, on dit que ρ et ρ' sont unitairement équivalentes. Étant donné un groupe de Lie $(G, \cdot)$ possédant des propriétés topologiques raisonnables (localement compact, séparable) ainsi qu'une propriété algébrique sur laquelle on ne s'étendra pas (l'unimodularité), on note $\widehat{G}$ l'ensemble de ses représentations irréductibles unitaires, quotienté par l'équivalence unitaire de représentations. L'ensemble $\widehat{G}$ s'appelle le dual unitaire de G et a, en toute généralité, une structure extrêmement compliquée. Sauf dans des cas particuliers, $\widehat{G}$ n'est pas naturellement muni d'une structure de groupe ; ce n'est par exemple pas le cas lorsque $(G, \cdot)$ est un groupe d'Heisenberg $(\mathbb{H}^d, \cdot)$ ou le groupe matriciel $(SL_2(\mathbb{R}), \cdot)$. *A contrario*, les duals unitaires de l'espace $(\mathbb{R}^d, +)$ et du tore $(\mathbb{T}^d, +)$ sont naturellement muni de structures de groupes les rendant isomorphes, respectivement, à $((\mathbb{R}^d)^*, +)$ et $(\mathbb{Z}^d, +)$. Ici, $((\mathbb{R}^d)^*, +)$ désigne l'espace vectoriel dual de $(\mathbb{R}^d, +)$.

Dans le cas de l'espace $\mathbb{R}^d$, les représentations unitaires irréductibles sont paramétrées de la façon suivante. Étant donné un complexe z , notons M_z l'opérateur de multiplication par z . Vu comme endomorphisme de $\mathbb{C}$ muni du produit scalaire usuel, M_z est unitaire pour tout z de module unité. Pour ξ dans $(\mathbb{R}^d)^*$, on définit alors la représentation $(M_{e^{-i\langle \xi, \cdot \rangle}}, \mathbb{C})$ par

$$M_{e^{-i\langle \xi, \cdot \rangle}} : \begin{cases} \mathbb{R}^d & \longrightarrow & \mathcal{U}(\mathbb{C}) \\ x_0 & \longmapsto & M_{e^{-i\langle \xi, x_0 \rangle}} \end{cases}$$

Par définition, pour ξ dans $(\mathbb{R}^d)^*$, x_0 dans $\mathbb{R}^d$ et w dans $\mathbb{C}$,

$$M_\xi(x_0)w := e^{-i\langle \xi, x_0 \rangle} w.$$

Ces notations introduites, si $(\rho, \mathcal{H}_\rho)$ est une représentation unitaire irréductible de $(\mathbb{R}^d, +)$, alors il existe ξ dans $(\mathbb{R}^d)^*$ tel que $(\rho, \mathcal{H}_\rho)$ soit unitairement équivalente à $(M_{e^{-i\langle \xi, \cdot \rangle}}, \mathbb{C})$.

3.4 Transformation de Fourier

Revenons maintenant au cas général. Soit μ une mesure de Haar sur G , $f : G \rightarrow \mathbb{C}$ μ -intégrable et $(\rho, \mathcal{H}_\rho)$ dans $\widehat{G}$. On rappelle que μ est une mesure de Haar sur G si μ est une mesure invariante par translation à gauche au sens où pour toute fonction f μ -intégrable et tout g_0 de G ,

$$\int_G f(g_0 \cdot g) d\mu(g) = \int_G f(g) d\mu(g).$$

Dans le cas d'un groupe dont l'ensemble sous-jacent est $\mathbb{R}^n$, les mesures de Haar sont exactement les multiples positifs de la mesure de Lebesgue usuelle. La transformée de Fourier de f en $(\rho, \mathcal{H}_\rho)$, notée $\mathcal{F}^G(f)(\rho)$, est par définition,

$$\mathcal{F}^G(f)(\rho) := \int_G f(g) \rho(g) d\mu(g) \in \mathcal{L}(\mathcal{H}_\rho).$$

Ainsi, pour u dans $\mathcal{H}_\rho$, on a

$$\mathcal{F}^G(f)(\rho) \cdot u := \int_G f(g) (\rho(g) \cdot u) d\mu(g) \in \mathcal{H}_\rho.$$

Une propriété fondamentale de la transformée de Fourier est d'échanger la convolution sur le groupe d'origine avec la composition d'opérateurs sur $\mathcal{H}_\rho$. Si

$$f_1, f_2 : G \longrightarrow \mathbb{C}$$

sont deux fonctions μ -intégrables, on définit leur produit de convolution $f_1 * f_2$ par

$$(f_1 * f_2)(g) := \int_G f_1(g') f_2(g'^{-1}g) d\mu(g') \text{ pour presque tout } g \text{ dans } G.$$

On dispose alors de l'identité de convolution suivante, valable pour toute représentation unitaire irréductible $(\rho, \mathcal{H}_\rho)$ de $\widehat{G}$,

$$\mathcal{F}^G(f_1 * f_2)(\rho) = \mathcal{F}^G(f_1)(\rho) \circ \mathcal{F}^G(f_2)(\rho).$$

Dans le cas de l'espace $(\mathbb{R}^d, +)$ et d'une représentation $(M_{e^{-i\langle \xi, \cdot \rangle}}, \mathbb{C})$, pour w dans $\mathbb{C}$,

$$\mathcal{F}^{\mathbb{R}^d}(f)(M_{e^{-i\langle \xi, \cdot \rangle}}) \cdot w = \int_{\mathbb{R}^d} f(x) (M_{e^{-i\langle \xi, x \rangle}} \cdot w) dx.$$

Notant alors

$$\hat{f} : \xi \longmapsto \int_{\mathbb{R}^d} f(x) e^{-i\langle \xi, x \rangle} dx \in \mathcal{C}_b^0((\mathbb{R}^d)^*),$$

on dispose de l'égalité entre opérateurs linéaires sur $\mathbb{C}$

$$\mathcal{F}^{\mathbb{R}^d}(f)(M_{e^{-i\langle \xi, \cdot \rangle}}) = M_{\hat{f}(\xi)}.$$

Dans le cas de l'espace, la transformation de Fourier écrite dans le langage des représentations unitaires irréductibles est donc équivalente à la transformation de Fourier usuelle, définie et pensée comme une transformation entre fonctions. Dans cet exemple, on a pris soin de différencier dans les notations la fonction f , définie sur $\mathbb{R}^d$, de sa transformée de Fourier $\hat{f}$, définie sur $(\mathbb{R}^d)^*$. Ce choix tient à une raison : en général, il n'existe pas d'identification naturelle entre un groupe et son dual unitaire. À titre de contre-exemple simple, le dual unitaire du tore $(\mathbb{T}^d, +)$ s'identifie au réseau $\mathbb{Z}^d$ et les deux ensembles sous-jacents sont nettement différents ; par exemple, une fois munis de leurs topologies canoniques, l'un est discret non compact tandis que l'autre est compact non discret.

3.5 Décomposition en coefficients matriciels

Donnons-nous une fonction f de $L^1(G, \mu)$, un élément g de G et $(\rho, \mathcal{H}_\rho)$ dans $\widehat{G}$. Plutôt que d'étudier directement l'opérateur unitaire $\rho(g)$, il peut être plus simple de considérer, pour v, w dans $\mathcal{H}_\rho$ et g dans G la quantité

$$m_{v,w}(g) := \langle \rho(g) \cdot v, w \rangle_{L^2(\mathcal{H}_\rho)},$$

appelée *coefficient matriciel* (de la représentation $(\rho, \mathcal{H}_\rho)$ en l'élément g). La théorie autour de ces coefficients est vaste et nous renvoyons le lecteur désireux de mieux connaître la théorie autour de ces fonctions au livre [106]. On définit alors, en suivant l'idée principale de [86], le coefficient matriciel de l'opérateur $\mathcal{F}^G(f)(\rho)$ par

$$\mathcal{F}^G(f)(\rho, v, w) := \langle \mathcal{F}^G(f)(\rho) \cdot v, w \rangle_{L^2(\mathcal{H}_\rho)}.$$

L'espace $\mathcal{H}_\rho$ étant un espace de Hilbert séparable, la connaissance des $\mathcal{F}^G(f)(\rho, v, w)$ lorsque v et w parcourent une base hilbertienne $\mathcal{B}_\rho$ de $\mathcal{H}_\rho$ suffit pour déterminer entièrement $\mathcal{F}^G(f)(\rho)$. Le choix de $\mathcal{B}_\rho$ est alors crucial si l'on souhaite développer une réduction de la théorie de Fourier écrite dans le langage des représentations à une deuxième théorie, souhaitée plus simple à manipuler et plus proche de celle que l'on connaît sur $\mathbb{R}^d$. Ce choix est motivé dans la sous-section suivante par son lien avec le laplacien invariant à gauche, expliquant au passage ce qu'est l'incarnation du laplacien dans ce contexte.

3.6 Lien avec le laplacien

Dans l'espace $\mathbb{R}^d$, une propriété fondamentale de la transformée de Fourier est la diagonalisation du laplacien usuel par l'égalité

$$-\widehat{\Delta_{\mathbb{R}^d} f}(\xi) = |\xi|^2 \hat{f}(\xi).$$

Réécrite en terme d'opérateurs agissant sur $\mathbb{C}$, cette égalité devient

$$\mathcal{F}^{\mathbb{R}^d}(-\Delta_{\mathbb{R}^d} f)(M_{e^{-i\langle \xi, \cdot \rangle}}) = \mathcal{F}^{\mathbb{R}^d}(f)(M_{e^{-i\langle \xi, \cdot \rangle}}) \circ M_{|\xi|^2}.$$

L'opérateur de multiplication que l'on obtient comme conjugué du laplacien sur $\mathbb{R}^d$ par la transformation de Fourier est un opérateur scalaire sur $\mathbb{C}$, en particulier diagonal. Il est donc impossible de le simplifier plus. Dans le cas d'un groupe de Heisenberg $\mathbb{H}^d$ muni de son laplacien invariant à gauche $-\Delta_{\mathbb{H}^d}$, l'opérateur conjugué de $-\Delta_{\mathbb{H}^d}$ sous la transformation de Fourier (qui remplace l'opérateur $M_{|\xi|^2}$ dans ce contexte) est, à un changement d'échelle près, celui associé à l'oscillateur harmonique quantique $-\Delta_{\mathbb{R}^d}^{\text{osc}}$. Ainsi, en oubliant temporairement ce changement d'échelle, on a

$$\mathcal{F}^{\mathbb{H}^d}(-\Delta_{\mathbb{H}^d} f)(\rho) = \mathcal{F}^{\mathbb{H}^d}(f)(\rho) \circ (-\Delta_{\mathbb{R}^d}^{\text{osc}}).$$

Les fonctions propres de $-\Delta_{\mathbb{R}^d}^{\text{osc}}$ sont connues : ce sont les fonctions d'Hermite, notées ici $(H_n)_{n \in \mathbb{N}^d}$. Si l'on note λ_n la valeur propre associée à H_n , i.e. le réel positif tel que

$$-\Delta_{\mathbb{R}^d}^{\text{osc}} H_n = \lambda_n H_n,$$

alors la transformée de Fourier sur $\mathbb{H}^d$ doit satisfaire une égalité du type

$$\mathcal{F}^{\mathbb{H}^d}(-\Delta_{\mathbb{H}^d} f)(\rho) \cdot H_n = \mathcal{F}^{\mathbb{H}^d}(f)(\rho) \circ (-\Delta_{\mathbb{R}^d}^{\text{osc}}) \cdot H_n = \lambda_n \mathcal{F}^{\mathbb{H}^d}(f)(\rho) \cdot H_n,$$

où ρ est une représentation irréductible unitaire quelconque de $\mathbb{H}^d$. En passant aux coefficients matriciels sur la base des fonctions d'Hermite, on obtient alors une égalité à l'aspect familier

$$\mathcal{F}^{\mathbb{H}^d}(-\Delta_{\mathbb{H}^d} f)(\rho, H_m, H_n) = \lambda_m \mathcal{F}^{\mathbb{H}^d}(f)(\rho, H_m, H_n).$$

Ainsi, le choix d'une base hilbertienne adapté au conjugué du laplacien invariant à gauche sur $\mathbb{H}^d$ a permis de le diagonaliser, au sens de l'égalité précédente. Le cas d'un groupe de Lie nilpotent simplement connexe d'indice 2 se traite de manière analogue. On insiste toutefois sur le fait que l'on a omis, dans cette écriture, un changement d'échelle dépendant de ρ qui modifie l'allure des fonctions d'Hermite ainsi que les valeurs propres λ_n . Pour la clarté de l'exposition, on a fait le choix de repousser l'explicitation de ces modifications à une partie ultérieure du manuscrit.

3.7 Résultats

Dans cette dernière partie, nous commençons par préciser la topologie de l'espace des fréquences du groupe et donnons une construction explicite de sa complétion reposant sur une réalisation de cet espace comme un sous-ensemble de l'espace euclidien (Proposition 4.3.1 page 100). Nous munissons ensuite le complété d'une mesure qui est essentiellement une mesure de comptage sur les fibres discrètes et une mesure de Lebesgue sur les fibres continues. Nous montrons que le choix de cette mesure est compatible avec la topologie de l'espace (Proposition 4.3.2 page 103). L'étude de la transformée de Fourier sur le groupe se ramène alors à la connaissance fine des propriétés de régularité, de décroissance ainsi que des identités satisfaites par ce qu'il convient d'appeler le 'noyau de Fourier', analogue dans ce contexte non commutatif de l'exponentielle complexe pour l'espace euclidien. Cette étude est menée de la section 4.4 à la fin de cette dernière partie et culmine dans l'obtention de l'identité (4.11) page 118.

Première partie

Mécanique des fluides incompressibles

Chapitre 1

Un lemme d'unicité et ses applications en mécanique des fluides incompressibles

1.1 Introduction

In their seminal paper [15], R. J. DiPerna and P.-L. Lions proved the existence and uniqueness of solutions to transport equations on $\mathbb{R}^d$. We recall here a slightly simplified version of their statement.

Theorem 1.1.1 (DiPerna-Lions). *Let $d \geq 1$ be an integer. Let $1 \leq p \leq \infty$ and p' its Hölder conjugate. Let a_0 be in $L^p(\mathbb{R}^d)$. Let v be a fixed divergence free vector field in $L^1_{loc}(\mathbb{R}_+, \dot{W}^{1,p'}(\mathbb{R}^d))$. Then there exists a unique distributional solution a in $L^\infty(\mathbb{R}_+, L^p(\mathbb{R}^d))$ of the Cauchy problem*

$$\begin{cases} \partial_t a + \nabla \cdot (av) = 0 \\ a(0) = a_0, \end{cases} \quad (1.1)$$

with the initial condition understood in the sense of $\mathcal{C}^0(\mathbb{R}_+, \mathcal{D}'(\mathbb{R}^d))$. We recall that a is a distributional solution of the aforementioned Cauchy problem if and only if, for any φ belonging to $\mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$ and any $T > 0$, there holds

$$\int_0^T \int_{\mathbb{R}^d} a(t, x) (\partial_t \varphi(t, x) + v(t, x) \cdot \nabla \varphi(t, x)) dx dt = \int_{\mathbb{R}^d} a(T, x) \varphi(T, x) dx - \int_{\mathbb{R}^d} a_0(x) \varphi(0, x) dx. \quad (1.2)$$

Beyond this theorem, many authors have since proved similar existence and (non-)uniqueness theorems, see for instance [1], [2], [4], [5], [6], [14], [23], [24], [26] and references therein. In particular, the papers [4], [5] and [6] use a duality method which is close in spirit to our results. Our key result, which relies on the maximum principle for the *adjoint* equation, is both more general and more restrictive than the DiPerna-Lions theorem. The generality comes from the wider range of exponents allowed, along with the affordability of additional scaling-invariant and/or dissipative terms in the equation. We thus extend the result from [27], where the setting was restricted to the $L^2_{t,x}$ case and no right-hand side was considered. On the other hand, we do not fully extend the original theorem, since we are unable to prove the existence of solutions in the uniqueness classes. Here is the statement.

Theorem 1.1.2. *Let $d \geq 1$ be an integer. Let $\nu \geq 0$ be a positive parameter. Let $1 \leq p, q \leq \infty$ be real numbers with Hölder conjugates p' and q' . Let $v = v(t, x)$ be a fixed, divergence free vector*

field in $L^{p'}(\mathbb{R}_+, \dot{W}^{1,q'}(\mathbb{R}^d))$. Given a time $T^* > 0$, let a be in $L^p([0, T^*], L^q(\mathbb{R}^d))$. Assume that a is a distributional solution of the Cauchy problem

$$(C) \begin{cases} \partial_t a + \nabla \cdot (av) - \nu \Delta a = 0 \\ a(0) = 0, \end{cases} \quad (1.3)$$

with the initial condition understood in the sense of $\mathcal{C}^0([0, T^*], \mathcal{D}'(\mathbb{R}^d))$. That is, we assume that, for any function φ in $\mathcal{D}(\mathbb{R}_+ \times \mathbb{R}^d)$ and any $T > 0$, there holds

$$\int_{\mathbb{R}_+ \times \mathbb{R}^d} a(t, x) (\partial_t \varphi(t, x) + v(t, x) \cdot \nabla \varphi(t, x) + \nu \Delta \varphi(t, x)) dx dt = \int_{\mathbb{R}^d} u(T, x) \varphi(T, x) dx. \quad (1.4)$$

Then a is identically zero on $[0, T^*] \times \mathbb{R}^d$.

Though one may fear that the lack of existence might render the theorem unapplicable in practice, it does not. For instance, when working with the Navier-Stokes equations, the vorticity of a Leray solution only belongs, a priori, to

$$L^\infty(\mathbb{R}_+, \dot{H}^{-1}(\mathbb{R}^d)) \cap L^2(\mathbb{R}_+ \times \mathbb{R}^d).$$

In particular, the only Lebesgue-type space to which this vorticity belongs is $L^2(\mathbb{R}_+ \times \mathbb{R}^d)$. Our theorem is well suited for solutions possessing *a priori* no integrable derivative whatsoever.

As such, our theorem appears a regularization tool. The philosophy is that, if an equation has smooth solutions, then any sufficiently integrable *weak* solution is automatically smooth. We illustrate our theorem with an application to the regularity result of J. Serrin [32] and subsequent authors [3], [8], [10], [17], [18], [19], [21], [35], [38]. The key point in our proof is the maximum principle of the *adjoint equation*. The validity of the maximum principle partially depends on the vorticity equation having only differential operators rather than pseudodifferential ones.

Another standpoint on this theorem, which we owe to a private communication from N. Masmoudi, is that we now have two ways to recover regularity on the vorticity field Ω from the velocity. We may either use the defining identity

$$\Omega := \nabla \wedge u$$

or that Ω is a solution of the linear problem

$$(NSV) \begin{cases} \partial_t \Omega + \nabla \cdot (\Omega \otimes u) - \Delta \Omega = \nabla \cdot (u \otimes \Omega) \\ \Omega(0) = \nabla \wedge u_0. \end{cases}$$

The second choice makes a strong use of the peculiar algebra of the Navier-Stokes equations, while the first one is general and requires no other assumption on u than the divergence-free condition. Thus, we may hope to garner more information from the vorticity uniqueness, even though it may seem circuitous.

1.2 Results

Let us comment a bit on the strategy we shall use. First, because a lies in a low-regularity class of distributions, energy-type estimates seem out of reach. Thus, a duality argument is much more adapted to our situation. Given the assumptions on a , which for instance imply that Δa is in $L^p(\mathbb{R}_+, \dot{W}^{-2,q}(\mathbb{R}^d))$, we need to prove the following existence result.

Theorem 1.2.1. *Let $\nu \geq 0$ be a positive real number. Let $v = v(t, x)$ be a fixed, divergence free vector field in $L^{p'}(\mathbb{R}_+, \dot{W}^{1, q'}(\mathbb{R}^d))$. Let φ_0 be a smooth, compactly supported function in $\mathbb{R}^d$. There exists a function φ in $L^\infty(\mathbb{R}_+ \times \mathbb{R}^d)$ solving*

$$(C') \begin{cases} \partial_t \varphi - \nabla \cdot (\varphi v) - \nu \Delta \varphi = 0 \\ \varphi(0) = \varphi_0 \end{cases} \quad (1.5)$$

in the sense of distributions and satisfying the estimate

$$\|\varphi(t)\|_{L^\infty(\mathbb{R}^d)} \leq \|\varphi_0\|_{L^\infty(\mathbb{R}^d)}.$$

Picking some positive time $T > 0$ and considering $\varphi(T - \cdot)$ instead of φ , Theorem 1.2.1 amounts to build, for $T > 0$, a solution on $[0, T] \times \mathbb{R}^d$ of the Cauchy problem

$$(-C') \begin{cases} -\partial_t \varphi - \nabla \cdot (\varphi v) - \nu \Delta \varphi = 0 \\ \varphi(T) = \varphi_0. \end{cases} \quad (1.6)$$

This theorem is a slight generalization of the analogue theorem in the Note [27]. The proof we provide here follows the same lines but retains only the key estimate, which is the boundedness of the solution. The additional estimate in the Note was inessential and had the inconvenient to degenerate when the viscosity coefficient is small. In contrast, the boundedness is unaffected by such changes. The techniques used in the proof of Theorem 1.2.1 are robust. This robustness is encouraging for future work, as many generalizations are possible depending on the needs. We will not try to list them all; instead, we give some examples of possible adaptations to other contexts. The most direct one is its analogue for diagonal systems, for uniqueness in this case reduces to applying the scalar case to each component of the solution. Alternatively, one may add various linear, scaling invariant terms on the right hand side, or any dissipative term (such as a fractional laplacian) on the left hand side. Also, in view of application to compressible fluid mechanics, the main theorems remain true without the divergence freeness of the transport field provided that the negative part of its divergence belongs to $L^1(\mathbb{R}_+, L^\infty(\mathbb{R}^d))$. This extension was already present in the original paper [15] from R.J. DiPerna and P.-L. Lions.

1.3 Proofs

We state here a commutator lemma, similar to Lemma II.1 in [15], which we will use in the proof of Theorem 1.1.2.

Lemma 1.3.1. *Let $T > 0$. Let v be a fixed, divergence free vector field in $L^{p'}(\mathbb{R}_+, \dot{W}^{1, q'}(\mathbb{R}^d))$. Let a be a fixed function in $L^p(\mathbb{R}_+, L^q(\mathbb{R}^d))$. Let $\rho = \rho(x)$ be some smooth, positive and compactly supported function on $\mathbb{R}^d$. Normalize ρ to have unit norm in $L^1(\mathbb{R}^d)$ and define $\rho_\varepsilon := \varepsilon^{-d} \rho(\frac{\cdot}{\varepsilon})$. Define the commutator C^ε by*

$$C^\varepsilon(t, x) := v(t, x) \cdot (\nabla \rho_\varepsilon * a(t))(x) - (\nabla \rho_\varepsilon * (v(t)a(t)))(x).$$

Then, as $\varepsilon \rightarrow 0$,

$$\|C^\varepsilon\|_{L^1(\mathbb{R}_+ \times \mathbb{R}^d)} \rightarrow 0.$$

Proof. For almost all (t, x) in $\mathbb{R}_+ \times \mathbb{R}^d$, we have

$$C^\varepsilon(t, x) = \int_{\mathbb{R}^d} \frac{1}{\varepsilon^d} a(t, y) \frac{v(t, x) - v(t, y)}{\varepsilon} \cdot \nabla \rho\left(\frac{x - y}{\varepsilon}\right) dy.$$

Performing the change of variable $y = x + \varepsilon z$ yields

$$C^\varepsilon(t, x) = \int_{\mathbb{R}^d} a(t, x + \varepsilon z) \frac{v(t, x) - v(t, x + \varepsilon z)}{\varepsilon} \cdot \nabla \rho(z) dz.$$

Using the Taylor formula

$$v(\cdot, x + \varepsilon z) - v(\cdot, x) = \int_0^1 \nabla v(\cdot, x + r\varepsilon z) \cdot (\varepsilon z) dr,$$

which is true for smooth functions and extends to $\dot{W}^{1, q'}(\mathbb{R}^d)$ thanks to the continuity of both sides on this space and owing to Fubini's theorem to exchange integrals, we get the nicer formula

$$C^\varepsilon(t, x) = - \int_0^1 \int_{\mathbb{R}^d} a(t, x + \varepsilon z) \nabla v(t, x + r\varepsilon z) : (\nabla \rho(z) \otimes z) dz dr,$$

where $:$ denotes the contraction of rank two tensors. Because q and q' are dual Hölder exponents, at least one of them is finite. We assume for instance that $q < \infty$, the case $q' < \infty$ being completely similar.

Let

$$\tilde{C}^\varepsilon(t, x) := - \int_0^1 \int_{\mathbb{R}^d} a(t, x + r\varepsilon z) \nabla v(t, x + r\varepsilon z) : (\nabla \rho(z) \otimes z) dz dr.$$

We claim that, as $\varepsilon \rightarrow 0$,

$$\|C^\varepsilon - \tilde{C}^\varepsilon\|_{L^1(\mathbb{R}_+ \times \mathbb{R}^d)} \rightarrow 0.$$

Integrating both in space and time and owing to Hölder's inequality, we have

$$\begin{aligned} \|C^\varepsilon - \tilde{C}^\varepsilon\|_{L^1(\mathbb{R}_+ \times \mathbb{R}^d)} &\leq \\ &\int_0^1 \int_{\mathbb{R}^d} \int_0^\infty \|a(t, \cdot + \varepsilon z) - a(t, \cdot + r\varepsilon z)\|_{L^q(\mathbb{R}^d)} \|\nabla v(t)\|_{L^{q'}(\mathbb{R}^d)} |\nabla \rho(z) \otimes z| dt dz dr. \end{aligned}$$

Since $a \in L^p(\mathbb{R}_+, L^q(\mathbb{R}^d))$ and $q < \infty$, for almost any $t \in \mathbb{R}_+$, for all $z \in \mathbb{R}^d$ and $r \in [0, 1]$,

$$\|a(t, \cdot + \varepsilon z) - a(t, \cdot + r\varepsilon z)\|_{L^q(\mathbb{R}^d)} \rightarrow 0$$

as $\varepsilon \rightarrow 0$. Thanks to the uniform bound

$$\begin{aligned} \|a(t, \cdot + \varepsilon z) - a(t, \cdot + r\varepsilon z)\|_{L^q(\mathbb{R}^d)} \|\nabla v(t)\|_{L^{q'}(\mathbb{R}^d)} |\nabla \rho(z) \otimes z| &\leq \\ &2 \|a(t)\|_{L^q(\mathbb{R}^d)} \|\nabla v(t)\|_{L^{q'}(\mathbb{R}^d)} |\nabla \rho(z) \otimes z|, \end{aligned}$$

we may invoke the dominated convergence theorem to get the desired claim.

From this point on, we denote by $U(t, x)$ the quantity $a(t, x) \nabla v(t, x)$. We notice that U is a fixed function in $L^1(\mathbb{R}_+ \times \mathbb{R}^d)$ and that, by definition,

$$\tilde{C}^\varepsilon(t, x) = - \int_0^1 \int_{\mathbb{R}^d} U(t, x + r\varepsilon z) : (\nabla \rho(z) \otimes z) dz dr.$$

The normalization on ρ yields the identity

$$-\int_{\mathbb{R}^d} \nabla \rho(z) \otimes z dz = \left(\int_{\mathbb{R}^d} \rho(z) dz \right) I_d = I_d,$$

where I_d is the d -dimensional identity matrix. This identity in turn entails that

$$\tilde{C}^0(t, x) = a(t, x) \nabla v(t, x) : I_d = a(t, x) \operatorname{div} v(t, x) = 0.$$

A second application of the dominated convergence theorem to the function U gives

$$\|\tilde{C}^\varepsilon - \tilde{C}^0\|_{L^1(\mathbb{R}_+ \times \mathbb{R}^d)} \rightarrow 0$$

as $\varepsilon \rightarrow 0$, from which the lemma follows. $\square$

Proof of Theorem 1.2.1. Let us choose some mollifying kernel $\rho = \rho(x)$ and denote $v_\delta := \rho_\delta * v$, where $\rho_\delta(x) := \delta^{-d} \rho(\frac{x}{\delta})$. Let (C'_δ) be the Cauchy problem (C') where we replaced v by v_δ . The existence of a (smooth) solution φ^δ to (C'_δ) is then easily obtained thanks to, for instance, a Friedrichs method combined with heat kernel estimates. We now turn to the L^∞ bound uniform in δ .

Let $r \geq 2$ be a real number. Multiplying the equation on φ^δ by $\varphi^\delta |\varphi^\delta|^{r-2}$ and integrating in space and time, we get

$$\frac{1}{r} \|\varphi^\delta(t)\|_{L^r(\mathbb{R}^d)}^r + (r-1) \int_0^t \|\nabla \varphi^\delta(s) |\varphi^\delta(s)|^{\frac{r-2}{2}}\|_{L^2(\mathbb{R}^d)}^2 ds = \frac{1}{r} \|\varphi_0\|_{L^r(\mathbb{R}^d)}^r.$$

Discarding the gradient term, taking r -th root in both sides and letting r go to infinity gives

$$\|\varphi^\delta(t)\|_{L^\infty(\mathbb{R}^d)} \leq \|\varphi_0\|_{L^\infty(\mathbb{R}^d)}. \quad (1.7)$$

Thus, the family $(\varphi^\delta)_\delta$ is bounded in $L^\infty(\mathbb{R}_+ \times \mathbb{R}^d)$. Up to an extraction, $(\varphi^\delta)_\delta$ converges weak-* in $L^\infty(\mathbb{R}_+ \times \mathbb{R}^d)$ to some function φ .

As a consequence, because $v_\delta \rightarrow v$ strongly in $L^1_{loc}(\mathbb{R}_+ \times \mathbb{R}^d)$ as $\delta \rightarrow 0$, the following convergences hold :

$$\begin{aligned} \Delta \varphi^\delta &\rightharpoonup^* \Delta \varphi \text{ in } L^\infty(\mathbb{R}_+, \dot{W}^{-2,\infty}(\mathbb{R}^d)); \\ \varphi^\delta v^\delta &\rightharpoonup \varphi v \text{ in } L^1_{loc}(\mathbb{R}_+ \times \mathbb{R}^d). \end{aligned}$$

In particular, such a φ is a distributional solution of (C') with the desired regularity. $\square$

We are now in position to prove the main theorem of this paper.

Proof of Theorem 1.1.2. Let $\rho = \rho(x)$ be a radial mollifying kernel and define $\rho_\varepsilon(x) := \varepsilon^{-d} \rho(\frac{x}{\varepsilon})$. Convoluting the equation on a by ρ_ε gives, denoting $a_\varepsilon := \rho_\varepsilon * a$,

$$(C_\varepsilon) \quad \partial_t a_\varepsilon + \nabla \cdot (a_\varepsilon v) - \nu \Delta a_\varepsilon = C^\varepsilon,$$

where the commutator C^ε has been defined in Lemma 1.3.1. Notice that even without any smoothing in time, $a_\varepsilon, \partial_t a_\varepsilon$ lie respectively in $L^\infty(\mathbb{R}_+, \mathcal{C}^\infty(\mathbb{R}^d))$ and $L^1(\mathbb{R}_+, \mathcal{C}^\infty(\mathbb{R}^d))$, which is enough to make the upcoming computations rigorous. In what follows, we let φ^δ be a solution of the Cauchy problem $(-C'_\delta)$, where $(-C'_\delta)$ is $(-C')$ with v replaced by v_δ . Let us now multiply, for $\delta, \varepsilon > 0$ the equation (C_ε) by φ^δ and integrate in space and time. After integrating by parts (which is justified by the high regularity of the terms we have written), we get

$$\int_0^T \int_{\mathbb{R}^d} \partial_t a_\varepsilon(s, x) \varphi^\delta(s, x) dx ds = \langle a_\varepsilon(T), \varphi_0 \rangle_{\mathcal{D}'(\mathbb{R}^d), \mathcal{D}(\mathbb{R}^d)} - \int_0^T \int_{\mathbb{R}^d} a_\varepsilon(s, x) \partial_t \varphi^\delta(s, x) dx ds.$$

From this identity, it follows that

$$\begin{aligned} \langle a_\varepsilon(T), \varphi_0 \rangle_{\mathcal{D}'(\mathbb{R}^d), \mathcal{D}(\mathbb{R}^d)} &= \int_0^T \int_{\mathbb{R}^d} \varphi^\delta(s, x) C^\varepsilon(s, x) dx ds \\ &\quad - \int_0^T \int_{\mathbb{R}^d} a_\varepsilon(s, x) \left(-\partial_t \varphi^\delta(s, x) - \nabla \cdot (v(s, x) \varphi^\delta(s, x)) - \nu \Delta \varphi^\delta(s, x) \right) dx ds. \end{aligned}$$

From Lemma 1.3.1, we know in particular that C^ε belongs to $L^1(\mathbb{R}_+ \times \mathbb{R}^d)$ for each fixed $\varepsilon > 0$. Thus, in the limit $\delta \rightarrow 0$, we have, for each $\varepsilon > 0$,

$$\int_0^T \int_{\mathbb{R}^d} \varphi^\delta(s, x) C^\varepsilon(s, x) dx ds \rightarrow \int_0^T \int_{\mathbb{R}^d} \varphi(s, x) C^\varepsilon(s, x) dx ds.$$

On the other hand, the definition of φ^δ gives

$$-\partial_t \varphi^\delta - \nabla \cdot (v \varphi^\delta) - \nu \Delta \varphi^\delta = \nabla \cdot ((v_\delta - v) \varphi^\delta).$$

Thus, the last integral in the above equation may be rewritten, integrating by parts,

$$- \int_0^T \int_{\mathbb{R}^d} \varphi^\delta (v_\delta - v) \cdot \nabla a_\varepsilon(s, x) dx ds.$$

For each fixed ε , the assumption on a entails that ∇a_ε belongs to $L^p(\mathbb{R}_+, L^q(\mathbb{R}^d))$. Furthermore, it is an easy exercise to show that

$$\|v_\delta - v\|_{L^{p'}(\mathbb{R}_+, L^{q'}(\mathbb{R}^d))} \leq \delta \|\nabla v\|_{L^{p'}(\mathbb{R}_+, L^{q'}(\mathbb{R}^d))} \|\cdot\|_{L^1(\mathbb{R}^d)}.$$

Now, taking the limit $\delta \rightarrow 0$ while keeping $\varepsilon > 0$ fixed, we have

$$\langle a_\varepsilon(T), \varphi_0 \rangle_{\mathcal{D}'(\mathbb{R}^d), \mathcal{D}(\mathbb{R}^d)} = \int_0^T \int_{\mathbb{R}^d} \varphi(s, x) C^\varepsilon(s, x) dx ds.$$

Taking the limit $\varepsilon \rightarrow 0$ and using Lemma 1.3.1, we finally obtain

$$\langle a(T), \varphi_0 \rangle_{\mathcal{D}'(\mathbb{R}^d), \mathcal{D}(\mathbb{R}^d)} = 0.$$

This being true for any test function φ_0 , $a(T)$ is the zero distribution and finally $a \equiv 0$. $\square$

Chapitre 2

Sur un critère de Serrin anisotrope pour les solutions faibles des équations de Navier-Stokes

2.1 Presentation of the problem

The present paper deals with the regularity of the Leray solutions of the incompressible Navier-Stokes equations in dimension three in space. We recall that these equations are

$$\begin{cases} \partial_t u + \nabla \cdot (u \otimes u) - \Delta u = -\nabla p, & t \geq 0, x \in \mathbb{X}^3, \\ \operatorname{div} u \equiv 0, \\ u(0) = u_0. \end{cases} \quad (2.1)$$

Here, $u = (u^1, u^2, u^3)$ stands for the velocity field of the fluid, p is the pressure and we have set for simplicity the viscosity equal to 1. We use the letter $\mathbb{X}$ to denote $\mathbb{R}$ and $\mathbb{T}$ whenever the current claim or proposition applies to both of them. Let us first recall the existence theorem proved by J. Leray in his celebrated paper [25].

Theorem 2.1.1 (J. Leray, 1934). *Let us assume that u_0 belongs to the energy space $L^2(\mathbb{X}^3)$. Then there exists at least one vector field u in the energy space $L^\infty(\mathbb{R}_+, L^2(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, H^1(\mathbb{X}^3))$ which solves the system (2.1) in the weak sense. Moreover, the solution u satisfies for all $t \geq 0$ the energy inequality*

$$\frac{1}{2} \|u(t)\|_{L^2(\mathbb{X}^3)}^2 + \int_0^t \|\nabla u(s)\|_{L^2(\mathbb{X}^3)}^2 ds \leq \frac{1}{2} \|u_0\|_{L^2(\mathbb{X}^3)}^2.$$

Uniqueness of such solutions, however, remains an outstanding open problem to this day. In his paper from 1961 [32], J. Serrin proved that, if one assumes that there exists a weak solution which is mildly regular, then it is actually smooth in space and time. More precisely, J. Serrin proved that if a weak solution u belongs to $L^p([T_1, T_2], L^q(D))$ for a time interval $]T_1, T_2[$ and some bounded domain $D \Subset \mathbb{X}$ with the restriction that $\frac{2}{p} + \frac{3}{q}$ is strictly smaller than 1, then this weak solution is $\mathcal{C}^\infty$ on $]T_1, T_2[\times D$. Following his path, many other authors proved results in the same spirit, with different regularity assumptions and/or covering limit cases. Let us cite for instance [3], [8], [17], [18], [19], [21], [35], [38] and references therein.

In this paper, we prove two results of the type we mentioned above : the first one is stated in the torus, while the second one is in a spatial domain in the usual Euclidean space. Thanks to the compactness of the torus, the first result is easier to prove than its local-in-space counterpart.

For this reason, we will use the torus case as a toy model, thus avoiding many technicalities and enlightening the overall strategy of the proof.

In the torus, the theorem writes as follows.

Theorem 2.1.2. *Let u be a Leray solution of the Navier-Stokes equations set in $\mathbb{R}_+ \times \mathbb{T}^3$*

$$\begin{cases} \partial_t u + \nabla \cdot (u \otimes u) - \Delta u = -\nabla p \\ u(0) = u_0 \end{cases}$$

with initial data u_0 in $L^2(\mathbb{T}^3)$ and assume that there exists a time interval $]T_1, T_2[$ such that its third component u^3 satisfies

$$u^3 \in L^2(]T_1, T_2[, W^{2, \frac{3}{2}}(\mathbb{T}^3)).$$

Then u is actually smooth in time and space on $]T_1, T_2[\times \mathbb{T}^3$ and satisfies the Navier-Stokes equations in the classical strong sense.

In a subdomain of the whole space, we need to add a technical assumption on the initial data, namely that it belongs to some particular L^p space with p strictly smaller than 2. Notice that such an assumption is automatically satisfied in the torus, thank to its compactness.

Theorem 2.1.3. *Let u be a Leray solution of the Navier-Stokes equations set in $\mathbb{R}_+ \times \mathbb{R}^3$*

$$\begin{cases} \partial_t u + \nabla \cdot (u \otimes u) - \Delta u = -\nabla p \\ u(0) = u_0 \end{cases}$$

with initial data u_0 in $L^2(\mathbb{R}^3) \cap L^{\frac{3}{2}}(\mathbb{R}^3)$ and assume that there exists a time interval $]T_1, T_2[$ and a spatial domain $D \Subset \mathbb{R}^3$ of compact closure such that its third component u^3 satisfies

$$u^3 \in L^2(]T_1, T_2[, W^{2, \frac{3}{2}}(D)).$$

Then, on $]T_1, T_2[\times D$, u is actually smooth in time and space and satisfies the Navier-Stokes equations in the classical strong sense.

Compared to the classical case, our result may seem weaker, as we require two space derivatives in $L^{\frac{3}{2}}$. However, the space in which we assume to have u^3 is actually at the same scaling than $L^2(]T_1, T_2[, L^\infty(D))$ or $L^2(]T_1, T_2[, BMO(D))$, which are more classically found in regularity theorems such as the one of J. Serrin. In the scaling sense, our assumption is as strong as the usual Serrin criterion. We demand a bit more in terms of spatial regularity because of the anisotropic nature of the criterion.

2.2 Overview of the proof

Our strategy draws its inspiration from the anisotropic rewriting of the Navier-Stokes system done in [10], though it also bears resemblance to the work of [1], [2], [14], [23], [26]. Letting

$$\Omega := \text{rot } u = (\omega_1, \omega_2, \omega_3), \quad \omega := \omega_3,$$

we notice that ω solves a transport-diffusion equation with $\Omega \cdot \nabla u^3$ as a forcing term. This equation writes

$$\begin{cases} \partial_t \omega + \nabla \cdot (\omega u) - \Delta \omega = \Omega \cdot \nabla u^3 \\ \omega(0) = \omega_0, \end{cases} \quad (2.2)$$

for some ω_0 which we do not specify. Actually, because we will assume more regularity on u^3 than given by the J.Leray theorem on a time interval which does not contain 0 in its closure, we will focus our attention on a truncated version of ω , for which the initial data is equal to 0. For the clarity of the discussion to follow, we drop any mention of the cut-off terms in this section. In the same vein, we will act as if Lebesgue spaces on $\mathbb{R}^3$ were ordered, which is of course only true on compact subdomains of $\mathbb{R}^3$.

Viewing Equation (2.2) as some abstract PDE problem, we are able to show, by a classical approximation procedure, the existence of *some* solution, call it $\tilde{\omega}$, which belongs to what we shall call the energy space associated to $L^{\frac{6}{5}}(\mathbb{X}^3)$, namely

$$L^\infty(\mathbb{R}_+, L^{\frac{6}{5}}(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, \dot{W}^{1, \frac{6}{5}}(\mathbb{X}^3)).$$

Thanks to Sobolev embeddings, we have $L^{\frac{6}{5}}(\mathbb{X}^3) \hookrightarrow \dot{H}^{-1}(\mathbb{X}^3)$ and $\dot{W}^{1, \frac{6}{5}}(\mathbb{X}^3) \hookrightarrow L^2(\mathbb{X}^3)$. In particular, this energy space is a subspace of $L^2(\mathbb{R}_+ \times \mathbb{X}^3)$. We then conclude that $\tilde{\omega}$ is actually equal to ω thanks to a uniqueness result in $L^2(\mathbb{R}_+ \times \mathbb{X}^3)$ for Equation (2.2). In particular, our ω has now an improved regularity, a fact which we will prove useful in the sequel.

At this stage, two things are to be emphasized. The first one is that the uniqueness result comes alone, without any existential counterpart. To put it plainly, we are *not* able to prove existence of solutions in the class where we are seeking uniqueness, contrary to, for instance, the now classical results from DiPerna-Lions *et al.* The existence here is given from the outside by the very properties of the Navier-Stokes equations.

The second one is the absence of any L^p bound uniform in time in the uniqueness class. From the algebra of the equation and the regularity assumption we made, one could indeed deduce boundedness in time but only in a Sobolev space of strongly negative index, like $H^{-2}(\mathbb{X}^3)$. The author is unaware of any uniqueness result for similar equations in such low-regularity spaces of distributions.

We then proceed to decompose the full vorticity Ω only in terms of ω and $\partial_3 u^3$, thanks to the div-curl decomposition, otherwise known as the Biot-Savart law. This decomposition essentially relies on the fact that a $2D$ vector field is determined by its $2D$ vorticity and divergence. In the case of (u^1, u^2) , its $2D$ divergence is $-\partial_3 u^3$, because u is divergence free and its $2D$ vorticity is exactly ω .

Let us introduce some piece of notation, which is taken from [10]. We denote

$$\nabla_h := (\partial_1, \partial_2), \quad \nabla_h^\perp := (-\partial_2, \partial_1), \quad \Delta_h := \partial_1^2 + \partial_2^2.$$

Hence, we can write, denoting $u^h := (u^1, u^2)$,

$$u^h = u_{\text{curl}}^h + u_{\text{div}}^h,$$

where

$$u_{\text{curl}}^h := \nabla_h^\perp \Delta_h^{-1} \omega, \quad u_{\text{div}}^h := \nabla_h \Delta_h^{-1} (-\partial_3 u^3).$$

We thus obtain a decomposition of the force $\Omega \cdot \nabla u^3$ into a sum of terms which are of two types. The first are linear in both ω and u^3 , while the others are quadratic in u^3 and contain no occurrence of ω . The first ones write as

$$\omega \partial_3 u^3 + \partial_2 u^3 \partial_3 u_{\text{curl}}^1 - \partial_1 u^3 \partial_3 u_{\text{curl}}^2,$$

while the terms quadratic in u^3 are

$$\partial_2 u^3 \partial_3 u_{\text{div}}^1 - \partial_1 u^3 \partial_3 u_{\text{div}}^2.$$

In other words, our ω is now the solution of some modified, anisotropic transport-diffusion equation with forcing terms. The forcing terms are exactly those quadratic in u^3 mentioned above and by our assumption on u^3 , they lie in $L^1(\mathbb{R}_+, L^{\frac{3}{2}}(\mathbb{X}^3))$.

We use again our strategy based on uniqueness. On this new, anisotropic equation, we prove a uniqueness result *in a regularity class in which ω now lies*, that is, in

$$L^\infty(\mathbb{R}_+, L^{\frac{6}{5}}(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, \dot{W}^{1, \frac{6}{5}}(\mathbb{X}^3)),$$

which is a space of functions more regular than the mere $L^2(\mathbb{R}_+ \times \mathbb{R}^3)$ given by J. Leray existence theorem. We then proceed to prove the existence of a solution to this anisotropic equation in the energy space associated to $L^{\frac{3}{2}}(\mathbb{R}^3)$, which is

$$L^\infty(\mathbb{R}_+, L^{\frac{3}{2}}(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, W^{1, \frac{3}{2}}(\mathbb{X}^3)).$$

Again, Sobolev and Lebesgue embeddings (see the remark in the beginning of this section) entail that the energy space associated to $L^{\frac{3}{2}}(\mathbb{X}^3)$ embeds in that associated to $L^{\frac{6}{5}}(\mathbb{X}^3)$. Thanks to the second uniqueness result, we deduce once again that ω has more regularity than assumed. More precisely, we have proved that ω lies in

$$L^\infty(\mathbb{R}_+, L^{\frac{3}{2}}(\mathbb{X}^3)) \cap L^2(\mathbb{R}_+, W^{1, \frac{3}{2}}(\mathbb{X}^3)).$$

Now that we have lifted the regularity of ω (which, we recall, is a shorthand for ω_3) to that of ∇u^3 , it remains to improve the two other components of the vorticity. Keeping in mind that we now control two independant quantities in a high regularity space instead of one as we originally assumed, the remainder of the proof shall be easier than its beginning.

At first sight, ω_1 and ω_2 solve two equations which both look very similar to Equation (2.2). Indeed, we have

$$\begin{cases} \partial_t \omega_1 + \nabla \cdot (\omega_1 u) - \Delta \omega_1 = \Omega \cdot \nabla u^1 \\ \partial_t \omega_2 + \nabla \cdot (\omega_2 u) - \Delta \omega_2 = \Omega \cdot \nabla u^2. \end{cases} \quad (2.3)$$

We again make use of the div-curl decomposition, but in a somewhat *adaptive* manner. Recall that, when we improved the regularity of ω_3 , we performed a div-curl decomposition with respect to the third variable. Such a decomposition has the drawback of forcing the appearance of anisotropic operators, which make lose regularity in some variables and gain regularity in others.

Let us pause for a moment to notice something interesting. From the div-curl decomposition with respect to the third variable, we know that we may write

$$u^h := (u^1, u^2) = \nabla_h^\perp \Delta_h^{-1} \omega + \nabla_h \Delta_h^{-1} (-\partial_3 u^3).$$

Taking the horizontal gradient then gives

$$\nabla_h u^h = \nabla_h \nabla_h^\perp \Delta_h^{-1} \omega + \nabla_h^2 \Delta_h^{-1} (-\partial_3 u^3).$$

That is, $\nabla_h u^h$ may be written as a linear combination of zero order *isotropic* differential operators applied to ω_3 and $\partial_3 u^3$. In other words, as a consequence of the Hörmander-Mikhlin theorem in three dimensions, the four components of the jacobian matrix $\partial_i u^j$ for i and j between 1 and 2 have the same regularity as ω_3 and $\partial_3 u^3$.

Now that we have some regularity on both u^3 and ω_3 , we may choose to perform the div-curl decomposition with respect to the second variable for u^1 and to the first variable for u^2 . Since the 2D divergence of (u^3, u^1) is $-\partial_2 u^2$ and its 2D vorticity is ω_2 , we have

$$u^1 = \partial_3 \Delta_{(1,3)}^{-1} \omega_2 - \partial_1 \Delta_{(1,3)}^{-1} \partial_2 u^2.$$

In turn, taking the derivative with respect to the third variable gives

$$\partial_3 u^1 = \partial_3^2 \Delta_{(1,3)}^{-1} \omega_2 - \partial_3 \partial_1 \Delta_{(1,3)}^{-1} \partial_2 u^2.$$

That is, $\partial_3 u^1$ may be expressed as the sum of a term linear in ω_2 and a source term which is, for instance, in $L^2(\mathbb{R}_+, L^3(\mathbb{X}^3))$. A similar decomposition also applies to $\partial_3 u^2$. Consequently, the system on (ω_1, ω_2) may be recast informally in the following form.

$$\begin{cases} \partial_t \omega_1 + \nabla \cdot (\omega_1 u) - \Delta \omega_1 = (\text{lin. term in } \omega_2) + (\text{source terms in } L^1(\mathbb{R}_+, L^{\frac{3}{2}}(\mathbb{X}^3))) \\ \partial_t \omega_2 + \nabla \cdot (\omega_2 u) - \Delta \omega_2 = (\text{lin. term in } \omega_1) + (\text{source terms in } L^1(\mathbb{R}_+, L^{\frac{3}{2}}(\mathbb{X}^3))). \end{cases}$$

Thus, it only remains to prove a uniqueness lemma similar to what we did for Equation (2.2), along with an existence statement in the energy space associated to $L^{\frac{3}{2}}(\mathbb{X}^3)$. We will then have proved that the full vorticity Ω was actually in, say, $L^4(\mathbb{R}_+, L^2(\mathbb{X}^3))$, entailing that the whole velocity field lies in $L^1(\mathbb{R}_+, \dot{H}^1(\mathbb{X}^3))$. A direct application of the standard Serrin criterion concludes the proof.

2.3 Notations

We define here the notations we shall use in this paper, along with some useful shorthands which we shall make a great use thereof.

If a is a real number or a scalar function, we define for any real, strictly positive p the generalized power a^p by

$$a^p := a|a|^{p-1}$$

if a is nonzero and 0 otherwise. Such a definition has the advantage of being reversible, in that we have the equality

$$a = (a^p)^{\frac{1}{p}}.$$

Spaces like $L^p(\mathbb{R}_t, L^q(\mathbb{X}_x^3))$ or $L^p(\mathbb{R}_t, W^{s,q}(\mathbb{X}_x^3))$ will have their name shortened simply to $L_t^p L_x^q$ and $L_t^q W_x^{s,q}$.

As we will have to deal with anisotropy, spaces such as $L^p(\mathbb{R}_t, L^q(\mathbb{X}_z, L^r(\mathbb{X}_{x,y}^2)))$ shall be simply written $L_t^p L_z^q L_h^r$ when the context prevents any ambiguity.

When dealing with regularizations procedures, often done through convolutions, we will denote the smoothing parameter by δ and the mollifying kernels by $(\rho_\delta)_\delta$.

If X is either a vector or scalar field which we want to regularize, we denote by X^δ the convolution $\rho_\delta * X$.

Conversely, assume that we have some scalar or vector field Y which is a solution of some (partial) differential equation whose coefficients are generically denoted by X . Both X and Y are to be thought as having low regularity. We denote by Y_δ the unique smooth solution of the same (partial) differential equation where all the coefficients X are replaced by their regularized counterparts X^δ .

If k lies between 1 and n , the horizontal variable associated to the vertical variable k in $\mathbb{R}^n$ is the $n-1$ tuple of variables $(1, \dots, k-1, k+1, \dots, n)$. In practice n will be equal to 3, in which case the horizontal variable associated to, say, 3 is none other than $(1, 2)$.

Now, for i, j, k between 1 and 3, we denote by $A_{i,j}^k$ the operator $\partial_i \partial_j \Delta_{h_k}^{-1}$, with h_k being the horizontal variable associated to the vertical variable k . We divide these 18 operators into three subsets.

First, we say that $A_{i,j}^k$ is *isotropic* if neither i nor j is equal to k . This corresponds to the case where the two derivatives lost through the derivations are actually gained by the inverse laplacian.

Applying the Hörmander-Mikhlin multiplier theorem in two dimensions shows that these operators are bounded from $L^p(\mathbb{X}^3)$ to itself for any p strictly between 1 and ∞ . There are 9 such operators.

The second class is that of the $A_{i,j}^k$ for which exactly one on the two indices i and j is equal to k while the other is not. We say that such operators are *weakly anisotropic*. Here, we lose one derivative in the vertical variable and gain one in the horizontal variable. There are 6 such operators.

The third and last class, which we will not have to deal with in this paper thanks to the peculiar algebraic structure of the equations, is formed by the three $A_{k,k}^k = \partial_k^2 \Delta_{h_k}^{-1}$ for k between 1 and 3. To keep a consistent terminology, we call them *strongly anisotropic*. The fact that we lose two derivatives in the vertical variable and gain two derivatives in the horizontal variable while working in three dimensions should make this last family quite nontrivial to study.

If A and B are two linear operators, their commutator is defined by

$$[A, B] := AB - BA.$$

We emphasize that, when dealing with commutators, we do not distinguish between a smooth function and the multiplication operator by the said function.

2.4 Preliminary lemmas

We collect in this section various results, sometimes taken from other papers which we will use while proving the main theorems. We begin by an analogue of the usual energy estimate, whose proof may be found in [10] except it is performed in L^p with $p \neq 2$.

Lemma 2.4.1. *Let $1 < p < \infty$ and a_0 in L_x^p . Let f be in $L_t^1 L_x^p$ and v be a divergence-free vector field in $L_t^2 L_x^\infty$. Assume that a is a smooth solution of*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \Delta a = f \\ a(0) = a_0. \end{cases}$$

Then, $|a|^{\frac{p}{2}}$ belongs to $L_t^\infty L_x^2 \cap L_t^2 H_x^1$ and we have the L^p energy equality

$$\begin{aligned} \frac{1}{p} \|a(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a(s)|^{\frac{p-2}{2}} \nabla a(s) \|_{L_x^2}^2 ds \\ = \frac{1}{p} \|a_0\|_{L_x^p}^p + \int_0^t \int_{\mathbb{R}^3} f(s, x) a(s, x) |a(s, x)|^{p-2} dx ds. \end{aligned}$$

Our next lemma is, along with the energy estimate above, one of the cornerstones of our paper. Thanks to it, we are able to prove that the solutions of some PDEs are more regular than expected. It may be found in [27] and appear as a particular case of Theorem 2 in [28], to which we refer the reader for a detailed proof.

Lemma 2.4.2. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let $\nu \geq 0$ be a real constant. Let a be a $L_{loc,t}^2 L_x^2$ solution of*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \nu \Delta a = 0 \\ a(0) = 0. \end{cases}$$

Then $a \equiv 0$.

The following lemma has a somewhat probabilistic flavor to it, partly due to the use of the Egorov's theorem.

Lemma 2.4.3. *Let $(a_\delta)_\delta$ be a sequence of bounded functions in $L_t^p L_x^q$, with $1 \leq p, q \leq \infty$. Let a be in $L_t^p L_x^q$ and assume that*

$$\begin{cases} a_\delta \rightarrow a \text{ in } \mathcal{D}'_{t,x} \\ a_\delta \rightarrow a \text{ a.e.} \end{cases}$$

as δ goes to 0.

Then, for any α in $]0, 1[$,

$$a_\delta^\alpha \rightharpoonup^* a^\alpha \text{ in } L_t^{\frac{p}{\alpha}} L_x^{\frac{q}{\alpha}}.$$

Proof. Let us fix some α in $]0, 1[$ and let us denote $(1 - \frac{\alpha}{p})^{-1}$ and $(1 - \frac{\alpha}{q})^{-1}$ by $\tilde{p}$ and $\tilde{q}$ respectively. Let g be a smooth function with compact support in space, which we denote by S . From our assumptions, $a_\delta^\alpha \rightarrow a^\alpha$ almost everywhere. By Egorov's theorem, since $[0, T] \times S$ has finite Lebesgue measure, for any real, strictly positive ε , there exists a subset A_ε of $[0, T] \times S$ of Lebesgue measure at most ε such that

$$\|a_\delta^\alpha - a^\alpha\|_{L_{t,x}^\infty(A_\varepsilon^c)} \rightarrow 0 \text{ as } \delta \rightarrow 0,$$

where we use A_ε^c as a shorthand for $([0, T] \times S) \setminus A_\varepsilon$. Out of the bad set A_ε , we can simply write

$$\left| \int_0^T \int_S (a_\delta^\alpha - a^\alpha) g \mathbb{1}_{A_\varepsilon^c} dx dt \right| \leq \|a_\delta^\alpha - a^\alpha\|_{L_{t,x}^\infty(A_\varepsilon^c)} \|g\|_{L_t^1 L_x^1},$$

and this last quantity goes to 0 as δ goes to 0, for any fixed ε . Define the function μ_ε by

$$\mu_\varepsilon(t) := \int_S \mathbb{1}_{A_\varepsilon}(t, x) dx \quad \text{for } t \in [0, T].$$

We notice that

$$\|\mu\|_{L_t^1} \leq \varepsilon,$$

while $\|\mu\|_{L_t^\infty}$ is uniformly bounded in ε . By interpolation, for any r between 1 and ∞ ,

$$\|\mu\|_{L_t^r} \lesssim \varepsilon^{\frac{1}{r}}.$$

On A_ε , we have

$$\begin{aligned} \left| \int_0^T \int_S a_\delta^\alpha \mathbb{1}_{A_\varepsilon} g dx dt \right| &\leq \int_0^T \|a_\delta^\alpha\|_{L_x^{\frac{q}{\alpha}}(S)} \|g\|_{L_x^\infty} \mu_\varepsilon^{\frac{1}{\tilde{q}}} dt \\ &\leq \|a_\delta^\alpha\|_{L_t^{\frac{p}{\alpha}} L_x^{\frac{q}{\alpha}}} \|g\|_{L_t^\infty L_x^\infty} \|\mu\|_{L_t^{\frac{\tilde{p}}{\tilde{q}}}}^{\frac{1}{\tilde{q}}} \\ &\lesssim \varepsilon^{\frac{1}{\tilde{p}}}. \end{aligned}$$

Similarly,

$$\left| \int_0^T \int_S a^\alpha \mathbb{1}_{A_\varepsilon} g dx dt \right| \lesssim \varepsilon^{\frac{1}{\tilde{p}}}.$$

Letting first δ then ε go to 0, thanks to the finiteness of $\tilde{p}$, we get the desired convergence. The case of a general g in $L_t^{\tilde{p}} L_x^{\tilde{q}}$ is handled by a standard approximation procedure, which is made possible by the finiteness of both $\tilde{p}$ and $\tilde{q}$. $\square$

Lemma 2.4.4. *Let F be in $L_t^1 L_x^1$ spatially supported in the ball $B(0, R)$ for some $R > 0$. Let a be the unique tempered distribution solving*

$$\begin{cases} \partial_t a - \Delta a = F \\ a(0) = 0. \end{cases}$$

Then there exists a constant $C = C_R > 0$ such that, for $|x| > 2R$, we have

$$|a(t, x)| \leq C_R \|F\|_{L_t^1 L_x^1} |x|^{-3}. \quad (2.4)$$

Proof. Let us write explicitly the Duhamel formula for a . We have, thanks to the support assumption on F ,

$$a(t, x) = \int_0^t \int_{B(0, R)} (2\pi(t-s))^{-\frac{3}{2}} e^{-\frac{|x-y|^2}{4(t-s)}} F(s, y) dy ds.$$

As the quantity $\tau^{-3/2} e^{-A^2/\tau}$ reaches its maximum for $\tau = \frac{2A^2}{3}$, we have

$$|a(t, x)| \lesssim \int_0^t \int_{B(0, R)} |x-y|^{-3} |F(s, y)| dy ds.$$

If x lies far away from the support of F , for instance if $|x| > 2R$ in our case, we further have

$$|a(t, x)| \leq C_R \int_0^t \int_{B(0, R)} |x|^{-3} |F(s, y)| dy ds = C_R |x|^{-3} \|F\|_{L_t^1 L_x^1}.$$

□

The following lemma is an easy exercise in functional analysis, whose proof we omit.

Lemma 2.4.5. *Let us define, for some fixed $R > 0$ and $p > 1$, the space*

$$\widetilde{W}^{1,p}(\mathbb{R}^3) := \{u \in W^{1,p}(\mathbb{R}^3) \text{ s.t. } \sup_{|x| > 2R} |x|^3 |u(x)| < \infty\}.$$

Then the embedding of $\widetilde{W}^{1,p}$ into L^p is compact.

The next lemma combines some of the previous ones and plays a key role in the paper. It allows us to gain regularity on solutions of transport-diffusion equations for free.

Lemma 2.4.6. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let p be a real number between $\frac{6}{5}$ and 2. Let $F = (F_i)_i$ be in $L_t^1 L_x^p$ and assume that $a = (a_i)_i$ is a solution in $L_t^2 L_x^2$ of*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \Delta a = F \\ a(0) = 0. \end{cases}$$

Then a is actually in $L_t^\infty L_x^p \cap L_t^2 W_x^{1,p}$ and moreover, its i -th component a_i satisfies the energy inequality

$$\frac{1}{p} \|a_i(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a_i(s)|^{\frac{p-2}{2}} \nabla a_i(s) \|_{L_x^2}^2 ds \leq \int_0^t \int_{\mathbb{R}^3} a_i^{p-1}(s) F_i(s) dx ds.$$

Proof. Before delving into the proof itself, we begin with a simplifying remark. As the equation on a_i simply writes

$$\partial_t a_i + \nabla \cdot (a_i v) - \Delta a_i = F_i,$$

the equations on the a_i are uncoupled, which allows us prove to prove the lemma only in the scalar case. Thus, we assume in the rest of the proof the a is actually a scalar function.

Let $(\rho_\delta)_\delta$ be a sequence of space-time mollifiers. Let a_δ be the unique solution of the PDE system

$$\begin{cases} \partial_t a_\delta + \nabla \cdot (a_\delta v^\delta) - \Delta a_\delta = F^\delta \\ a_\delta(0) = 0. \end{cases}$$

Performing an energy-type estimate in L^p , which is made possible thanks to Lemma 2.4.1, we get for all strictly positive t the equality

$$\frac{1}{p} \|a_\delta(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a_\delta(s)|^{\frac{p-2}{2}} \nabla a_\delta(s) \|_{L_x^2}^2 ds = \int_0^t \int a_\delta^{p-1}(s) F^\delta(s) dx ds$$

In turn, it entails

$$\|a_\delta(t)\|_{L_x^p} \leq p \int_0^t \|F^\delta(s)\|_{L_x^p} ds,$$

which finally gives

$$\frac{1}{p} \|a_\delta(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a_\delta(s)|^{\frac{p-2}{2}} \nabla a_\delta(s) \|_{L_x^2}^2 ds \leq p^{p-2} \left(\int_0^t \|F^\delta(s)\|_{L_x^p} ds \right)^p.$$

From the definition of F^δ , we infer that

$$\frac{1}{p} \|a_\delta(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a_\delta(s)|^{\frac{p-2}{2}} \nabla a_\delta(s) \|_{L_x^2}^2 ds \leq p^{p-2} \left(\int_0^t \|F(s)\|_{L_x^p} ds \right)^p,$$

where the last term is independent of δ . Because p is strictly smaller than 2, we have a bound on a_δ in $L_t^\infty L_x^p \cap L_t^2 W_x^{1,p}$ uniform in δ , thanks to the identity

$$\nabla a = (\nabla |a|^{\frac{p-2}{2}}) |a|^{\frac{2-p}{2}}.$$

We now take the limit $\delta \rightarrow 0$. First of all, because F^δ is nothing but a space-time mollification of F , we have

$$\|F^\delta - F\|_{L_t^1 L_x^p} \rightarrow 0 \text{ as } \delta \rightarrow 0.$$

Moreover, the weak-* accumulation points of $(a_\delta)_\delta$ in $L_t^\infty L_x^p$ and $L_t^2 W_x^{1,p}$ respectively are, in particular, solutions of the problem

$$\begin{cases} \partial_t b + \nabla \cdot (bv) - \Delta b = F \\ b(0) = 0. \end{cases}$$

Because p is greater than $\frac{6}{5}$, the space $W^{1,p}(\mathbb{R}^3)$ embeds into $L^q(\mathbb{R}^3)$ for some q greater than 2. By Lemma 2.4.2, the only possible accumulation point is none other than a . Thus, as $\delta \rightarrow 0$,

$$\begin{cases} a_\delta \rightharpoonup^* a \text{ in } L^\infty L^p \\ a_\delta \rightharpoonup a \text{ in } L^2 W^{1,p}. \end{cases}$$

From Lemma 2.4.4, we also have

$$|a_\delta(t, x)| \lesssim |x|^{-3}$$

for large enough x , with constants independant of δ . Combining the bounds we have on $(a_\delta)_\delta$, we have shown that this family is bounded in $L^2_{\text{loc},t} \widetilde{W}_x^{1,p}$. On the other hand, the equation on a_δ may be rewritten as

$$\partial_t a_\delta = -\nabla \cdot (a_\delta \otimes v^\delta) + \Delta a_\delta + F^\delta$$

and the right-hand side is bounded in, say, $L^1_{\text{loc},t} H_x^{-2}$, because p is greater than $\frac{6}{5}$. By Aubin-Lions lemma, it follows that the family $(a_\delta)_\delta$ is strongly compact in, say, $L^2_{\text{loc},t} L_x^p$. Furthermore, once again thanks to Lemma 2.4.2, it follows that a is the only strong accumulation point of $(a_\delta)_\delta$ in $L^2_{\text{loc},t} L_x^p$. Thus,

$$a_\delta \rightarrow a \text{ in } L^2_{\text{loc},t} L_x^p.$$

Thanks to this strong convergence, up to extracting a subsequence $(\delta_n)_n$, we have

$$a_{\delta_n} \rightarrow a \text{ a.e. as } n \rightarrow \infty.$$

We are now in position to apply Lemma 2.4.3 to the sequence $(a_{\delta_n})_n$. With $\alpha = \frac{p}{2}$, we have

$$a_{\delta_n}^{\frac{p}{2}} \rightharpoonup^* a^{\frac{p}{2}} \text{ in } L_t^\infty L_x^2 \text{ as } n \rightarrow \infty,$$

while $\alpha = p-1$ leads to

$$a_{\delta_n}^{p-1} \rightharpoonup^* a^{p-1} \text{ in } L_t^\infty L_x^{\frac{p}{p-1}} \text{ as } n \rightarrow \infty.$$

Using the identity

$$\nabla(a^{\frac{p}{2}}) = \frac{p}{2} a^{\frac{p-2}{2}} \nabla a$$

and the energy inequality, we have

$$\sup_{n \in \mathbb{N}} \int_0^t \|\nabla(a_{\delta_n}^{\frac{p}{2}})\|_{L_x^2}^2 ds < \infty.$$

Since $a_{\delta_n}^{\frac{p}{2}} \rightharpoonup^* a^{\frac{p}{2}}$ in $L_t^\infty L_x^2$ as $n \rightarrow \infty$, applying Fatou's lemma to $a^{\frac{p}{2}}$ shows that

$$\int_0^t \|\nabla(a^{\frac{p}{2}})\|_{L_x^2}^2 ds \leq \liminf_{n \rightarrow \infty} \int_0^t \|\nabla(a_{\delta_n}^{\frac{p}{2}})\|_{L_x^2}^2 ds < \infty.$$

Taking the limit in the energy inequality, we finally have

$$\frac{1}{p} \|a(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a(s)|^{\frac{p-2}{2}} \nabla a(s) \|_{L_x^2}^2 ds \leq p^{p-2} \left(\int_0^t \|F(s)\|_{L_x^p} ds \right)^p.$$

More interestingly, taking the limit in the energy equality gives us the stronger statement

$$\frac{1}{p} \|a(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a(s)|^{\frac{p-2}{2}} \nabla a(s) \|_{L_x^2}^2 ds \leq \int_0^t \int_{\mathbb{R}^3} a^{p-1}(s) F(s) dx ds.$$

The proof of the lemma is now complete. $\square$

Lemma 2.4.7. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let A be a matrix-valued function in $L_t^2 L_x^3$. Let K be a matrix whose coefficients are homogeneous Fourier multipliers of order 0, smooth outside the origin. Let a be a solution in $(L_t^2 L_x^2)^2$ of the equation*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \Delta a = AKa \\ a(0) = 0. \end{cases}$$

Then $a = 0$.

Proof. From the assumptions we made, the right-hand side AKa lies in $L_t^1 L_x^{\frac{6}{5}}$. Thanks to Lemma 2.4.6, a is actually in $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$. Moreover, we also have a set of energy estimates in $L^{\frac{6}{5}}$ on the components a_i of a , which are

$$\frac{5}{6} \|a_i(t)\|_{L_x^{\frac{6}{5}}}^{\frac{6}{5}} + \frac{1}{5} \int_0^t \| |a_i(s)|^{-\frac{2}{5}} \nabla a_i(s) \|_{L_x^2}^2 ds \leq \int_0^t \int_{\mathbb{R}^3} a_i^{\frac{1}{5}}(s) (A(s)Ka(s))_i dx ds.$$

By the Hölder inequality and Sobolev embeddings, we have

$$\begin{aligned} \int_0^t \int_{\mathbb{R}^3} a_i^{\frac{1}{5}}(s) (A(s)Ka(s))_i dx ds &\lesssim \sum_j \int_0^t \|A(s)\|_{L_x^3} \|a_i(s)\|_{L_x^6}^{\frac{1}{5}} \|Ka_j(s)\|_{L_x^2} ds \\ &\lesssim \sum_j \int_0^t \|A(s)\|_{L_x^3} \|a_i(s)\|_{L_x^{\frac{6}{5}}}^{\frac{1}{5}} \|a_j(s)\|_{L_x^2} ds \\ &\lesssim \sum_j \int_0^t \|A(s)\|_{L_x^3} \|a_i(s)\|_{L_x^{\frac{6}{5}}}^{\frac{1}{5}} \|\nabla a_j(s) |a_j(s)|^{-\frac{2}{5}}\|_{L_x^2} \|a_j(s)\|_{L_x^{\frac{6}{5}}}^{\frac{2}{5}} ds \\ &\lesssim \sum_j \int_0^t \|A(s)\|_{L_x^3} \|a(s)\|_{L_x^{\frac{6}{5}}}^{\frac{3}{5}} \|\nabla a_j(s) |a_j(s)|^{-\frac{2}{5}}\|_{L_x^2} ds. \end{aligned}$$

Young inequality now ensures that

$$\begin{aligned} \int_0^t \|A(s)\|_{L_x^3} \|a(s)\|_{L_x^{\frac{6}{5}}}^{\frac{3}{5}} \|\nabla a_j(s) |a_j(s)|^{-\frac{2}{5}}\|_{L_x^2} ds \\ \leq \frac{1}{10} \int_0^t \|\nabla a_j(s) |a_j(s)|^{-\frac{2}{5}}\|_{L_x^2}^2 ds + C \int_0^t \|A(s)\|_{L_x^3}^2 \|a(s)\|_{L_x^{\frac{6}{5}}}^{\frac{6}{5}} ds. \end{aligned}$$

Adding these inequalities and cancelling out the gradient terms, we get

$$\frac{5}{6} \|a(t)\|_{L_x^{\frac{6}{5}}}^{\frac{6}{5}} \lesssim \int_0^t \|A(s)\|_{L_x^3}^2 \|a(s)\|_{L_x^{\frac{6}{5}}}^{\frac{6}{5}} ds.$$

The Grönwall inequality now implies that a vanishes identically. $\square$

Lemma 2.4.8. *Let p be a real number between $\frac{6}{5}$ and 2. Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let A be a matrix-valued function in $L_t^2 L_x^3$. Let K be a matrix whose coefficients are homogeneous Fourier multipliers of order 0, smooth outside the origin. Let F be a fixed function in $L_t^1 L_x^p$. Let a be a solution in $(L_t^2 L_x^2)^2$ of the equation*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \Delta a = AKa + F \\ a(0) = 0. \end{cases}$$

Then a is actually in $L_t^\infty L_x^p \cap L_t^2 W_x^{1,p}$.

Proof. The proof follows closely the steps of Lemma 2.4.6, so we shall skip it. $\square$

Lemma 2.4.9. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let a be a $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$ solution of the linear system*

$$\begin{cases} \partial_t a + \nabla \cdot (av) - \Delta a = \alpha a + \sum_{i,j=1,2} \varepsilon_{i,j} (\partial_j \beta_i) A_{3,i}^3 a \\ a(0) = 0, \end{cases} \quad (2.5)$$

with $\varepsilon_{i,j}$ being equal to 0 or 1 for any i, j between 1 and 2. We also assume that α lies in $L_t^2 L_x^3$ and that all the β_i 's are in $L_t^2 H_x^{\frac{3}{2}}$. Then a is identically 0.

Proof. For the sake of readability, we assume in the proof that only one coefficient $\varepsilon_{i,j}$ is not zero. We denote the corresponding $\partial_j \beta_i$ simply by $\partial_j \beta$. Let us denote by F the right-hand side of (2.5). From the assumptions and anisotropic Sobolev embeddings, it follows that F belongs to $L^1 L^{\frac{6}{5}}$. By Lemma 2.4.6, a satisfies an energy inequality which writes, in our case,

$$\frac{5}{6} \|a(t)\|_{L_x^{\frac{6}{5}}}^{\frac{6}{5}} + \frac{1}{5} \int_0^t \| |a(s)|^{-\frac{2}{5}} \nabla a(s) \|_{L_x^2}^2 ds \leq \int_0^t \int_{\mathbb{R}^3} \left(a^{\frac{6}{5}}(s) \alpha(s) + a^{\frac{1}{5}}(s) \partial_j \beta(s) A_{3,i}^3 a(s) \right) dx ds.$$

By Hölder inequalities, we have

$$\begin{aligned} \int_0^t \int_{\mathbb{R}^3} a^{\frac{6}{5}}(s) \alpha(s) dx ds &\lesssim \int_0^t \|a^{\frac{3}{5}}(s)\|_{L^3}^2 \|\alpha(s)\|_{L^3} ds \\ &\lesssim \int_0^t \|a^{\frac{3}{5}}(s)\|_{L^2} \| |a(s)|^{-\frac{2}{5}} \nabla a(s) \|_{L^2} \|\alpha(s)\|_{L^3} ds \\ &\leq \frac{1}{10} \int_0^t \| |a(s)|^{-\frac{2}{5}} \nabla a(s) \|_{L^2}^2 ds + C \int_0^t \|a^{\frac{3}{5}}(s)\|_{L^2}^2 \|\alpha(s)\|_{L^3}^2 ds. \end{aligned}$$

To bound the other term, we begin by using a trace theorem on β , which gives that β lies in $L_t^2 L_z^\infty H_h^1$. Taking a horizontal derivative, we get $\partial_j \beta \in L_t^2 L_z^\infty L_h^2$. We emphasize that such a trace embedding would not be true in general, because $H^{\frac{1}{2}}(\mathbb{X})$ does not embed in $L^\infty(\mathbb{X})$. Here, the fact that the multiplier $\partial_j \beta$ appears as a derivative of some function is crucial. Regarding the weakly anisotropic term $A_{3,i}^3 a$, the assumption on a gives $\partial_3 a \in L_t^2 L_x^{\frac{6}{5}} = L_t^2 L_z^{\frac{6}{5}} L_h^{\frac{6}{5}}$. Since in two dimensions the space $W^{1,\frac{6}{5}}$ embeds into L^3 , we get that $A_{3,i}^3 a$ belongs to $L_t^2 L_z^{\frac{6}{5}} L_h^3$. Combining these embeddings with Hölder inequality, we arrive at

$$\begin{aligned} \int_0^t \int_{\mathbb{R}^3} a^{\frac{1}{5}}(s) \partial_j \beta(s) A_{3,i}^3 a(s) dx ds &\leq \int_0^t \|a^{\frac{1}{5}}(s)\|_{L_z^6 L_h^6} \|\partial_j \beta(s)\|_{L_z^\infty L_h^2} \|A_{3,i}^3 a(s)\|_{L_z^{\frac{6}{5}} L_h^3} ds \\ &\lesssim \int_0^t \|a^{\frac{1}{5}}(s)\|_{L_x^6} \|\beta(s)\|_{H_x^{\frac{3}{2}}} \|\nabla a(s)\|_{L_x^{\frac{6}{5}}} ds. \end{aligned}$$

Using once again the identity

$$\nabla a = \left(|a|^{-\frac{2}{5}} \nabla a \right) |a|^{\frac{2}{5}}$$

together with the Hölder inequality, we get

$$\int_0^t \int_{\mathbb{R}^3} a^{\frac{1}{5}}(s) \partial_j \beta(s) A_{3,i}^3 a(s) dx ds \lesssim \int_0^t \|a^{\frac{3}{5}}(s)\|_{L_x^2} \|\beta(s)\|_{H_x^{\frac{3}{2}}} \| |a(s)|^{-\frac{2}{5}} \nabla a(s) \|_{L_x^2} ds.$$

Now, Young inequality for real numbers entails, for some constant C ,

$$\int_0^t \int_{\mathbb{R}^3} a^{\frac{1}{5}}(s) \partial_j \beta(s) A_{3,i}^3 a(s) dx ds \leq \frac{1}{10} \int_0^t \| |a(s)|^{-\frac{2}{5}} \nabla a(s) \|_{L_x^2}^2 ds + C \int_0^t \|a^{\frac{3}{5}}(s)\|_{L_x^2}^2 \|\beta(s)\|_{H_x^{\frac{3}{2}}}^2 ds.$$

Cancelling out the gradient terms, we finally get

$$\|a^{\frac{3}{5}}(t)\|_{L_x^2}^2 \lesssim \int_0^t \|a^{\frac{3}{5}}(s)\|_{L_x^2}^2 (\|\alpha(s)\|_{L_x^3}^2 + \|\beta(s)\|_{H_x^{\frac{3}{2}}}^2) ds.$$

Grönwall's inequality then ensures that a vanishes identically. $\square$

The three following lemmas allow us, in the spirit of Lemmas 2.4.6 and 2.4.9, to enhance the regularity of the solutions to some equations. As their proofs are akin to those of the aforementioned Lemmas we only sketch them.

Lemma 2.4.10. *Let p be a real number between $\frac{6}{5}$ and 2. Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let a be a solution in $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$ of the linear system*

$$\begin{cases} \partial_t a + \nabla \cdot (av) - \Delta a = \alpha a + \sum_{i,j=1,2} \varepsilon_{i,j} (\partial_j \beta_i) A_{3,i}^3 a + F \\ a(0) = 0, \end{cases}$$

where $\varepsilon_{i,j}$ equal to 0 or 1 for any i, j between 1 and 2. We also assume that α lies in $L_t^2 L_x^3$, that all the β_i 's are in $L_t^2 H_x^{\frac{3}{2}}$ and that the force F belongs to $L_t^1 L_x^p \cap L_t^1 L_x^{\frac{6}{5}}$. Then a is actually in $L_t^\infty L_x^p \cap L_t^2 W_x^{1,p}$.

Proof. [Sketch of proof] We again assume that only one coefficient $\varepsilon_{i,j}$ is nonzero and write $\partial_j \beta$ instead of $\partial_j \beta_i$. We abbreviate the whole right-hand side of the equation by $\tilde{F}$. First, we mollify the force fields $\alpha, \partial_j \beta, F$ and the weakly anisotropic operator $A_{3,i}^3$ by some regularizing kernel ρ_δ . This mollified right-hand side will be denoted by $\tilde{F}^\delta$, even though it is not exactly equal to $\rho_\delta * \tilde{F}$. This regularization allows us to build smooth solutions a_δ to the modified equation. In a second step, Lemma 2.4.1 gives us estimates in the energy space associated to L^p which are uniform in δ . These estimates write, recalling that $a_\delta(0)$ is equal to 0,

$$\frac{1}{p} \|a_\delta(t)\|_{L_x^p}^p + (p-1) \int_0^t \| |a_\delta(s)|^{\frac{p-2}{2}} \nabla a_\delta(s) \|_{L_x^2}^2 ds = \int_0^t \int_{\mathbb{R}^3} a_\delta(s, x)^{p-1} \tilde{F}^\delta(s, x) dx ds.$$

Repeating the computations we did for Lemma 2.4.9 and using Hölder inequality to deal with F^δ , we get

$$\|a_\delta(t)\|_{L_x^p}^p \lesssim \int_0^t \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds + \int_0^t \|a_\delta(s)\|_{L_x^p}^{p-1} \|F^\delta(s)\|_{L_x^p} ds.$$

We detail how to deal with the new term added by F^δ . Let us denote, for any strictly positive T ,

$$M_\delta(T) := \sup_{0 \leq t \leq T} \|a_\delta(t)\|_{L_x^p}.$$

For t between 0 and T , we have

$$\begin{aligned} \|a_\delta(t)\|_{L_x^p}^p &\lesssim \int_0^t \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds + M_\delta(T)^{p-1} \int_0^t \|F^\delta(s)\|_{L_x^p} ds \\ &\lesssim \int_0^t \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds + M_\delta(T)^{p-1} \|F\|_{L_t^1 L_x^p}. \end{aligned}$$

Taking the supremum over t in the time interval $[0, T]$ in the left-hand side gives

$$\|M_\delta(T)\|_{L_x^p}^p \lesssim \int_0^T \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds + M_\delta(T)^{p-1} \|F\|_{L_t^1 L_x^p}.$$

Viewing the above equation as an algebraic inequality between positive numbers, we get

$$\|M_\delta(T)\|_{L_x^p} \lesssim \left(\int_0^T \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds \right)^{\frac{1}{p}} + \|F\|_{L_t^1 L_x^p}.$$

Taking again the p -th power and owing to the inequality $(a+b)^p \lesssim a^p + b^p$, we have

$$\|M_\delta(T)\|_{L_x^p}^p \lesssim \left(\int_0^T \|a_\delta(s)\|_{L_x^p}^p (\|\alpha^\delta(s)\|_{L_x^3}^2 + \|\beta^\delta(s)\|_{H_x^{\frac{3}{2}}}^2) ds \right) + \|F\|_{L_t^1 L_x^p}^p.$$

Finally, since $\|a_\delta(T)\|_{L_x^p} \leq M_\delta(T)$ for all strictly positive T , Grönwall's inequality entails that, for some constant C ,

$$\|a_\delta(T)\|_{L_x^p} \leq C \|F\|_{L_t^1 L_x^p} \exp \left(C \int_0^T \|\alpha(s)\|_{L_x^3}^2 + \|\beta(s)\|_{H_x^{\frac{3}{2}}}^2 ds \right).$$

Having this bound and its analogue when the exponent p is equal to $\frac{6}{5}$, thanks to the assumptions we did on F , we get a solution of our problem in both the energy spaces associated to $L^{\frac{6}{5}}$ and L^p . We conclude that this new solution is actually equal to a thanks to Lemma 2.4.9. $\square$

Lemma 2.4.11. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let a be a $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$ solution of the linear system*

$$\begin{cases} \partial_t a + \nabla \cdot (av) - \Delta a = \alpha a + \sum_{i,j=1,2} \varepsilon_{i,j} (\partial_j \beta_i) A_{3,i}^3 a + F_1 + F_2 \\ a(0) = 0, \end{cases}$$

where $\varepsilon_{i,j}$ equal to 0 or 1 for any i, j between 1 and 2. We assume that α lies in $L_t^2 L_x^3$ and that all the β_i 's are in $L_t^2 H_x^{\frac{3}{2}}$. The forces F_1 and F_2 belong respectively to $L_t^1 L_x^{\frac{3}{2}} \cap L_t^1 L_x^{\frac{6}{5}}$ and $L_t^{\frac{4}{3}} L_x^{\frac{6}{5}} \cap L_t^1 L_x^{\frac{6}{5}}$. Then a is actually in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$.

Proof. [Sketch of proof] We essentially have to repeat the proof of Lemma 2.4.10, apart from estimating the term coming from F_2 . Keeping the same notations as in the last proof, we have

$$\int_0^t \int_{\mathbb{R}^3} a_\delta(s, x)^{\frac{1}{2}} F^\delta(s, x) dx ds \leq \int_0^t \|F^\delta(s)\|_{L_x^{\frac{6}{5}}} \|a_\delta(s)^{\frac{1}{2}}\|_{L_x^6} ds.$$

Using the identity

$$\|a_\delta(s)^{\frac{1}{2}}\|_{L_x^6} = \|a_\delta(s)^{\frac{3}{4}}\|_{L_x^4}^{\frac{2}{3}}$$

and the Sobolev embedding $H^{\frac{3}{4}} \hookrightarrow L^4$, we get

$$\int_0^t \|F^\delta(s)\|_{L_x^{\frac{6}{5}}} \|a_\delta(s)^{\frac{1}{2}}\|_{L_x^6} ds \lesssim \int_0^t \|F^\delta(s)\|_{L_x^{\frac{6}{5}}} \|a_\delta(s)^{\frac{3}{4}}\|_{L_x^2}^{\frac{1}{6}} \| |a(s)|^{-\frac{1}{4}} \nabla a(s) \|_{L_x^2}^{\frac{1}{2}} ds.$$

Now, Young inequality gives us, for some positive constant C ,

$$\begin{aligned} \int_0^t \|F^\delta(s)\|_{L_x^{\frac{6}{5}}} \|a_\delta(s)^{\frac{3}{4}}\|_{L_x^2}^{\frac{1}{6}} \| |a(s)|^{-\frac{1}{4}} \nabla a(s) \|_{L_x^2}^{\frac{1}{2}} ds &\leq \frac{1}{10} \int_0^t \| |a(s)|^{-\frac{1}{4}} \nabla a(s) \|_{L_x^2}^2 ds \\ &\quad + \int_0^t \|a_\delta(s)^{\frac{3}{4}}\|_{L_x^2}^2 \|F^\delta(s)\|_{L_x^{\frac{6}{5}}}^{\frac{4}{3}} ds + C \int_0^t \|F^\delta(s)\|_{L_x^{\frac{6}{5}}}^{\frac{4}{3}} ds. \end{aligned}$$

Plugging this finaly bound in the energy estimate performed in $L^{\frac{3}{2}}$, the rest of the proof is the same as for Lemma 2.4.10. $\square$

Lemma 2.4.12. *Let v be a fixed, divergence free vector field in $L_t^2 H_x^1$. Let A be a matrix-valued function in $L_t^2 L_x^3$. Let K be a matrix whose coefficients are homogeneous, isotropic Fourier multipliers of order 0. Let F_1 be a fixed function in $L_t^1 L_x^{\frac{3}{2}} \cap L_t^1 L_x^{\frac{6}{5}}$ and F_2 be fixed in $L_t^{\frac{4}{3}} L_x^{\frac{6}{5}} \cap L_t^1 L_x^{\frac{6}{5}}$. Let a be a solution in $(L_t^2 L_x^2)^2$ of the equation*

$$\begin{cases} \partial_t a + \nabla \cdot (a \otimes v) - \Delta a = AKa + F_1 + F_2 \\ a(0) = 0. \end{cases}$$

Then a is actually in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$.

Proof. This lemma essentially combines the proofs of Lemmas 2.4.6, 2.4.10 and 2.4.11, so we shall not repeat them. $\square$

Lemma 2.4.13. *Let v_0 be a divergence free vector field in $L_x^{\frac{3}{2}} \cap L_x^2$. Then any Leray solution of the Navier-Stokes system*

$$\begin{cases} \partial_t v + \nabla \cdot (v \otimes v) - \Delta v = -\nabla p \\ \operatorname{div} v = 0 \\ v(0) = v_0 \end{cases}$$

belongs, in addition to the classical energy space $L_t^\infty L_x^2 \cap L_t^2 H_x^1$, to $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$.

Proof. Let v be a Leray solution of the Navier-Stokes system, which exists by classical approximation arguments. Then, letting

$$F := -\mathbb{P} \nabla \cdot (v \otimes v) = -\mathbb{P}(v \cdot \nabla v)$$

where $\mathbb{P}$ denotes the Leray projection on divergence free vector fields, v solves the heat equation

$$\begin{cases} \partial_t v - \Delta v = F \\ v(0) = v_0. \end{cases}$$

That F belongs to $L_t^1 L_x^{\frac{3}{2}}$ is easily obtained by the continuity of $\mathbb{P}$ on $L^{\frac{3}{2}}$. The result follows from an energy estimate in $L^{\frac{3}{2}}$. $\square$

2.5 Case of the torus

Let us now state the first main theorem of this paper.

Theorem 2.5.1. *Let u be a Leray solution of the Navier-Stokes equations set in $\mathbb{R}_+ \times \mathbb{T}^3$*

$$\begin{cases} \partial_t u + \nabla \cdot (u \otimes u) - \Delta u = -\nabla p \\ u(0) = u_0 \end{cases}$$

with initial data u_0 in $L^2(\mathbb{T}^3)$. Assume the existence of a time interval $]T_1, T_2[$ such that its third component u^3 satisfies

$$u^3 \in L^2(T_1, T_2[, W^{2, \frac{3}{2}}(\mathbb{T}^3)).$$

Then u is actually smooth in time and space on $]T_1, T_2[\times \mathbb{T}^3$ and satisfies the Navier-Stokes equations in the classical, strong sense.

Let χ, φ be smooths cutoffs in time, localised inside $]T_1, T_2[$. Let ω be the third component of $\Omega := \text{rot } v$. Denote $\chi\omega$ by ω' . The equation satisfied by ω' writes

$$\partial_t \omega' + \nabla \cdot (\omega' u) - \Delta \omega' = \chi \Omega \cdot \nabla u^3 + \omega \partial_t \chi.$$

Denote $F := \chi \Omega \cdot \nabla u^3 + \omega \partial_t \chi$. As u is a Leray solution of the Navier-Stokes equations, we know that Ω belongs to $L_t^2 L_x^2$. Thus, ω' also lies in $L_t^2 L_x^2$. On the other hand, the assumption made on u^3 tells us in particular that $\Omega \cdot \nabla u^3$ belongs to $L_t^1 L_x^{\frac{6}{5}}$. That $\omega \partial_t \chi$ also belongs to $L_t^1 L_x^{\frac{6}{5}}$ follows directly from the compactness of $\mathbb{T}^3$.

We are now in position to apply Lemma 2.4.6, which tells us that ω' is actually in $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$. Let us now expand the quantity $\Omega \cdot \nabla u^3$ in terms of ω and u^3 . We have, after some simplifications,

$$\Omega \cdot \nabla u^3 = \partial_3 u^3 \omega + \partial_2 u^3 \partial_3 u^1 - \partial_1 u^3 \partial_3 u^2.$$

Performing a horizontal div-curl decomposition of u^1 and u^2 in terms of $\partial_3 u^3$ and ω , we have

$$\begin{aligned} \Omega \cdot \nabla u^3 &= \partial_3 u^3 \omega + \partial_2 u^3 (-A_{1,3}^3 \partial_3 u^3 - A_{2,3}^3 \omega) - \partial_1 u^3 (-A_{2,3}^3 \partial_3 u^3 + A_{1,3}^3 \omega) \\ &= \partial_3 u^3 \omega + \mathcal{A}(\omega, u^3) + \mathcal{B}(u^3, u^3), \end{aligned}$$

where we defined as shorthands the operators

$$\mathcal{A}(\omega, u^3) := -\partial_2 u^3 A_{2,3}^3 \omega - \partial_1 u^3 A_{1,3}^3 \omega \quad (2.6)$$

$$\mathcal{B}(u^3, u^3) := -\partial_2 u^3 A_{1,3}^3 \partial_3 u^3 + \partial_1 u^3 A_{2,3}^3 \partial_3 u^3. \quad (2.7)$$

Notice that the div-curl decomposition forces the appearance of weakly anisotropic operators acting either on ω or u^3 . Assume from now on that the condition

$$\text{supp } \chi \subset \{\varphi \equiv 1\}.$$

holds. Under this condition, the equation on ω' then reads

$$\begin{aligned} \partial_t \omega' + \nabla \cdot (\omega' u) - \Delta \omega' &= \chi \omega \partial_3 u^3 + \chi \mathcal{A}(\omega, u^3) + \chi \mathcal{B}(u^3, u^3) + \omega \partial_t \chi \\ &= \omega' \partial_3 u^3 + \mathcal{A}(\omega', \varphi u^3) + \mathcal{B}(\chi u^3, \varphi u^3) + \omega \partial_t \chi, \end{aligned}$$

because the cutoffs χ and φ act only on time. It follows from the assumptions on u^3 that $\mathcal{B}(\chi u^3, \varphi u^3)$ belongs to $L_t^1 L_x^{\frac{3}{2}}$. Moreover, $\omega \partial_t \chi$ also belongs to $L_t^1 L_x^{\frac{3}{2}}$. Thanks to Lemma 2.4.10, ω' is actually in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$. Let us now write the system of equations satisfied by the other components of the vorticity, which we respectively denote by ω_1 and ω_2 . We have

$$\begin{cases} \partial_t \omega_1 + \nabla \cdot (\omega_1 u) - \Delta \omega_1 = \partial_3 u^1 \partial_1 u^2 - \partial_2 u^1 \partial_1 u^3 \\ \partial_t \omega_2 + \nabla \cdot (\omega_2 u) - \Delta \omega_2 = \partial_1 u^2 \partial_2 u^3 - \partial_3 u^2 \partial_2 u^1. \end{cases}$$

We now perform a horizontal div-curl decomposition of u^1 with respect to the second variable. That is, we write that

$$u^1 = \partial_3 \Delta_{(1,3)}^{-1} \omega_2 - \partial_1 \Delta_{(1,3)}^{-1} \partial_2 u^2.$$

In turn, we have

$$\begin{aligned} \partial_3 u^1 &= \partial_3^2 \Delta_{(1,3)}^{-1} \omega_2 - \partial_3 \partial_1 \Delta_{(1,3)}^{-1} \partial_2 u^2 \\ &= A_{3,3}^2 \omega_2 - A_{1,3}^2 \partial_2 u^2. \end{aligned}$$

What we wish to emphasize is that $\partial_3 u^1$ may be expressed as an order zero *isotropic* Fourier multiplier applied to ω_2 and $\partial_2 u^2$. The same reasoning applies to $\partial_3 u^2$, which may be decomposed in terms of ω_1 et $\partial_1 u^1$. The fact that there is no (weakly) anisotropic operator here is a great simplification compared to the study of ω_3 , for which such a complication was unavoidable. The system on (ω_1, ω_2) may be recast in the following form :

$$\begin{cases} \partial_t \omega_1 + \nabla \cdot (\omega_1 u) - \Delta \omega_1 = (A_{3,3}^2 \omega_2 - A_{1,3}^2 \partial_2 u^2) \partial_1 u^2 - \partial_2 u^1 \partial_1 u^3 \\ \partial_t \omega_2 + \nabla \cdot (\omega_2 u) - \Delta \omega_2 = \partial_1 u^2 \partial_2 u^3 + (A_{3,3}^1 \omega_1 + A_{2,3}^1 \partial_1 u^1) \partial_2 u^1. \end{cases}$$

Informally, the above system behaves roughly like its simplified version

$$\begin{cases} \partial_t \omega_1 + \nabla \cdot (\omega_1 u) - \Delta \omega_1 = (\omega_2 - \partial_2 u^2) \partial_1 u^2 - \partial_2 u^1 \partial_1 u^3 \\ \partial_t \omega_2 + \nabla \cdot (\omega_2 u) - \Delta \omega_2 = \partial_1 u^2 \partial_2 u^3 + (\omega_1 + \partial_1 u^1) \partial_2 u^1, \end{cases}$$

which is much simpler to understand and shall make the upcoming computations clearer. Let us denote, as we did for ω ,

$$\omega'_1 := \chi \omega_1 \text{ and } \omega'_2 := \chi \omega_2.$$

Applying the time cutoff χ to the system on (ω_1, ω_2) , we get

$$\begin{cases} \partial_t \omega'_1 + \nabla \cdot (\omega'_1 u) - \Delta \omega'_1 = \varphi \partial_1 u^2 A_{3,3}^2 \omega'_2 - \varphi \partial_1 u^2 A_{1,3}^2 (\chi \partial_2 u^2) - (\chi \partial_2 u^1) (\varphi \partial_1 u^3) + \omega_1 \partial_t \chi \\ \partial_t \omega'_2 + \nabla \cdot (\omega'_2 u) - \Delta \omega'_2 = \varphi \partial_2 u^1 A_{3,3}^1 \omega'_1 + \varphi \partial_2 u^1 A_{2,3}^1 (\chi \partial_1 u^1) + (\chi \partial_1 u^2) (\varphi \partial_2 u^3) + \omega_2 \partial_t \chi. \end{cases}$$

Finally, applying the same decomposition to u^1 and u^2 , we have four equations of the type

$$\partial_1 u^1 = -A_{1,1}^3 \omega_3 - A_{1,2}^3 \partial_3 u^3,$$

which allow us to control, for i, j between 1 and 2, $\partial_i u^j$ in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{6}{5}}$ in terms of ω_3 and $\partial_3 u^3$ in the same space. Thus, what we have gained through the regularity enhancement on ω_3 is the control of four components of the jacobian of u , in addition to the three provided by the assumption on u^3 . For this reason, the system we have on (ω_1, ω_2) may be viewed as an affine and isotropic one with all exterior forces in scaling invariant spaces. For instance, $\varphi \partial_2 u^1$ belongs to $L_t^2 L_x^3$, while the exterior forces lie in $L_t^1 L_x^{\frac{3}{2}}$. Lemma 2.4.8 now implies that both ω'_1 and ω'_2 are in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$.

We now have proven that the whole vorticity Ω belongs to $L_t^4 L_x^2$ by Sobolev embeddings. In turn, it implies that the whole velocity field belongs to $L_t^4 H_x^1$. The main theorem then follows from the application of the usual Serrin criterion.

2.6 Local case in $\mathbb{R}^3$.

We state the second main theorem of this paper.

Theorem 2.6.1. *Let u be a Leray solution of the Navier-Stokes equations set in $\mathbb{R}_+ \times \mathbb{R}^3$*

$$\begin{cases} \partial_t u + \nabla \cdot (u \otimes u) - \Delta u = -\nabla p \\ u(0) = u_0 \end{cases}$$

with initial data u_0 in $L^2(\mathbb{R}^3) \cap L^{\frac{3}{2}}(\mathbb{R}^3)$. Assume the existence of a time interval $]T_1, T_2[$ and a spatial domain $D \Subset \mathbb{R}^3$ of compact closure such that its third component u^3 satisfies

$$u^3 \in L^2(T_1, T_2[, W^{2, \frac{3}{2}}(D)).$$

Then, on $]T_1, T_2[\times D$, u is actually smooth in time and space and satisfies the Navier-Stokes equations in the classical, strong sense.

Let us describe in a few words our strategy for this case. Compared to the torus, there are two main differences to notice. First, since the assumption on u^3 was made on the whole space, the cutoffs acted only in time. The difference between the original Navier-Stokes equation and its truncated version was thus only visible in one term, rendering our strategy easier to apply. On the other hand, since the torus has finite measure, the Lebesgue spaces form a decreasing family of spaces. This fact allowed us to lose some integrability when we wanted to embed different forcing terms in the same space. This last difference will become visible when dealing with commutators between Fourier multipliers and the cutoff functions, thus lengthening a little bit the proof, compared to the torus case. For that technical reason, we added an assumption on the initial data which was trivially true in the torus case, thanks to the aforementioned embedding of Lebesgue spaces.

Let χ, φ be smooths cutoffs in space and time, localised inside $]T_1, T_2[\times D$. Denote $\text{rot } v$ by Ω and let ω be its third component. Denote $\chi\omega$ by ω' . The equation satisfied by ω' writes

$$\partial_t \omega' + \nabla \cdot (\omega' u) - \Delta \omega' = \chi \Omega \cdot \nabla u^3 + \mathcal{C}(\omega, \chi),$$

where $\mathcal{C}(\omega, \chi)$ stands for all the cutoff terms. Namely, we have

$$\mathcal{C}(\omega, \chi) := \omega \partial_t \chi + \omega u \cdot \nabla \chi - \omega \Delta \chi - 2 \nabla \omega \cdot \nabla \chi.$$

As χ is smooth and has compact support, we claim that $\mathcal{C}(\omega, \chi)$ belongs to $L_t^1 L_x^{\frac{3}{2}} + L_t^2 \dot{H}_x^{-1}$. Indeed, that ω belongs to $L_t^2 L_x^2$ entails that the term $\nabla \omega \cdot \nabla \chi$ belongs to $L_t^2 \dot{H}_x^{-1}$. Regarding the other terms, that ω belongs to $L_t^2 L_x^2$ and u to $L_t^2 L_x^6$ is enough to sustain the claim, thanks to the compactness of the support of χ . Because χ has compact support in space, the terms in $L_t^1 L_x^{\frac{3}{2}}$ also lie in $L_t^1 L_x^{\frac{6}{5}}$. Finally, the quantity $\chi \Omega \cdot \nabla u^3$ clearly belongs to $L_t^1 L_x^{\frac{6}{5}}$. Let now $\omega'_{(1)}$ be the unique solution in $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$ of the equation

$$\partial_t \omega'_{(1)} + \nabla \cdot (\omega'_{(1)} u) - \Delta \omega'_{(1)} = \chi \Omega \cdot \nabla u^3 + \omega \partial_t \chi + \omega u \cdot \nabla \chi - \omega \Delta \chi$$

with the initial condition $\omega'_{(1)}(0)$ being set to 0, which exists thanks to Lemma 2.4.1 and is unique thanks to Lemma 2.4.2. Similarly, let $\omega'_{(2)}$ be the unique solution in $L_t^\infty L_x^2 \cap L_t^2 H_x^1$ of

$$\partial_t \omega'_{(2)} + \nabla \cdot (\omega'_{(2)} u) - \Delta \omega'_{(2)} = -2 \nabla \omega \cdot \nabla \chi.$$

with the initial condition $\omega'_{(2)}(0)$ being set to 0. Let

$$\tilde{\omega}' := \omega'_{(1)} + \omega'_{(2)} - \omega'.$$

From the regularity we have on each term, $\tilde{\omega}'$ belongs to $L_{\text{loc},t}^2 L_x^2$ and satisfies

$$\partial_t \tilde{\omega}' + \nabla \cdot (\tilde{\omega}' u) - \Delta \tilde{\omega}' = 0$$

with a vanishing initial condition $\tilde{\omega}'(0)$. Lemma 2.4.2 then implies that $\tilde{\omega}' \equiv 0$, from which it follows that

$$\omega' = \omega'_{(1)} + \omega'_{(2)}.$$

By local embeddings of Lebesgue spaces, $\omega'_{(2)}$ also belongs to $L_t^\infty L_{\text{loc},x}^{\frac{6}{5}} \cap L_t^2 W_{\text{loc},x}^{1, \frac{6}{5}}$. On the other hand, it is rather trivial that $\omega'_{(1)}$ also belongs to $L_t^\infty L_{\text{loc},x}^{\frac{6}{5}} \cap L_t^2 W_{\text{loc},x}^{1, \frac{6}{5}}$. Now, since ω' has compact

support in space, it follows that ω' belongs to the full space $L_t^\infty L_x^{\frac{6}{5}} \cap L_t^2 W_x^{1, \frac{6}{5}}$. In particular, the forcing term $\nabla \omega \cdot \nabla \chi$ is now an integrable vector field, instead of a mere $L_t^2 \dot{H}_x^{-1}$ distribution. At this stage, because the reasoning is valid for *any* cutoff χ supported in $]T_1, T_2[\times D$, we have proved that the third component ω of the vorticity of u has the regularity

$$\omega \in L_{\text{loc}}^\infty(]T_1, T_2[, L_{\text{loc}}^{\frac{6}{5}}(D)) \cap L_{\text{loc}}^2(]T_1, T_2[, W_{\text{loc}}^{1, \frac{6}{5}}(D)).$$

In particular, such a statement allows us to improve the regularity of $\mathcal{C}(\omega, \chi)$ to $L_t^1 L_x^{\frac{3}{2}} + L_t^2 L_x^{\frac{6}{5}}$. Such a gain will be of utmost importance near the end of the proof. Expanding again the product $\Omega \cdot \nabla u^3$ in terms of ω and u^3 only, we have

$$\partial_t \omega' + \nabla \cdot (\omega' u) - \Delta \omega' = \chi \omega \partial_3 u^3 + \chi \mathcal{A}(\omega, u^3) + \chi \mathcal{B}(u^3, u^3) + \mathcal{C}(\omega, \chi).$$

We refer the reader to Equations (2.6) and (2.7) on page 46 for the definition of the remainders $\mathcal{A}$ and $\mathcal{B}$. From now on, we enforce the condition

$$\text{supp } \chi \subset \{\varphi \equiv 1\}.$$

Now, because the cutoff χ acts both in space and time, we have to carefully compute the associated commutators with the operators $\mathcal{A}$ and $\mathcal{B}$. First, let us notice that $\mathcal{A}$ is local in its variable u^3 , which allows us to write that

$$\chi \mathcal{A}(\omega, u^3) = \chi \mathcal{A}(\omega, \varphi u^3).$$

On the other hand, for $i = 1, 2$,

$$\begin{aligned} \chi A_{i,3}^3 \omega &= \chi \partial_i \Delta_{(1,2)}^{-1} (\partial_3 \omega) \\ &= [\chi, \partial_i \Delta_{(1,2)}^{-1}] (\partial_3 \omega) + \partial_i \Delta_{(1,2)}^{-1} (\chi \partial_3 \omega) \\ &= [\chi, \partial_i \Delta_{(1,2)}^{-1}] (\partial_3 \omega) + A_{i,3}^3 (\chi \omega) - \partial_i \Delta_{(1,2)}^{-1} (\omega \partial_3 \chi) \end{aligned}$$

We now estimate the two remainder terms in $L_t^1 L_x^{\frac{3}{2}}$. By Sobolev embeddings in $\mathbb{R}^2$, we have, for any strictly positive t and any real x_3 ,

$$\|(\partial_i \Delta_{(1,2)}^{-1} (\omega \partial_3 \chi))(t, \cdot, x_3)\|_{L_h^6} \lesssim \|(\omega \partial_3 \chi)(t, \cdot, x_3)\|_{L_h^{\frac{3}{2}}}.$$

Thus,

$$\|\partial_i \Delta_{(1,2)}^{-1} (\omega \partial_3 \chi)\|_{L_t^2 L_z^{\frac{3}{2}} L_h^6} \lesssim \|\omega \partial_3 \chi\|_{L_t^2 L_x^{\frac{3}{2}}} \lesssim \|\omega\|_{L_t^2 L_x^2} \|\nabla \chi\|_{L_t^\infty L_x^6}.$$

The commutator is a little bit trickier. First, we write

$$\partial_3 \omega = \partial_3 (\partial_1 u^2 - \partial_2 u^1) = \partial_1 (\partial_3 u^2) - \partial_2 (\partial_3 u^1).$$

In order to continue the proof, we need a commutator lemma, which we state and prove below for the sake of completeness, despite its ordinary nature.

Lemma 2.6.1. *Let f be in $L^{\frac{3}{2}}(\mathbb{R}^2)$ and χ be a test function. The following commutator estimates hold*

$$\begin{aligned} \|[\chi, \nabla \Delta^{-1}](\nabla f)\|_{L^6(\mathbb{R}^2)} &\lesssim \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)} \|f\|_{L^{\frac{3}{2}}(\mathbb{R}^2)} \quad \text{and} \\ \|[\chi, \nabla^2 \Delta^{-1}](f)\|_{L^6(\mathbb{R}^2)} &\lesssim \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)} \|f\|_{L^{\frac{3}{2}}(\mathbb{R}^2)}. \end{aligned}$$

Proof. We notice that the first estimate may be deduced from the second thanks to the identity

$$[\chi, \nabla \Delta^{-1}](\nabla f) = [\chi, \nabla^2 \Delta^{-1}](f) + \nabla \Delta^{-1}(f \nabla \chi).$$

The operator $\nabla \Delta^{-1}$ is continuous from $L^{\frac{3}{2}}(\mathbb{R}^2)$ to $L^6(\mathbb{R}^2)$ thanks to the Hardy-Littlewood-Sobolev inequality. Hence, we get

$$\|\nabla \Delta^{-1}(f \nabla \chi)\|_{L^6(\mathbb{R}^2)} \lesssim \|f \nabla \chi\|_{L^{\frac{3}{2}}(\mathbb{R}^2)} \lesssim \|f\|_{L^{\frac{3}{2}}(\mathbb{R}^2)} \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)}.$$

It only remains to study the second commutator, which we denote by C_χ . There exist numerical constants c_1, c_2 such that, for almost every x in $\mathbb{R}^2$,

$$C_\chi(x) = \int_{\mathbb{R}^2} \left(c_1 \frac{(x-y) \otimes (x-y)}{|x-y|^4} + \frac{c_2}{|x-y|^2} I_2 \right) (\chi(x) - \chi(y)) f(y) dy.$$

This yields

$$|C_\chi(x)| \lesssim \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)} \int_{\mathbb{R}^2} \frac{|f(y)|}{|x-y|} dy = \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)} (|f| * |\cdot|^{-1})(x).$$

Applying the Hardy-Littlewood-Sobolev inequality to f , we get

$$\|C_\chi\|_{L^6(\mathbb{R}^2)} \lesssim \|\nabla \chi\|_{L^\infty(\mathbb{R}^2)} \|f\|_{L^{\frac{3}{2}}(\mathbb{R}^2)}$$

as we wanted. $\square$

We now return to the proof of Theorem 2.6.1. Thanks to Lemma 2.6.1, we have the estimate

$$\|[\chi, \partial_i \Delta_{(1,2)}^{-1}](\partial_1(\partial_3 u^2))\|_{L^6(\mathbb{R}^2)} \lesssim \|\nabla \chi\|_{L^\infty} \|\partial_3 u^2\|_{L^{\frac{3}{2}}(\mathbb{R}^2)},$$

which translates into

$$\|[\chi, \partial_i \Delta_{(1,2)}^{-1}](\partial_1(\partial_3 u^2))\|_{L_t^2 L_z^{\frac{3}{2}} L_h^6} \lesssim \|\nabla \chi\|_{L_{t,x}^\infty} \|\partial_3 u^2\|_{L_t^2 L_x^{\frac{3}{2}}}.$$

From Lemma 2.4.13 applied to u , we deduce that $\partial_3 u^2$ belongs to $L_t^2 L_x^{\frac{3}{2}}$. Moreover, we may bound $\|\partial_3 u^2\|_{L_t^2 L_x^{\frac{3}{2}}}$ by a quantity depending only on u_0 through its L^2 and $L^{\frac{3}{2}}$ norms. Gathering these estimates, we may write

$$\chi \mathcal{A}(\omega, \varphi u^3) = \mathcal{A}(\chi \omega, \varphi u^3) + \mathcal{R},$$

where $\mathcal{R}$ stands for a generic remainder satisfying a bound of the type

$$\|\mathcal{R}\|_{L_t^1 L_x^{\frac{3}{2}}} \lesssim_\chi \|u_0\|_{L_x^2 \cap L_x^{\frac{3}{2}}} \|u^3\|_{L_t^2 (H_x^1 \cap W_x^{2, \frac{3}{2}})}.$$

In this case, the bound holds thanks to Lemma 2.4.13 and the trace theorem

$$\|\nabla u^3\|_{L_t^2 L_z^\infty L_h^2} \lesssim \|u^3\|_{L_t^2 W_x^{2, \frac{3}{2}}}.$$

In particular, $\mathcal{R}$ may be regarded as an exterior force independant of ω' in the sequel and scaling invariant. The same reasoning applies to $\mathcal{B}$: we have

$$\chi \mathcal{B}(u^3, \varphi u^3) = \mathcal{B}(\chi u^3, \varphi u^3) + \mathcal{R}.$$

Finally, the equation on ω' has been rewritten as

$$\partial_t \omega' + \nabla \cdot (\omega' u) - \Delta \omega' = \omega' \partial_3 u^3 + \mathcal{A}(\omega', \varphi u^3) + \mathcal{B}(\chi u^3, \varphi u^3) + \mathcal{C}(\omega, \chi) + \mathcal{R}.$$

Applying Lemma 2.4.11, we deduce that the truncated vorticity ω' is actually in $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$. Again, thanks to the horizontal div-curl decomposition, it follows that space-time truncations of $\partial_i u^j$ are controlled in the same space in terms of ω' and u^3 , for i, j between 1 and 2. We now turn to the other components of the vorticity, namely ω_1 and ω_2 . Truncating the equations and using the div-curl decomposition, we have

$$\begin{cases} \partial_t \omega'_1 + \nabla \cdot (\omega'_1 u) - \Delta \omega'_1 = \chi(A_{3,3}^2 \omega_2 - A_{1,3}^2 \partial_2 u^2) \partial_1 u^2 - \chi \partial_2 u^1 \partial_1 u^3 + \mathcal{C}(\omega_1, \chi) \\ \partial_t \omega'_2 + \nabla \cdot (\omega'_2 u) - \Delta \omega'_2 = \chi \partial_1 u^2 \partial_2 u^3 + \chi(A_{3,3}^1 \omega_1 + A_{2,3}^1 \partial_1 u^1) \partial_2 u^1 + \mathcal{C}(\omega_2, \chi). \end{cases}$$

Let us now write and estimate the necessary commutators. By Lemma 2.6.1, whenever k is neither i nor j ,

$$\|[\chi, A_{i,j}^k](\omega_2)\|_{L^6(\mathbb{R}^2)} \lesssim \|\nabla \chi\|_{L_h^\infty} \|\omega_2\|_{L_h^{\frac{3}{2}}(\mathbb{R}^2)}.$$

Thus,

$$\|[\chi, A_{i,j}^k](\omega_2)\|_{L_t^2 L_x^{\frac{3}{2}} L_h^6} \lesssim \|\nabla \chi\|_{L_x^\infty} \|\omega_2\|_{L_t^2 L_x^{\frac{3}{2}}}.$$

On the other hand, by a trace theorem, we have, for a in $W^{1, \frac{3}{2}}(\mathbb{R}^3)$,

$$\|a\|_{L^\infty(\mathbb{R}, L^2(\mathbb{R}^2))} \lesssim \|a\|_{W^{1, \frac{3}{2}}(\mathbb{R}^3)}.$$

These two estimates together entail that, for i, j between 1 and 2,

$$\|\partial_i(\varphi u^j)[\chi, A_{i,j}^k](\omega_2)\|_{L_t^1 L_x^{\frac{3}{2}}} \lesssim \|\nabla \chi\|_{L_x^\infty} \|\omega_2\|_{L_t^2 L_x^{\frac{3}{2}}} \|\partial_i(\varphi u^j)\|_{L_t^2 W_x^{1, \frac{3}{2}}}.$$

The system on (ω'_1, ω'_2) may be recast as

$$\begin{cases} \partial_t \omega'_1 + \nabla \cdot (\omega'_1 u) - \Delta \omega'_1 = (A_{3,3}^2 \omega'_2 - A_{1,3}^2 \partial_2(\chi u^2)) \partial_1(\varphi u^2) - \partial_2(\chi u^1) \partial_1(\varphi u^3) + \mathcal{C}(\omega_1, \chi) + \mathcal{R} \\ \partial_t \omega'_2 + \nabla \cdot (\omega'_2 u) - \Delta \omega'_2 = \partial_1(\chi u^2) \partial_2(\varphi u^3) + (A_{3,3}^1 \omega'_1 + A_{2,3}^1 \partial_1(\chi u^1)) \partial_2(\varphi u^1) + \mathcal{C}(\omega_2, \chi) + \mathcal{R}. \end{cases}$$

Because χ has compact support in time, the term $-2\nabla \omega \cdot \nabla \chi$ is in $L_t^{\frac{4}{3}} L_x^{\frac{6}{5}}$. Applying Lemma 2.4.12, it follows that both ω'_1 and ω'_2 belong to $L_t^\infty L_x^{\frac{3}{2}} \cap L_t^2 W_x^{1, \frac{3}{2}}$. The conclusion of the theorem now follows from the standard Serrin criterion.

Deuxième partie

Graphes quantiques

Chapitre 3

Graphes quantiques optimisant leur trou spectral.

3.1 Introduction

The spectral gap is a vastly explored quantity due to its importance both for applicative purposes and theoretic ones. The applicative aspects range from estimates of convergence to equilibrium to behavior of quantum many body systems. The theoretic study concerns with connecting the shape of an object to a fundamental spectral property. Such relations stand in the heart of spectral geometry and motivate the current work.

A compact quantum graph can be thought of as a three-fold object, consisting of a topology, a metric and an operator. The topology is described by an underlying discrete graph and the metric is simply the assignment of a positive length to each of the edges. The operator together with its domain complete this description. In the current work we adopt the most common choice and fix the operator to be the one-dimensional Laplacian acting on functions which satisfy the so called Neumann conditions at the graph vertices (see [43, 56]). It is then most natural to fix a certain graph topology and explore how the graph spectral properties depend on the choice of edge lengths [55, 51, 44]. In particular, we examine the spectral gap which, in our case, is the first positive eigenvalue of the Laplacian. Picking a particular graph topology, we ask which edge lengths minimize or maximize the spectral gap. We notice that as our space of edge lengths is not compact, it is possible that the minimum or maximum are not obtained at all. The space of edge lengths is thus extended by allowing zero length edges so that the minima (maxima) of this new length space are the infimums (supremums) of the previous. This leads to a most interesting exploration direction : sending edge lengths to zero changes the topology of the original graph and makes us wonder what are the topologies which are obtained as optimizers (either maximizers or minimizers) of other graphs. This is the central question of the current paper.

Already in 1987, Nicaise showed that among all graphs with a fixed length, the minimal spectral gap is obtained for the single edge graph [73]. In 2005, Friedlander proved a more general result, showing that the minimum of the k^{th} eigenvalue is uniquely obtained for a star graph with k edges [54]. More recently, Exner and Jex showed how the change of graph edge lengths may increase or decrease the spectral gap, depending on the graph's topology [51]. In the last couple of years, a series of works on the subject came to light. Kurasov and Naboko [69] treated the spectral gap minimization and together with Malenová they explored how the spectral gap changes with various modifications of the graph connectivity [68]. Kennedy, Kurasov, Malenová and Mugnolo provided a broad survey on bounding the spectral gap in terms of various geometric quantities of the graph [59].

Karreskog, Kurasov and Trygg Kupersmidt generalized the minimization results mentioned above to Schrödinger operators with potentials and δ -type vertex conditions [58]. Del Pezzo and Rossi proved upper and lower bounds for the spectral gap of the p-Laplacian and evaluated its derivatives with respect to change of edge lengths [49]. Rohleder solved the spectral gap maximization problem for all eigenvalues of tree graphs [76]. We complement this literature review by mentioning some interesting and recent works on the spectral gap of metric graphs, whose scope is different than ours. Post [75], Kurasov [67], Kennedy and Mugnolo [60] all treated various estimates of the spectral gap in terms of the Cheeger constant (a line of research which already originated in [73] for quantum graphs). Buttazzo, Ruffini and Velichkov optimize over spectral gap of graphs given some prescribed set of Dirichlet vertices embedded in $\mathbb{R}^d$ [45].

The spectral gap optimization we consider in this paper is close in nature to the first line of works mentioned above. Nevertheless, our point of view is different as we wish to solve the optimization problem for each and every topology. This broad phrasing of the question provides a unified framework for several of the works mentioned above. In particular, it allows to take a step forward and complement those.

3.1.1 Discrete graphs and graph topologies

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ be a connected graph with finite sets of vertices $\mathcal{V}$ and edges $\mathcal{E}$ and we denote $V := |\mathcal{V}|$, $E := |\mathcal{E}|$. We allow edges to connect either two distinct vertices or a vertex to itself. In the latter case, this edge is called a loop, or sometimes a petal.

For a vertex $v \in \mathcal{V}$, its *degree*, d_v , equals the number of edges connected to it. Vertices of degree one are called leaves. Furthermore, we abuse this naming and frequently also use the name leaf for an edge which is connected to a vertex of degree one.

An important topological quantity of the graph is

$$\beta := E - V + 1, \quad (3.1)$$

which counts the number of “independent” cycles on the graph (assuming the graph is connected). This is also known as the first Betti number, which is the dimension of the graph’s first homology. In particular, tree graphs are characterized by $\beta = 0$.

We consider the following two ways for treating the graph connectivity. The graph’s edge connectivity is the minimal number of edges one needs to remove in order to disconnect the graph. If the graph’s edge connectivity equals one, then an edge whose removal disconnects the graph is called a *bridge*. In particular, leaf edges are bridges. Similarly, the graph’s vertex connectivity is the number of vertices needed to be removed in order to disconnect the graph. In particular, we show the special role played by graphs of edge connectivity one (Theorem 3.2.1) and of vertex connectivity one (Theorem 3.2.6).

3.1.2 Spectral theory of quantum graphs

A *metric graph* is a discrete graph with each of whose edges, $e \in \mathcal{E}$, being identified with a one-dimensional interval $[0, l_e]$ of positive finite length l_e . We assign to each edge $e \in \mathcal{E}$ a coordinate, x_e , which measures the distance along the edge from the starting vertex of e . We denote a coordinate by x , when its precise nature is unimportant.

A function on the graph is described by its restrictions to the edges, $\{f|_e\}_{e \in \mathcal{E}}$, where $f|_e : [0, l_e] \rightarrow \mathbb{C}$. We equip the metric graphs with a self-adjoint differential operator,

$$\mathcal{H} : f|_e(x_e) \mapsto -\frac{d^2}{dx_e^2} f|_e(x_e), \quad (3.2)$$

which in our case is just the one-dimensional negative Laplacian on every edge¹. It is most common to call this setting of a metric graph and an operator by the name quantum graph.

To complete the definition of the operator we need to specify its domain. We denote by $H^2(\Gamma)$ the following direct sum of Sobolev spaces

$$H^2(\Gamma) := \bigoplus_{e \in \mathcal{E}} H^2([0, l_e]) . \quad (3.3)$$

In addition we require the following matching conditions on the graph vertices. A function $f \in H^2(\Gamma)$ is said to satisfy the Neumann vertex conditions at a vertex v if

1. f is continuous at $v \in \mathcal{V}$, i.e.,

$$\forall e_1, e_2 \in \mathcal{E}_v \quad f|_{e_1}(0) = f|_{e_2}(0), \quad (3.4)$$

where $\mathcal{E}_v$ is the set of edges connected to v , and for each $e \in \mathcal{E}_v$ we choose the coordinate such that $x_e = 0$ at v .

2. the outgoing derivatives of f at v satisfy

$$\sum_{e \in \mathcal{E}_v} \left. \frac{df}{dx_e} \right|_e (0) = 0. \quad (3.5)$$

Another common vertex condition is called the Dirichlet condition. Imposing Dirichlet condition at vertex $v \in \mathcal{V}$ means

$$\forall e \in \mathcal{E}_v \quad f|_e(0) = 0. \quad (3.6)$$

Requiring either of these conditions at each vertex leads to the operator (3.2) being self-adjoint and its spectrum being real and bounded from below [43]. In addition, since we only consider compact graphs, the spectrum is discrete. We number the eigenvalues in the ascending order and denote them with $\{\lambda_n\}_{n=0}^\infty$ and their corresponding real eigenfunctions with $\{f_n\}_{n=0}^\infty$.

In this paper, we almost solely consider graphs whose vertex conditions are Neumann at all vertices. Those are called *Neumann graphs*. The spectrum of a Neumann graph is non-negative, which means that we may represent the spectrum by the non-negative square roots of the eigenvalues, $k_n = \sqrt{\lambda_n}$, and say that $\{k_n\}_{n=0}^\infty$ are the k -eigenvalues of the graph. For convenience, we express most of our results and proofs in terms of the k -eigenvalues. This choice makes all expressions of this paper look nicer. A Neumann graph has $k_0 = 0$ with multiplicity which equals the number of graph components (which is taken to be one throughout this paper). It is k_1 which is in the focus of this paper and is called the spectral gap².

3.1.3 Graph Optimizers

Definition 3.1.1. Let $\mathcal{G}$ be a discrete graph with E edges.

1. Denote by

$$\mathcal{L}_{\mathcal{G}} := \left\{ (l_1, \dots, l_E) \in \mathbb{R}^E \left| \sum_{e=1}^E l_e = 1 \text{ and } \forall e, l_e > 0 \right. \right\}$$

the space of all possible lengths we may assign to the edges of $\mathcal{G}$. We further denote by $\overline{\mathcal{L}}_{\mathcal{G}}$ the closure of $\mathcal{L}$ in $\mathbb{R}^E$ and by $\partial \mathcal{L}$ its boundary.

1. Note that more general operators appear in the literature. See for example the book [43] and the survey [56].

2. This terminology is justified, as a spectral gap is a common name for the difference between some trivial eigenvalue (which is $k_0 = 0$ in our case) and the next eigenvalue. We note that in this sense it is also common to call λ_1 the spectral gap.

2. Denote by $\Gamma(\mathcal{G}; \underline{l})$ the metric graph whose connectivity is the same as $\mathcal{G}$ and whose edge lengths are given by $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$. We take $\Gamma(\mathcal{G}; \underline{l})$ to be a Neumann graph. If $\underline{l} \in \partial\mathcal{L}$, then $\underline{l}$ has some vanishing entries and in this case the connectivity of $\Gamma(\mathcal{G}; \underline{l})$ is not the same as $\mathcal{G}$. For each vanishing entry, $l_e = 0$, the edge e does not exist in $\Gamma(\mathcal{G}; \underline{l})$, but rather the vertices at the endpoints of this edge are identified and form a single vertex when considered in $\Gamma(\mathcal{G}; \underline{l})$.

We emphasize that the definition above dictates a normalization choice we make in the optimization problems to follow - all graphs in this paper are considered to have total metric length equal to one.

This paper studies the spectral gap, $k_1[\Gamma(\mathcal{G}; \underline{l})]$, as a function of $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$. A first step is to show that the function $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is continuous on $\overline{\mathcal{L}}_{\mathcal{G}}$, which is done in Appendix A.1. Noting that $\overline{\mathcal{L}}_{\mathcal{G}}$ is a compact set we have the existence of a maximum and a minimum of the spectral gap on $\overline{\mathcal{L}}_{\mathcal{G}}$ (but not necessarily on $\mathcal{L}_{\mathcal{G}}$).

Indeed, the focus of the current paper is on the extremal points of $k_1[\Gamma(\mathcal{G}; \underline{l})]$. In particular we investigate whether the extremal points are obtained on $\mathcal{L}_{\mathcal{G}}$ or on $\partial\mathcal{L}_{\mathcal{G}}$ and to which metric graphs $\Gamma(\mathcal{G}; \underline{l})$ they correspond. This motivates the following.

Definition 3.1.2. Let $\mathcal{G}$ be a discrete graph.

1. $\Gamma(\mathcal{G}; \underline{l}^*)$ is called a maximizer of $\mathcal{G}$ if $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ and

$$\forall \underline{l} \in \mathcal{L}_{\mathcal{G}} \quad k_1[\Gamma(\mathcal{G}; \underline{l}^*)] \geq k_1[\Gamma(\mathcal{G}; \underline{l})].$$

In this case we call $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$ the maximal spectral gap of $\mathcal{G}$.

2. $\Gamma(\mathcal{G}; \underline{l}^*)$ is called a supremizer of $\mathcal{G}$ if $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ and

$$\forall \underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}} \quad k_1[\Gamma(\mathcal{G}; \underline{l}^*)] \geq k_1[\Gamma(\mathcal{G}; \underline{l})].$$

In this case we call $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$ the supremal spectral gap of $\mathcal{G}$.

3. $\Gamma(\mathcal{G}; \underline{l}^*)$ is called the unique maximizer of $\mathcal{G}$ if for all $\underline{l} \neq \underline{l}^*$, $\Gamma(\mathcal{G}; \underline{l})$ is not a maximizer of $\mathcal{G}$. The same definition holds for the unique supremizer.
4. Analogous definitions to the above hold for minimizers and infimizers.
5. $\Gamma(\mathcal{G}; \underline{l}^*)$ is called an optimizer of $\mathcal{G}$ if it is either a supremizer, a maximizer, an infimizer or a minimizer of $\mathcal{G}$.

Continuing the discussion preceding the definition, we note that there might be graphs which do not have a maximizer or a minimizer. Yet, a supremizer and an infimizer exist for any graph. Let $\mathcal{G}$ be a discrete graph and $\Gamma(\mathcal{G}; \underline{l}^*)$ be its supremizer (infimizer), with $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$. Denote by $\mathcal{G}^*$ the discrete graph which corresponds to $\Gamma(\mathcal{G}; \underline{l}^*)$. We note that if $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ then $\mathcal{G}^* = \mathcal{G}$ and if $\underline{l}^* \in \partial\mathcal{L}_{\mathcal{G}}$ then $\mathcal{G}^*$ is obtained from $\mathcal{G}$ by contracting all edges which correspond to the zero entries of $\underline{l}$.

The questions which motivate this work are the following : what are the metric graphs $\Gamma(\mathcal{G}; \underline{l}^*)$ which serve as supremizers (or infimizers) and what are all the possible topologies (i.e. the discrete graphs $\mathcal{G}^*$) obtained by these optimizations?

We start by presenting a few examples of topologies which form part of the answer to the questions above.

Example 3.1.3. Star graph

Let $\mathcal{G}$ be a graph with $V \geq 3$ vertices, and $E = V - 1$ edges, where one of the vertices (called the central vertex) is connected by edges to all the $V - 1$ other vertices (Figure 3.1(a)). $\mathcal{G}$ is called a star graph. The graph $\Gamma(\mathcal{G}; \underline{l})$ with $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$ is called the equilateral star. A simple calculation shows that $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2}E$. We show (Theorem 3.2.2) that the equilateral star is the unique

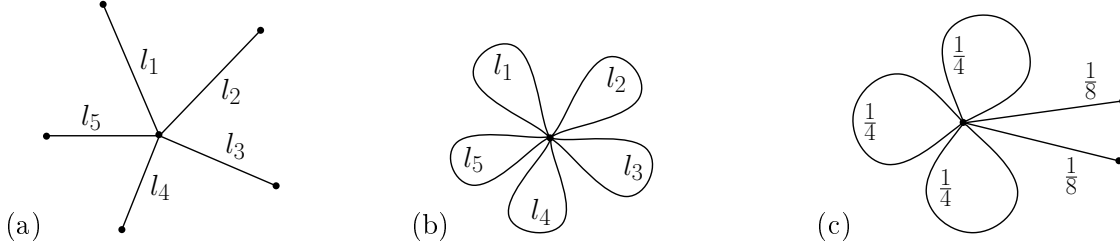


FIGURE 3.1 – A few basic examples. (a) star graph (b) flower graph (c) equilateral stower graph with $E_p = 3$, $E_l = 2$

maximizer of the star topology and that it is also the unique supremizer of any tree graph with E leaves. If we choose above $V = 2$, $E = 1$ we get an interval, which is the unique infimizer of any graph with a bridge (Theorem 3.2.1).

Example 3.1.4. Flower graph

Let $\mathcal{G}$ be a graph with a single vertex and $E \geq 2$ edges, where each edge is a loop (petal) connecting that single vertex to itself (Figure 3.1(b)). $\mathcal{G}$ is called a flower graph. The graph $\Gamma(\mathcal{G}; \underline{l})$ with $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$ is called the equilateral flower. A simple calculation shows that $k_1[\Gamma(\mathcal{G}; \underline{l})] = \pi E$. We show (Corollary 3.2.8) that the equilateral flower is the unique maximizer of the flower topology. If we choose above $E = 1$ we get a single loop graph, which is an infimizer for all bridgeless graphs (Theorem 3.2.1).

Example 3.1.5. Stower graph

Let $\mathcal{G}$ be a graph with V vertices and $E = E_p + E_l \geq 2$ edges. E_p of the edges are loops which connect a single vertex to itself (the same vertex for all those edges) and, as before, they are called petals. Each of the rest $E_l = V - 1$ edges connect this single vertex to another graph vertex and they are called dangling edges or just leaves (Figure 3.1(c)). Being a hybrid between a star graph and a flower graph, such $\mathcal{G}$ is called a stower graph. We note that a flower graph is a stower (with $E_l = 0$) and a star graph is a stower as well (with $E_p = 0$). The graph $\Gamma(\mathcal{G}; \underline{l})$ with $\underline{l} = \frac{1}{2E_p + E_l}(\underbrace{2, \dots, 2}_{E_p}, \underbrace{1, \dots, 1}_{E_l})$ is called the equilateral stower. Note that we abuse terminology and

call the graph equilateral, even though not all edges of the description above have the same length. A simple calculation shows that $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2}(2E_p + E_l)$. We show (Corollary 3.2.8) that the equilateral stower is the unique maximizer of the stower topology, except when $E_p = E_l = 1$, for which the supremizer is actually a single loop. Furthermore, spectral gaps of stowers obey a sort of additive property in the following sense : if two graphs whose supremizers are stowers are glued at non-leaf vertices to form a single graph, then this graph's supremizer is a stower graph obtained by adding the petals and the leaves of the two individual stower supremizers (Corollary 3.2.8).

Example 3.1.6. Mandarin graph

Let $\mathcal{G}$ be a graph with 2 vertices and E edges, each connecting those two vertices (Figure 3.2(a)). Such $\mathcal{G}$ is called a mandarin graph. In the literature it is also called a watermelon or a pumpkin, but we adopt the name mandarin which was used in a thorough exploration of spectral properties of these graphs, [40]. The graph $\Gamma(\mathcal{G}; \underline{l})$ with $\underline{l} = (\frac{1}{E}, \dots, \frac{1}{E})$ is called the equilateral mandarin. A

simple calculation shows that $k_1[\Gamma(\mathcal{G}; \underline{l})] = \pi E$. The equilateral mandarin is the unique maximizer of the mandarin topology, as was shown recently in [59] (theorem 4.2 there).

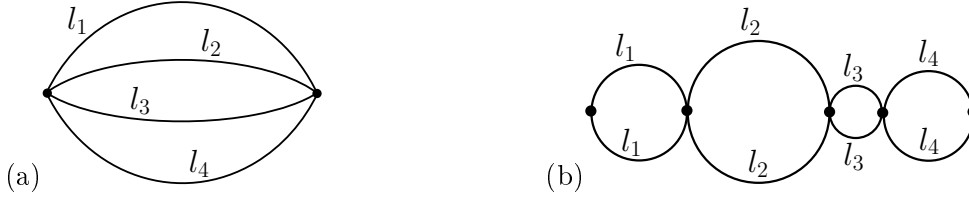


FIGURE 3.2 – (a) mandarin graph (b) symmetric necklace graph

Example 3.1.7. Necklace graph

Let $\mathcal{G}$ be a graph with V vertices and $E = 2(V - 1)$ edges, such that every two adjacent vertices, v_i, v_{i+1} ($1 \leq i \leq V - 1$) are connected by two edges (Figure 3.2(b)). If $\underline{l}$ is chosen such that every pair of parallel edges connecting two vertices have the same length, $\Gamma(\mathcal{G}; \underline{l})$ is called a symmetric necklace. Note that the two vertices at the endpoints of the necklace are redundant, being Neumann vertices of degree two (they are merely used here to shorten the graph description). Necklace graphs are the only graphs which may serve as infimizers of bridgeless graphs (Theorem 3.2.1).

3.2 Main Results

The main results of the current paper are stated below, arranged by subjects. In each of the following subsections, we mention which section of the paper contains the relevant proofs and discussions.

3.2.1 Infimizers (section 3.3)

Theorem 3.2.1.

1. Let $\mathcal{G}$ be a graph with a bridge. Then the infimal spectral gap of $\mathcal{G}$ equals π . Moreover, the unique infimizer is the unit interval.
2. Let $\mathcal{G}$ be a bridgeless graph. Then the infimal spectral gap of $\mathcal{G}$ equals 2π . Moreover, any infimizer is a symmetric necklace graph.

We note that it was already proved in [73, 54, 69] that π is a universal lower bound for the spectral gap, attained only by the interval. In [54] it is even shown that πn is a lower bound for k_n . The paper [69] proves that the lower bound may be improved to 2π if all vertices have even degrees. Theorem 3.2.1 extends the set of graph topologies whose spectral gap is bounded by 2π to all bridgeless graphs (indeed graphs whose all vertices are of even degrees form a particular case). Furthermore, combining Theorem 3.2.1 with the continuity of eigenvalues with respect to the graphs edge lengths (Appendix A.1) allows to conclude that our result cannot be improved by imposing further restrictions on the graph topology. For any bridgeless graph $\mathcal{G}$, there exists $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ for which $\Gamma(\mathcal{G}; \underline{l}^*)$ is a single cycle graph with spectral gap 2π . As $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is a continuous function of $\underline{l}$, the spectral gap may be as close to 2π as we wish, by choosing $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ close enough to $\underline{l}^*$. Similarly, the lower bound π cannot be improved for graphs with a bridge. Therefore, Theorem 3.2.1 complements the previous results and provides a complete answer to the infimization problem.

3.2.2 Supremizers of tree graphs (section 3.4)

Theorem 3.2.2. *Let $\mathcal{G}$ be a tree graph with $E_l \geq 2$ leaves. Then the unique supremizer of $\mathcal{G}$ is the equilateral star with E_l edges, whose spectral gap is $\frac{\pi}{2}E_l$. In particular, the uniqueness implies that this supremizer is a maximizer if and only if $\mathcal{G}$ is a star graph.*

Theorem 3.2.2 completely solves the optimization problem for tree graphs. While writing this paper, we became aware of the recent work, [76], which solves the maximization problem for trees (theorem 3.2 there). In the course of doing so, that work provides the upper bound $\frac{\pi}{2}E$ on the spectral gap of trees³. Our proof is close in spirit to that of theorem 3.4 in [76]. Yet, thanks to a basic geometric observation (Lemma 3.4.2 here), the better bound $\frac{\pi}{2}E_l$ is obtained⁴.

Theorem 3.2.2 allows to deduce the following.

Corollary 3.2.3. *Let $\mathcal{G}$ be a non-tree graph. Then its supremizer is not a tree graph.*

3.2.3 Supremizers whose spectral gap is a simple eigenvalue (section 3.5)

Whenever the spectral gap is a simple eigenvalue, it is differentiable with respect to edge lengths, which allows to search for local maximizers. There are indeed examples for critical values (not just maximizers) of the spectral gap, which we demonstrate in Proposition 3.5.8. If such local critical point is actually a supremizer it is possible to prove the following.

Theorem 3.2.4. *Let $\mathcal{G}$ be a discrete graph and let $\underline{l} \in \mathcal{L}_{\mathcal{G}}$. Assume that $\Gamma(\mathcal{G}; \underline{l})$ is a supremizer of $\mathcal{G}$ and that the spectral gap $k_1(\Gamma(\mathcal{G}; \underline{l}))$ is a simple eigenvalue. Then $\Gamma(\mathcal{G}; \underline{l})$ is not a unique supremizer. There exists a choice of lengths $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ such that $\Gamma(\mathcal{G}; \underline{l}^*)$ is an equilateral mandarin and*

$$k_1(\Gamma(\mathcal{G}; \underline{l})) = k_1(\Gamma(\mathcal{G}; \underline{l}^*)).$$

3.2.4 Supremizers of vertex connectivity one (sections 3.6, 3.7, 3.8)

Next, we describe a bottom to top construction which allows to find out a supremizer of a graph by knowing the supremizers of two of its subgraphs. This is possible for graphs of vertex connectivity one. In order to state the result, the following criteria are introduced.

Definition 3.2.5.

1. A Neumann graph Γ obeys the *Dirichlet criterion* with respect to its vertex v if imposing Dirichlet vertex condition at v does not change the value of k_1 (comparing to the one with Neumann condition at v).
2. A Neumann graph Γ obeys the *strong Dirichlet criterion* with respect to its vertex v if it obeys the Dirichlet criterion and if imposing the Dirichlet vertex condition at v strictly increases the eigenvalue multiplicity of k_1 .

Theorem 3.2.6. *Let $\mathcal{G}_1, \mathcal{G}_2$ be discrete graphs, let v_i ($i = 1, 2$) be a vertex of $\mathcal{G}_i$. Let $\mathcal{G}$ be the graph obtained by identifying v_1 and v_2 . Let $\underline{l}^{(i)} \in \overline{\mathcal{L}}_{\mathcal{G}_i}$ and $\Gamma_i := \Gamma(\mathcal{G}_i; \underline{l}^{(i)})$ be the corresponding metric graphs. Define $\underline{l} := (L\underline{l}^{(1)}, (1-L)\underline{l}^{(2)}) \in \overline{\mathcal{L}}_{\mathcal{G}}$, for some $L \in [0, 1]$. Then the graph $\Gamma := \Gamma(\mathcal{G}; \underline{l})$ is a supremizer of $\mathcal{G}$ if all the following conditions are met*

1. $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$.
2. Γ_i is a supremizer of $\mathcal{G}_i$ ($i = 1, 2$).

3. Theorem 3.2 in that paper is actually more general and provides the upper bound $\frac{\pi n}{2}E$ for k_n .

4. Furthermore, the same geometric observation may be used to improve the more general theorem 3.2 of [76].

3. Γ_i obeys the Dirichlet criterion with respect to v_i ($i = 1, 2$).

If we further assume either of the following :

- (a) For both $i = 1, 2$, Γ_i is a unique supremizer of $\mathcal{G}_i$ or
- (b) For both $i = 1, 2$, Γ_i obeys the strong Dirichlet criterion and any other supremizer of $\mathcal{G}_i$ violates the Dirichlet criterion.

then Γ is the unique supremizer of $\mathcal{G}$.

Remark. This theorem may be strengthened by weakening condition (3). Yet, the description of the weaker condition is more technical and we leave its specification, as well as the proof of the stronger version of this theorem, to section 3.6.

We note that the equilateral stower obeys the Dirichlet criterion with respect to its central vertex. Obviously, this observation also includes the equilateral star and equilateral flower as special cases. This observation together with theorem 3.2.6 allow to prove the following corollaries.

Corollary 3.2.7. *Let $\mathcal{G}_1, \mathcal{G}_2$ be discrete graphs. Denote by v_1, v_2 non-leaf vertices of each of those graphs and let $\mathcal{G}$ be the graph obtained by identifying v_1 and v_2 . If the (unique) supremizer of $\mathcal{G}_i$ is the equilateral stower with $E_p^{(i)}$ petals and $E_l^{(i)}$ leaves, such that $E_p^{(i)} + E_l^{(i)} \geq 2$, then the (unique) supremizer of $\mathcal{G}$ is an equilateral stower with $E_p^{(1)} + E_p^{(2)}$ petals and $E_l^{(1)} + E_l^{(2)}$ leaves.*

We note that as we have shown (Theorem 3.2.2) that equilateral stars are the unique supremizers of trees, the corollary above implies that gluing a tree (at its internal vertex) to any graph whose (unique) supremizer is a stower gives a graph whose (unique) supremizer is a stower as well.

Corollary 3.2.8. *Let $\mathcal{G}$ be a stower graph with E_p petals and E_l leaves, such that $E_p + E_l \geq 2$ and $(E_p, E_l) \neq (1, 1)$. Then it has a maximizer which is the equilateral stower graph with E_p petals and E_l dangling edges and the corresponding spectral gap is $\frac{\pi}{2} (2E_p + E_l)$. Furthermore, this maximizer is unique for all cases except $(E_p, E_l) \in \{(2, 0), (1, 2)\}$.*

We remark that a partial result of the above was already proved within the proof of theorem 4.2 in [59]. It was shown there that the equilateral flower is the unique maximizer among all flowers⁵. This was used there to prove the global bound $k_1[\Gamma] \leq \pi E$ (theorem 4.2 in [59]). Having corollary 3.2.8, it is possible to prove the following improved bound.

Corollary 3.2.9. *Let $\mathcal{G}$ be a graph with E edges, out of which E_l are leaves. Then*

$$\forall \underline{l} \in \mathcal{L}_{\mathcal{G}}, \quad k_1[\Gamma(\mathcal{G}; \underline{l})] \leq \pi \left(E - \frac{E_l}{2} \right), \quad (3.7)$$

provided that $(E, E_l) \notin \{(1, 1), (1, 0), (2, 1)\}$.

Assume in addition that $(E, E_l) \notin \{(2, 0), (3, 2)\}$. Then an equality above implies that the graph $\Gamma(\mathcal{G}; \underline{l})$ achieving the inequality is either an equilateral mandarin or an equilateral stower.

This latter bound is sharp as it is attained by most equilateral stower graphs (see Example 3.1.5 and Corollary 3.2.8).

5. It is claimed there that the equilateral flower is the unique maximizer for all flowers with $E \geq 2$. Actually, the uniqueness does not hold for the $E = 2$ case, as we show in the proof of Corollary 3.2.8.

3.3 Infimizers

Proof of Theorem 3.2.1. Let Γ be a metric graph whose total edge length equals one and let f be an eigenfunction corresponding to the spectral gap $k_1(\Gamma)$ and normalized such that its L^2 norm equals one. Denote

$$m := \min f < 0 \quad (3.8)$$

$$M := \max f > 0, \quad (3.9)$$

where the inequalities arise as f , being a Neumann eigenfunction is orthogonal to the constant function. In what follows we bound from below the Rayleigh quotient of f by using the rearrangement technique in a similar manner to the proof of lemma 3 in [54]. We further define

$$\mu_f(t) := |\{x \in \Gamma \mid f(x) < t\}| \quad \text{for } t \in [m, M]$$

where $|\cdot|$ denotes the Lebesgue measure of the corresponding set on the graph. This allows to define a continuous, non-decreasing function f^* on the interval $[0, 1]$, such that $\mu_{f^*} = \mu_f$. This property gives

$$1 = \int_{\Gamma} |f(x)|^2 dx = \int_m^M t^2 d\mu_f = \int_0^1 |f^*(x)|^2 dx \quad (3.10)$$

and

$$0 = \int_{\Gamma} f(x) dx = \int_m^M t d\mu_f = \int_0^1 f^*(x) dx, \quad (3.11)$$

where the first equality in (3.11) holds since f is orthogonal to the constant function.

Another ingredient we use in the proof is the co-area formula [46]. Let $t \in [m, M]$ such that if $f(x) = t$ then x is not a vertex and $f'(x) \neq 0$ and call this t a regular value. By Sard's theorem, the non-regular values are of zero measure. According to the co-area formula if t is a regular value then

$$\mu'_f(t) = \sum_{x; f(x)=t} \frac{1}{|f'(x)|}, \quad (3.12)$$

and for any L^1 function g on the graph

$$\int_{\Gamma} g(x) |f'(x)| dx = \int_m^M \left(\sum_{x; f(x)=t} g(t) \right) dt. \quad (3.13)$$

We now estimate the numerator of the Rayleigh quotient, $\int_{\Gamma} |f'(x)|^2 dx$, as follows. Denote by x_m, x_M two points for which $f(x_m) = m$, $f(x_M) = M$ (they are not necessarily unique). Let $t \in [m, M]$ be a regular value. As Γ is connected there is a path on the graph connecting x_m with x_M and by continuity of f it attains the value t at least once along this path, say at some point x_t . By the choice of t , x_t is not a vertex. If Γ is a bridgeless graph, then cutting the graph at x_t , the graph is still connected and we can find another path joining x_m and x_M . By the same reasoning f attains the value t along this path as well, so that t is attained by f at least twice on Γ . Denoting by $n(t)$ the number of times that the value t is attained by f on the graph, we get that

$$n(t) \geq \begin{cases} 1 & \text{if } \Gamma \text{ has a bridge,} \\ 2 & \text{if } \Gamma \text{ is bridgeless.} \end{cases} \quad (3.14)$$

We may also bound $n(t)$ from above

$$(n(t))^2 = \left(\sum_{x; f(x)=t} \frac{1}{\sqrt{|f'(x)|}} \sqrt{|f'(x)|} \right)^2 \quad (3.15)$$

$$\leq \left(\sum_{x; f(x)=t} \frac{1}{|f'(x)|} \right) \left(\sum_{x; f(x)=t} |f'(x)| \right) \quad (3.16)$$

$$= \mu'_f(t) \left(\sum_{x; f(x)=t} |f'(x)| \right), \quad (3.17)$$

by applying the Cauchy-Schwarz inequality and (3.12). Writing (3.13) with $g(x) = |f'(x)|$ gives

$$\int_{\Gamma} |f'(x)|^2 dx = \int_m^M \left(\sum_{x; f(x)=t} |f'(x)| \right) dt \geq \int_m^M \frac{(n(t))^2}{\mu'_f(t)} dt. \quad (3.18)$$

We may repeat the arguments above for f^* , which attains each regular value exactly once and obtain that (3.17),(3.18) hold for f^* as equalities and with $n^*(t) = 1$. Therefore

$$\int_{\Gamma} |f'(x)|^2 dx \geq \operatorname{ess\,inf}_{m \leq t \leq M} (n(t))^2 \int_{\Gamma} |(f^*)'(x)|^2 dx, \quad (3.19)$$

where the infimum above is taken only with respect to regular values. As f is the eigenfunction corresponding to $k_1(\Gamma)$ with unit L^2 norm we have $\int_{\Gamma} |f'(x)|^2 dx = (k_1(\Gamma))^2$. Considering f^* as a test function of unit L^2 norm (see (3.10)) and zero mean (see (3.11)) on the unit interval we get that its Rayleigh quotient is no less than the first positive eigenvalue, namely that $\int_{\Gamma} |(f^*)'(x)|^2 dx \geq \pi^2$. Combining this with (3.19) and (3.14) we get the lower bounds,

$$k_1(\Gamma) \geq \begin{cases} \pi & \text{if } \Gamma \text{ has a bridge,} \\ 2\pi & \text{if } \Gamma \text{ is bridgeless.} \end{cases} \quad (3.20)$$

All that remains to complete the proof is the characterization of the infimizers.

Assume first that Γ has a bridge. An equality in (3.20) is possible only if $n(t) = 1$ for all regular $t \in [m, M]$. This implies that Γ does not have vertices of degree 3 and above. Otherwise, due to continuity of f , we would have $n \neq 1$ in a vicinity of such a vertex. Γ cannot be a single cycle graph as it has a bridge and is therefore the unit interval, $[0, 1]$. Hence it is the unique candidate for an infimizer. Indeed, its spectral gap is π and starting from any discrete graph $\mathcal{G}$ with a bridge, $\Gamma(\mathcal{G}; \underline{l})$ is the unit interval if $\underline{l} \in \bar{\mathcal{L}}_{\mathcal{G}}$ is chosen such that all of its entries vanish, except the entry corresponding to the bridge.

Next, the possible minimizers of bridgeless graphs are characterized. By Menger's theorem [71], a graph is bridgeless if and only if there are at least two edge disjoint paths connecting any pair of points. We use that to deduce that if $\mathcal{G}$ is bridgeless then $\Gamma(\mathcal{G}; \underline{l})$ is bridgeless as well. Indeed, any path between a pair of points in $\Gamma(\mathcal{G}; \underline{l})$ corresponds to at least one path between those points in $\mathcal{G}$. Thus, to seek for a possible minimizer, we assume that Γ is bridgeless and $k_1(\Gamma) = 2\pi$. As a bridgeless graph is 2-edge-connected, we deduce from Menger's theorem that there are at least two edge disjoint paths connecting x_m with x_M . Pick two such paths and denote them by γ_1, γ_2 . A necessary condition for $k_1(\Gamma) = 2\pi$ is that $n(t) = 2$ for each regular value $t \in [m, M]$. By continuity, f attains each regular value at least once on γ_1 and at least once on γ_2 . As $n(t) = 2$ for a regular

value t , f attains the value t *exactly* once on each of γ_1 and γ_2 . Hence f is strictly increasing on γ_1 from x_m to x_M and the same holds for γ_2 . We further conclude that f may attain only non-regular values at $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$. In particular, if there exists an edge in $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$, f should be constant on that edge and due to $-f'' = (2\pi)^2 f$ this constant equals zero. Thus, the edges of $\Gamma \setminus \{\gamma_1 \cup \gamma_2\}$ may be removed from Γ , such that f still satisfies the Neumann conditions on the remaining graph $\gamma_1 \cup \gamma_2$ and it is an eigenfunction on that graph. However, by this we find an eigenfunction of k -eigenvalue 2π on a bridgeless graph whose total length smaller than one, which contradicts the lower bound, (3.20). Hence Γ consists of just the union of the paths γ_1, γ_2 . As γ_1, γ_2 are edge disjoint, $\gamma_1 \cap \gamma_2$ contains only vertices. We denote those vertices by $v_0, \dots, v_n$, with $v_0 = x_m$, $v_n = x_M$ and the indices are arranged in an increasing order along the path γ_1 . As f is strictly increasing along both γ_1, γ_2 , the order of those vertices along γ_2 is the same : $v_0, \dots, v_n$. Consider two adjacent vertices v_i, v_{i+1} ($0 \leq i \leq n-1$) and denote the corresponding path segments connecting them by $\gamma_1(v_i, v_{i+1}), \gamma_2(v_i, v_{i+1})$. As f takes the same values on the endpoints of $\gamma_1(v_i, v_{i+1}), \gamma_2(v_i, v_{i+1})$, is increasing and satisfies $-f'' = (2\pi)^2 f$ on both, we conclude $f|_{\gamma_1(v_i, v_{i+1})} = f|_{\gamma_2(v_i, v_{i+1})}$ and also that $\gamma_1(v_i, v_{i+1})$ has the same length as $\gamma_2(v_i, v_{i+1})$. Hence $\Gamma = \gamma_1 \cup \gamma_2$ is a symmetric necklace. $\square$

Remark. A further exploration of symmetric necklace graphs appears in Proposition 3.5.8. It is shown there that a symmetric necklace graph belongs to a family of graphs in which every graph has a simple spectral gap and its spectral gap $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is a critical value when considered as a function of $\underline{l} \in \mathcal{L}_{\mathcal{G}}$.

Theorem 3.2.1 provides a complete answer to the minimization problem. In particular, it states that any infimizer of a bridgeless graph is a symmetric necklace. A further task would be to classify the entire family of necklace graphs which serve as infimizers of a particular discrete graph. We start treating this by observing that the spectral gap of any symmetric necklace (of total length one) is 2π . This follows from noting that 2π is an eigenvalue of any symmetric necklace and combining this with Theorem 3.2.1. Now, let $\mathcal{G}$ be a bridgeless graph and let $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$, such that $\Gamma(\mathcal{G}; \underline{l}^*)$ is a symmetric necklace with some β number of cycles. By the observation above and Theorem 3.2.1 we have that $\Gamma(\mathcal{G}; \underline{l}^*)$ is an infimizer of $\mathcal{G}$. Furthermore, by choosing other values for $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ we may get $\Gamma(\mathcal{G}; \underline{l})$ to be any symmetric necklace with at most β cycles, and from the above this $\Gamma(\mathcal{G}; \underline{l})$ would also serve as an infimizer. Therefore, the answer to the classification problem above would be given once we find what is the maximal number of cycles among all symmetric necklaces that can be obtained from a given discrete graph $\mathcal{G}$. Solving this requires some elements from the theory of graph connectivity which we shortly present below. A graph is called k -edge-connected if it remains connected whenever less than k edges are removed. In particular, a bridgeless graph is 2-edge-connected. A cactus graph is a graph in which every edge is contained in exactly one cycle. Let $\mathcal{G}$ be a bridgeless graph. There exists $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ such that $\Gamma(\mathcal{G}; \underline{l})$ is a cactus graph with the following property. For every two edges e, e' which form a 2-edge-cut in $\mathcal{G}$ (two edges whose removal disconnects the graph), we have $l_e, l_{e'} \neq 0$. Namely, those two edges also appear in $\Gamma(\mathcal{G}; \underline{l})$. The theory leading to this result appears in [50, 53, 72] for general k -connected graphs and is very nicely explained for the particular case of 2-edge-connected graphs in section 10 of the recent paper [70]. Now, in order to determine the maximal number of cycles of a necklace obtained from $\mathcal{G}$ we perform the following procedure. Find all subgraphs of $\mathcal{G}$ which are 3-edge-connected and contract each of them to a vertex; for example by choosing $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ such that the corresponding entries vanish and considering $\Gamma(\mathcal{G}; \underline{l})$. This yields a cactus graph with the property mentioned above [70]. The cactus graph has a tree-like structure. This can be observed by considering an auxiliary graph Γ' , where each cycle of $\Gamma(\mathcal{G}; \underline{l})$ is represented by a vertex of Γ' and two vertices of Γ' are connected if the corresponding cycles in $\Gamma(\mathcal{G}; \underline{l})$ share a vertex (a cactus graph has the property that any two cycles of it, share at most one vertex). The obtained graph, Γ' turns to be a tree graph. Any path of this

tree graph then corresponds to a necklace which can be obtained from the cactus $\Gamma(\mathcal{G}; \underline{l})$ by further setting some edge lengths to zero. The longest possible necklace is found by identifying the longest path of the tree Γ' .

3.4 Supremizers of tree graphs

The proof of Theorem 3.2.2 is based on bounding the graph diameter, as follows.

Definition 3.4.1. Let Γ be a compact metric graph. The diameter of Γ is

$$d(\Gamma) := \max \{ \text{dist}(x, y) \mid x, y \in \Gamma \}$$

Lemma 3.4.2. Let Γ be a metric tree graph of total length 1 and with $E_l \geq 2$ leaves. Then

$$d(\Gamma) \geq \frac{2}{E_l} \tag{3.21}$$

with equality if and only if Γ is an equilateral star.

Démonstration. Choose two points, x_1, x_2 , in Γ such that the distance between them is exactly $d(\Gamma)$. We show that x_1, x_2 are necessarily leaves. Assume by contradiction that (w.l.o.g) x_1 is not a leaf. Then $\Gamma \setminus \{x_1\}$ has at least two connected components. Let Γ_1 be one of these components satisfying $x_2 \notin \Gamma_1$. Let z be a point of Γ_1 different from x_1 . As Γ is a tree, any path from z to x_2 contains x_1 , which yields

$$d(x_2, z) > d(x_2, x_1) = d(\Gamma),$$

thus contradicting the definition of $d(\Gamma)$. Let now $\mathcal{P}$ be the shortest path connecting x_1 to x_2 and denote by x_0 its middle, such that

$$d(x_1, x_0) = d(x_2, x_0) = \frac{d(\Gamma)}{2}.$$

We cover Γ with E_l paths, each starting at x_0 and ending at a leaf of Γ . The length of each of these paths is at most $d(x_1, x_0)$ (otherwise, we may replace x_1 by a different leaf and increase $d(\Gamma)$). As the union of these paths cover Γ , whose total length is 1, we have

$$1 \leq \sum_{v \text{ is a leaf}} d(x_0, v) \leq \sum_{v \text{ is a leaf}} d(x_0, x_1) = E_l \frac{d(\Gamma)}{2}, \tag{3.22}$$

from which the inequality of the lemma follows. The first inequality can be an equality if and only if Γ is a star and x_0 is its central vertex. Assuming this, the second inequality can be an equality if and only if the star is equilateral. $\square$

Aided with Lemma 3.4.2, we turn to the proof of the theorem.

Proof of Theorem 3.2.2. We show in the following that there exists a test function f on Γ such that its Rayleigh quotient satisfies

$$\mathcal{R}(f) \leq \left(\frac{\pi}{d(\Gamma)} \right)^2. \tag{3.23}$$

Indeed, let y, z be two leaves of Γ such that the distance between them is exactly $d(\Gamma)$. Let us denote by $\mathcal{P}$ a path of Γ , of length $d(\Gamma)$, connecting y and z . We consider $\mathcal{P}$ as the interval $[0, d(\Gamma)]$, for example by identifying y with 0 and z with $d(\Gamma)$ and define the following function on $\mathcal{P}$,

$$f(x) = \cos\left(\frac{\pi x}{d(\Gamma)}\right) \text{ for } x \in \mathcal{P}.$$

We extend f to be defined on the whole graph, Γ , by setting its value on each connected component of $\Gamma \setminus \mathcal{P}$ to the unique constant which preserves the continuity of f . Referring to Appendix A.3 and using $f - \langle f \rangle$ as our test function we have from (A.18),

$$\mathcal{R}(f - \langle f \rangle) = \frac{\int_{\Gamma} |f'(x)|^2 dx}{\int_{\Gamma} |f(x)|^2 dx - \left(\int_{\Gamma} f(x) dx\right)^2} \quad (3.24)$$

$$= \frac{\left(\frac{\pi}{d(\Gamma)}\right)^2 \frac{d(\Gamma)}{2}}{\frac{d(\Gamma)}{2} + \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx - \left(\int_{\Gamma} f(x) dx\right)^2} \quad (3.25)$$

As the integral of f on $\mathcal{P}$ vanishes, using Cauchy-Schwarz inequality we get

$$\left(\int_{\Gamma} f(x) dx\right)^2 = \left(\int_{\Gamma \setminus \mathcal{P}} f(x) dx\right)^2 \leq (1 - d(\Gamma)) \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx. \quad (3.26)$$

Plugging (3.26) in (3.25) gives

$$\mathcal{R}(f - \langle f \rangle) \leq \frac{\left(\frac{\pi}{d(\Gamma)}\right)^2 \frac{d(\Gamma)}{2}}{\frac{d(\Gamma)}{2} + d(\Gamma) \int_{\Gamma \setminus \mathcal{P}} |f(x)|^2 dx} \leq \left(\frac{\pi}{d(\Gamma)}\right)^2. \quad (3.27)$$

Using this and Lemma 3.4.2 we get

$$k_1(\Gamma) \leq \frac{\pi}{d(\Gamma)} \leq \frac{\pi}{2} E_l. \quad (3.28)$$

Let $\mathcal{G}$ be a tree graph with E_l leaves. We may choose $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$ such that $\Gamma(\mathcal{G}; \underline{l})$ is an equilateral star graph with E_l leaves, so that $k_1[\Gamma(\mathcal{G}; \underline{l})] = \frac{\pi}{2} E_l$ and from the bound above we get that $\Gamma(\mathcal{G}; \underline{l})$ is a supremizer. This is a unique supremizer as having equality in the right inequality of (3.28) implies by Lemma 3.4.2 that Γ is an equilateral star with E_l leaves. $\square$

Remark. We note that the upper bound $k_1(\Gamma) \leq \frac{\pi}{d(\Gamma)}$, which is obtained in the course of the proof above, is a particular case of a result proven recently in [76]. There it was shown that for any n , $k_n(\Gamma) \leq \frac{\pi n}{d(\Gamma)}$. Applying (3.21) to the latter we may get that for any $n \geq 1$, $k_n(\Gamma) \leq \frac{\pi n}{2} E_l$, which improves the bound $k_n(\Gamma) \leq \frac{\pi n}{2} E$ given in [76].

The theorem above yields the following.

Proof of Corollary 3.2.3. Let $\mathcal{G}$ be a graph with $\beta > 0$ cycles and E_l leaves. We start by observing that for $(\beta, E_l) \in \{(1, 0), (1, 1)\}$, the supremizer is the single cycle graph (see Lemma 3.8.5), which is not a tree. We continue assuming $(\beta, E_l) \notin \{(1, 0), (1, 1)\}$. Choose a maximal spanning tree of $\mathcal{G} \setminus \mathcal{E}_l$, where $\mathcal{E}_l$ is the set of the graph's E_l leaves. Choose $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ such that all of its entries corresponding to the spanning tree edges are set to zero. This makes $\Gamma(\mathcal{G}; \underline{l}^*)$ a stower with β petals and E_l leaves. Furthermore, $\underline{l}^*$ may be chosen such that $\Gamma(\mathcal{G}; \underline{l}^*)$ is an equilateral stower. The spectral gap of this graph is $\frac{\pi}{2} (2\beta + E_l)$ (see Example 3.1.5). Alternatively, if $\underline{l} \in \overline{\mathcal{L}}_{\mathcal{G}}$ is such that $\Gamma(\mathcal{G}; \underline{l})$ is a tree then the number of its leaves is at most E_l and by Theorem 3.2.2 its spectral gap is at most $\frac{\pi}{2} E_l$. Therefore, the stower graph $\Gamma(\mathcal{G}; \underline{l}^*)$ obtained above has a greater spectral gap than any tree graph $\Gamma(\mathcal{G}; \underline{l})$. $\square$

3.5 Spectral gaps as critical values

In this section we assume that the spectral gap, $k_1(\Gamma(\mathcal{G}; \underline{l}))$, is a simple eigenvalue. This allows to take derivatives of the eigenvalue with respect to the edge lengths, $\underline{l} \in \mathcal{L}_{\mathcal{G}}$, and to find critical points which serve as candidates for maximizers. We prove here Theorem 3.2.4 which shows that such local maximizers do not achieve a spectral gap higher than that achieved by turning the graph into a mandarin or a flower.

Lemma 3.5.1. *Let Γ be a metric graph and f an eigenfunction corresponding to the eigenvalue k^2 with arbitrary vertex conditions. Then the function $f'(x)^2 + k^2 f(x)^2$ is constant along each edge.*

Démonstration. The proof is immediate, once differentiating the function $f'(x)^2 + k^2 f(x)^2$ along an edge. $\square$

The last lemma motivates us to define the energy⁶ of an eigenfunction on an edge e as $\mathcal{E}_e := f'(x)^2 + k^2 f(x)^2$ for any $x \in e$. This energy shows up naturally when differentiating an eigenvalue with respect to an edge length. In order to evaluate such derivatives we extend Definition 3.1.1 so that $\Gamma(\mathcal{G}; \underline{l})$ is defined for all $\underline{l} \in \mathbb{R}^E$ with positive entries and relax the restriction $\sum_{e=1}^E l_e = 1$, imposed by $\underline{l} \in \mathcal{L}_{\mathcal{G}}$. The following lemma appears also as Lemma A.1 in [47] and within the proof of a lemma in [55].

Lemma 3.5.2. *Let $\mathcal{G}$ be a discrete graph and let $\underline{l} \in \mathbb{R}^E$ with positive entries. Assume that the spectral gap, $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is a simple eigenvalue and let f be the corresponding eigenfunction, normalized to have unit L^2 norm. Then $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is differentiable with respect to any edge length $l_{\tilde{e}}$ and*

$$\frac{\partial}{\partial l_{\tilde{e}}} \left((k_1[\Gamma(\mathcal{G}; \underline{l})])^2 \right) = -\mathcal{E}_{\tilde{e}}. \quad (3.29)$$

Démonstration. In this proof we use the analyticity of the eigenvalues and eigenfunctions with respect to the edge lengths. This is established for example in sections 3.1.2, 3.1.3 of [43]. Let $s \in \mathbb{R}$ and let $\tilde{e}$ be an edge of $\Gamma(\mathcal{G}; \underline{l})$. Denote $\underline{l}(s) := \underline{l} + s\vec{e}$, with $\vec{e} \in \mathbb{R}^E$ a vector with one at its $\tilde{e}^{\text{th}}$ position and zeros in all other entries. We use the notation $\Gamma(s) := \Gamma(\mathcal{G}; \underline{l}(s))$ and denote by $k_1(s)$ the spectral gap of $\Gamma(s)$. By assumption, $k_1(0)$ is a simple eigenvalue and hence there is a neighborhood of zero for which all $k_1(s)$ are simple eigenvalues. The corresponding eigenfunctions are denoted by $f(s; \cdot)$ and we further assume that all those eigenfunctions have unit L^2 norm,

$$\int_{\Gamma(s)} (f(s; x))^2 dx = \sum_{e=1}^E \int_0^{l_e(s)} (f(s; x_e))^2 dx_e = 1, \quad (3.30)$$

where $l_e(s) = l_e + \delta_{e,\tilde{e}}s$ and $\delta_{e,\tilde{e}}$ being the Kronecker delta function.

Taking a derivative of the above with respect to s ,

$$(f(s; l_{\tilde{e}}(s)))^2 + 2 \sum_{e=1}^E \int_0^{l_e(s)} f(s; x_e) \frac{\partial}{\partial s} f(s; x_e) dx_e = 0. \quad (3.31)$$

In addition, evaluating the Rayleigh quotient of f ,

$$k_1(s)^2 = \mathcal{R}[f(s; \cdot)] = \sum_{e=1}^E \int_0^{l_e(s)} \left(\frac{\partial}{\partial x_e} f(s; x_e) \right)^2 dx_e, \quad (3.32)$$

6. A simple harmonic oscillator whose spring constant is k and whose position is given by $f(x)$ has a total energy of $\frac{1}{2}\mathcal{E}_e$.

using that $f(s; \cdot)$ has unit norm. Differentiating this with respect to s gives

$$\frac{d}{ds} (k_1(s)^2) = \left(\frac{\partial}{\partial x_{\tilde{e}}} f(s; l_{\tilde{e}}(s)) \right)^2 + 2 \sum_{e=1}^E \int_0^{l_e(s)} \frac{\partial}{\partial x_e} f(s; x_e) \frac{\partial^2}{\partial s \partial x_e} f(s; x_e) dx_e. \quad (3.33)$$

Integrating by parts in the right hand side and using the eigenvalue equation, we get for each term in the sum above

$$\begin{aligned} \int_0^{l_e(s)} \frac{\partial}{\partial x_e} f(s; x_e) \frac{\partial^2}{\partial s \partial x_e} f(s; x_e) dx_e &= \\ &= \frac{\partial}{\partial x_e} f(s; l_e(s)) \left(\frac{\partial}{\partial s} f \right) (s; l_e(s)) - \frac{\partial}{\partial x_e} f(s; 0) \frac{\partial}{\partial s} f(s; 0) \\ &\quad + k_1(s)^2 \int_0^{l_e(s)} f(s; x_e) \frac{\partial}{\partial s} f(s; x_e) dx_e \\ &= \frac{\partial f}{\partial x_e} \left(\frac{df}{ds} - \delta_{e, \tilde{e}} \frac{\partial f}{\partial x_e} \right) \Big|_{(s; l_e(s))} - \frac{\partial f}{\partial x_e} \frac{df}{ds} \Big|_{(s; 0)} + k_1(s)^2 \int_0^{l_e(s)} f \frac{\partial f}{\partial s} \Big|_{(s; x_e)} dx_e, \end{aligned} \quad (3.34)$$

where the partial derivatives with respect to s are rewritten in terms of complete derivatives.

Summing the first two terms of the right hand side of (3.34) over all edges and rewriting it as a sum over all graph vertices we get

$$\begin{aligned} \sum_{e=1}^E \left\{ \frac{\partial f}{\partial x_e} f \left(\frac{df}{ds} - \delta_{e, \tilde{e}} \frac{\partial f}{\partial x_e} \right) \Big|_{(s; l_e(s))} - \frac{\partial f}{\partial x_e} \frac{df}{ds} \Big|_{(s; 0)} \right\} \\ = \sum_v \left(\sum_{e \sim v} \frac{\partial f}{\partial x_e} \right) \frac{df}{ds} \Big|_{(s; v)} - \left(\frac{\partial f}{\partial x_{\tilde{e}}} \Big|_{(s; l_{\tilde{e}}(s))} \right)^2 \\ = - \left(\frac{\partial f}{\partial x_{\tilde{e}}} \Big|_{(s; l_{\tilde{e}}(s))} \right)^2, \end{aligned} \quad (3.35)$$

where the sum $e \sim v$ above is taken over all edges adjacent to a chosen vertex v , the derivatives $\frac{\partial}{\partial x_e}$ in this sum are all taken towards the vertex v and $\sum_{e \sim v} \frac{\partial}{\partial x_e} f(s; v) = 0$, as f satisfies Neumann conditions at v .

Plugging (3.34), (3.35) and (3.31) in equation (3.33) we get

$$\frac{d}{ds} (k_1(s)^2) = - \left(\frac{\partial f}{\partial x_{\tilde{e}}} \Big|_{(s; l_{\tilde{e}}(s))} \right)^2 - (k_1(s))^2 \left(f|_{(s; l_{\tilde{e}}(s))} \right)^2 = -\mathcal{E}_{\tilde{e}},$$

which finishes the proof once $s = 0$ is taken. $\square$

We note that the derivative of an eigenvalue with respect to an edge length is derived in [49] (theorem 4.4) for the general case of the p -Laplacian on a graph. In the case of the 2-Laplacian, using Lemma 3.5.1 shows that the integral expression obtained in [49] simplifies to equal $-\mathcal{E}_{\tilde{e}}$.

The lemma above provides a practical tool for increasing the spectral gap once the corresponding eigenfunction is known. In order to do so, one should increase the length of edges with lower energy on the expense of shortening those with higher energy. In particular, focusing on a particular vertex, one should increase the lengths of the edges for which the eigenfunction derivative is the lowest and

vice versa. This method is useful as long as the spectral gap is not a critical point in the edge length space, $\mathcal{L}_{\mathcal{G}}$. An equilateral star with an odd number of edges illustrates the importance of simplicity : though we cannot increase the spectral gap, no eigenfunction on this graph will have equal energy at all edges.

The next lemma provides a necessary and sufficient condition for existence of a critical point in the edge length space, $\mathcal{L}_{\mathcal{G}}$.

Lemma 3.5.3. *Let $\mathcal{G}$ be a discrete graph and let $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$. Assume that the spectral gap, $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$ is a simple eigenvalue and let f be the corresponding eigenfunction. The function $k_1[\Gamma(\mathcal{G}; \underline{l})]$ has a critical value at $\underline{l} = \underline{l}^*$ if and only if both conditions below are satisfied*

1. The derivative of f vanishes at all vertices of odd degree.
2. The derivative of f satisfy, $\left| \frac{\partial}{\partial x_{e_1}} f(v) \right| = \left| \frac{\partial}{\partial x_{e_2}} f(v) \right|$, for all edges e_1, e_2 adjacent to a vertex of even degree, v .

Démonstration. We first observe that positivity of the spectral gap yields that $k_1[\Gamma(\mathcal{G}; \underline{l})]$ has a critical point at $\underline{l} = \underline{l}^*$ if and only if $(k_1[\Gamma(\mathcal{G}; \underline{l})])^2$ has a critical point there. From Lemma 3.5.2 we deduce that a critical point occurs if and only if the corresponding eigenfunction has equal energies on all graph edges. The last deduction comes as this is a critical point under the constraint $\sum_e l_e = 1$. Let v be a graph vertex and e_1, e_2 two edges adjacent to it. Since f is continuous (i.e., single valued) at v we conclude

$$\mathcal{E}_e = \mathcal{E}_{\bar{e}} \Leftrightarrow \left(\frac{\partial}{\partial x_e} f(v) \right)^2 = \left(\frac{\partial}{\partial x_{\bar{e}}} f(v) \right)^2,$$

which proves the second claim of the lemma. The first claim follows since the Neumann condition gives that the sum of all derivatives at v vanishes. $\square$

Obviously, graphs whose spectral gap is a critical point in the space $\mathcal{L}_{\mathcal{G}}$ serve as good candidates for maximizers. The next lemma characterizes those graphs and their corresponding eigenfunctions.

Lemma 3.5.4. *Let $\mathcal{G}$ be a discrete graph, $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ and denote $\Gamma := \Gamma(\mathcal{G}; \underline{l}^*)$. Assume that $k := k_1[\Gamma]$ is a critical value and let f be the corresponding eigenfunction. Then we have the following edge-disjoint decomposition*

$$\Gamma = \bigcup_{i=1}^P \mathcal{P}_i, \tag{3.36}$$

where

1. All $\mathcal{P}_i$'s are graphs which possess an Eulerian path or an Eulerian cycle. Namely, for each $\mathcal{P}_i$ there is a path (either open path or a cycle), which visits each edge exactly once.
2. Different $\mathcal{P}_i$'s may share only vertices, but not edges.
3. $f|_{\mathcal{P}_i}$ is a Neumann eigenfunction of $\mathcal{P}_i$, whose eigenvalue equals k .
4. Denote by μ_i the number of zeros of $f|_{\mathcal{P}_i}$, where each zero at a vertex of $\mathcal{P}_i$ is counted as half the degree of this vertex in $\mathcal{P}_i$. Denoting by L_i the metric length of $\mathcal{P}_i$, the following holds

$$kL_i = \pi\mu_i.$$

5. In addition,

$$k = \pi\mu, \quad (3.37)$$

where μ is the number of zeros of f on Γ , where each zero at a vertex of Γ is counted as half the degree of this vertex in Γ .

Démonstration. We use the claims of Lemma 3.5.3 to describe a recursive process, which produces this path decomposition.

- Assume first that Γ has at least one vertex of odd degree, v_0 . Take v_0 to be the starting point of a path $\mathcal{P}$ and add to $\mathcal{P}$ any edge, e_0 , which is adjacent to v_0 and the vertex connected at its other end, which we denote by v_1 . If v_1 is of even degree we seek for an edge e_1 connected to v_1 such that $f'|_{e_1}(v_1) = -f'|_{e_0}(v_1)$ (both derivatives are outgoing from v_1). Such edge exists by lemma 3.5.3.(2) and as the sum of derivatives of f at v vanish. Add e_1 and its other endpoint, v_2 to $\mathcal{P}$ and repeat the step above until reaching a vertex of odd degree. Once an odd degree vertex is reached, we end the construction of $\mathcal{P}$ and continue recursively to form the next path on $\Gamma \setminus \mathcal{P}$. Note that a certain vertex may be reached more than once during $\mathcal{P}$'s construction. Such a vertex would appear in $\mathcal{P}$ only once, but with a degree greater than two. This process of path constructions continues until we exhaust the whole of Γ or alternatively, until Γ does not have any more odd degree vertices, at which point we continue with performing the next stage.
- If Γ has no vertex of odd degree, the construction of $\mathcal{P}$ is as follows. We choose an arbitrary vertex, v_0 as the starting point of $\mathcal{P}$ and choose an arbitrary edge, e_0 which is connected to v_0 and add it to $\mathcal{P}$ as well, together with its other endpoint, v_1 . Now, just as we did in the first stage, we seek for an edge e_1 connected to v_1 such that $f'|_{e_1}(v_1) = -f'|_{e_0}(v_1)$. We keep constructing $\mathcal{P}$ as above, keeping in mind that all vertices are of even degree. At some point we reach again the vertex v_0 , arriving from some edge denoted e_n . If $f'|_{e_0}(v_0) = -f'|_{e_n}(v_0)$ (both derivatives are outgoing from v_0) then we end the construction of $\mathcal{P}$. Otherwise, continue the construction of $\mathcal{P}$ until the condition above is satisfied. This will indeed occur, as the graph is finite and f satisfies Neumann conditions on Γ . Once we finish constructing of $\mathcal{P}$ we continue recursively to form the next path on $\Gamma \setminus \mathcal{P}$.

We observe that by way of construction each $\mathcal{P}_i$ possesses an Eulerian path or an Eulerian cycle and also $f|_{\mathcal{P}_i}$ satisfies Neumann conditions on $\mathcal{P}_i$. Thus claims (1) and (3) are valid. Also, as each subgraph $\mathcal{P}_i$ is removed from Γ once constructed, it is clear that $\forall i \neq j, \mathcal{P}_i \cap \mathcal{P}_j$ may contain only vertices, which is stated in claim (2). A subgraph $\mathcal{P}_i$ of the first stage of the construction, where Γ has some odd degree vertices, possesses an Eulerian path and may be identified with an interval $[0, L_i]$, where L_i is the metric length of $\mathcal{P}_i$. Also by way of construction, $f|_{[0, L_i]}$ is a Neumann eigenfunction (notice that this is more restrictive than stating that $f|_{\mathcal{P}_i}$ is a Neumann eigenfunction, because of possible self-crossings). Hence $f|_{[0, L_i]} = \cos\left(\frac{\pi}{L_i}\mu_i x\right)$ for some positive integer, μ_i . Clearly, μ_i equals the number of zeros of $f|_{[0, L_i]}$. Furthermore, it also equals the number of zeros of $f|_{\mathcal{P}_i}$, where zero at a vertex is counted as many times as half the degree of that vertex in $\mathcal{P}_i$. A subgraph $\mathcal{P}_i$ of the second construction stage, where all Γ vertices are of even degrees possesses an Eulerian cycle and may be identified with an interval $[0, L_i]$, where L_i is the metric length of $\mathcal{P}_i$. Also by way of construction, $f|_{[0, L_i]}$ is a Neumann eigenfunction which satisfies periodic boundary conditions. Hence $f|_{[0, L_i]} = \cos\left(\frac{\pi}{L_i}\mu_i x\right)$ for some positive even integer, μ_i . As before, μ_i equals the number of zeros of $f|_{\mathcal{P}_i}$, counted according to vertex degrees. In both cases, we have that $k = \frac{\pi}{L_i}\mu_i$, which shows claim (4) of the theorem.

Finally, claim (5) is deduced from claim (4), by summing over all $\mathcal{P}_i$'s. $\square$

Having characterized local critical points, we wish to connect those to supremizers.

Lemma 3.5.5. *Let $\Gamma(\mathcal{G}; \underline{l})$ be a supremizer of a discrete graph $\mathcal{G}$, such that its spectral gap $k_1[\Gamma(\mathcal{G}; \underline{l})]$ is simple. Then, there exists a discrete graph $\mathcal{G}^*$ and positive edge lengths $\underline{l}^* \in \mathcal{L}_{\mathcal{G}^*}$ such that $\Gamma(\mathcal{G}; \underline{l}) = \Gamma(\mathcal{G}^*; \underline{l}^*)$ and the spectral gap $k_1[\Gamma(\mathcal{G}^*; \underline{l}^*)]$ is a critical value.*

Démonstration. Start by forming a new discrete graph $\mathcal{G}^*$ by contracting the edges of $\mathcal{G}$ which correspond to the vanishing values of $\underline{l}$, or setting $\mathcal{G}^* = \mathcal{G}$ if all entries of $\underline{l}$ are strictly positive. We get that there exists $\underline{l}^* \in \mathcal{L}_{\mathcal{G}^*}$ such that $\Gamma(\mathcal{G}; \underline{l}) = \Gamma(\mathcal{G}^*; \underline{l}^*)$. In effect, $\underline{l}^*$ entries are exactly the non-vanishing entries of $\underline{l}$. Since $\Gamma(\mathcal{G}; \underline{l})$ is a supremizer of $\mathcal{G}$ we get that $\Gamma(\mathcal{G}^*; \underline{l}^*)$ is a supremizer of $\mathcal{G}^*$. Furthermore, $\Gamma(\mathcal{G}^*; \underline{l}^*)$ is even a maximizer of $\mathcal{G}^*$ as all of $\underline{l}^*$ entries are positive. Since $k_1[\Gamma(\mathcal{G}^*; \underline{l}^*)]$ is a simple eigenvalue, it is analytic with respect to edge lengths and therefore must be a critical value. $\square$

Having Lemma 3.5.5 allows to conclude that all the claims in lemmata 3.5.3 and 3.5.4 hold for supremizers whose spectral gaps are simple. We use this in proving Theorem 3.2.4.

Proof of Theorem 3.2.4. We start by noting that the path decomposition of Lemma 3.5.4 is valid under the assumptions of the theorem. Denote for brevity $\Gamma := \Gamma(\mathcal{G}; \underline{l})$ and $k := k_1[\Gamma]$, with corresponding eigenfunction f . Denote $\Gamma_+ := \{x \in \Gamma \mid f(x) > 0\}$, $\Gamma_- := \{x \in \Gamma \mid f(x) < 0\}$ and denote by β_+, β_- their corresponding first Betti numbers. The connected components of Γ_+, Γ_- are called the nodal domains of f . As k is the second eigenvalue of Γ , we deduce from the Courant nodal theorem and the simplicity of k that f has only two nodal domains (see [48] for the original proof of Courant, or [57, 42] for its adaptation for graphs). Hence, the sets Γ_+ and Γ_- are connected (notice that $\Gamma_{\pm}$ are not exactly subgraphs, as they do not include the vertices at which f vanishes).

Next, note that f cannot completely vanish on an edge. Otherwise, the energy of that edge equals to zero and as k is a critical value, by the proof of Lemma 3.5.3 all edge energies are equal to zero which leads to $f \equiv 0$. Furthermore, we show that f cannot vanish more than once on the same edge, including its endpoints. Assume by contradiction that there exists an edge, $e = [u, v]$ on which f vanishes at least twice. As f has only two nodal domains, it can vanish at most twice on e . For each zero of f located on the interior of e , add a dummy vertex of degree two at the position of this zero. Those two zeros now coincide with two vertices of $\Gamma(\mathcal{G}; \underline{l})$, which we denote by v_1, v_2 and further denote the degrees of those vertices by d_1, d_2 . We note that both d_1 and d_2 are even and in particular not smaller than two. This holds as a zero at an odd degree vertex implies by Lemma 3.5.3 that the energy at this vertex vanishes as well. As k is a critical value, all energies are equal throughout the graph, which implies $f \equiv 0$. From Lemma 3.5.4, (5) we get $k = \frac{1}{2}(d_1 + d_2)\pi$. We modify Γ by contracting the edge segment connecting between v_1 and v_2 , turning them into a single vertex which we denote by v_0 . We get that in the new graph, the vertex v_0 has a degree $d_0 = d_1 + d_2 - 2$. This new graph is connected and we modify it by contracting all edges except those d_0 edges connected to v_0 . Doing so, we obtain a mandarin graph with $d_1 + d_2 - 2$ edges. By turning the mandarin into an equilateral mandarin it achieves a spectral gap of $(d_1 + d_2 - 2)\pi$ (see Example 3.1.6). As Γ is a supremizer we conclude $(d_1 + d_2 - 2)\pi \leq \frac{1}{2}(d_1 + d_2)\pi$, so that $d_1 + d_2 \leq 4$. Since we have seen above that $d_1 \geq 2, d_2 \geq 2$ we deduce $d_1 = d_2 = 2$. By the path decomposition in Lemma 3.5.4, each path must contain at least one zero of f . Hence only a single path is possible in the decomposition and Γ must be a single cycle graph. We arrive at a contradiction, as the spectral gap of this graph is not simple. Hence f vanishes at most once on each edge, which includes both the interior of the edge and its two endpoints.

If f vanishes at points which are not vertices, we turn those points into dummy vertices of degree two. Each zero of f is now located at some vertex of Γ . We introduce the following notation. Denote

by V_+ (V_-) the number of vertices at which f is positive (negative), which is just the number of vertices of Γ_+ (Γ_-). Denote by V_0 the number of vertices at which f vanishes (this includes the additional dummy vertices we added). Similarly, denote by E_{++} (E_{--}) the number of edges which connect two vertices from V_+ (V_-). Note that f does not vanish at all on those edges. Further denote by E_{0+} (E_{0-}) the number of edges which connect a vertex of V_0 to a vertex of V_+ (V_-). Note that due to the additional dummy vertices there are no edges which connect a positive vertex to a negative one. With those notations, the graph's first Betti number is

$$\begin{aligned}\beta &= E - V + 1 \\ &= (E_{++} + E_{--} + E_{0+} + E_{0-}) - (V_+ + V_- + V_0) + 1 \\ &= (E_{++} - V_+ + 1) + (E_{--} - V_- + 1) + (E_{0+} + E_{0-} - V_0) - 1 \\ &= \beta_+ + \beta_- + (E_{0+} + E_{0-} - V_0) - 1,\end{aligned}\tag{3.38}$$

where $\beta_+ := E_{++} - V_+ + 1$ is the first Betti number of Γ_+ and similarly for $\beta_- := E_{--} - V_- + 1$ and Γ_- . In addition,

$$E_{0+} + E_{0-} = \sum_{v \in V_0} d_v = 2V_0 + 2\delta,\tag{3.39}$$

where $\delta \geq 0$ is defined by the equality above. The sum above is even by Lemma 3.5.3 and hence δ has an integer value. In addition, $\delta = 0$ if and only if f does not vanish on the original vertices of Γ (i.e., it vanishes only on the added dummy vertices which are of degree two). The number of graph zeros, counted with their multiplicities as in Lemma 3.5.4 (namely, each zero is counted as many times as half the degree of the corresponding vertex) is

$$\mu = \frac{1}{2} \sum_{v \in V_0} d_v = E_{0+} + E_{0-} - V_0 - \delta,\tag{3.40}$$

where we used (3.39). Combining (3.37), (3.38), (3.40) we get

$$k = \pi(\beta + 1 - (\beta_+ + \beta_-) - \delta).\tag{3.41}$$

Let v be a vertex such that $f(v) = 0$. We concluded above such a vertex must be of even degree. Furthermore, from Lemma 3.5.3 we have that half of f derivatives at v are positive and half negative. Hence, v is connected to the same number of positive values vertices as to negative valued once. We conclude that $E_{0+} = E_{0-}$ and from the left equalities in (3.39) and (3.40) we get $\mu = E_{0-}$. Choose $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ such that all of its entries equal zero except those which correspond to the E_{0-} edges, which we set to be equal $\frac{1}{E_{0-}}$. We get that $\Gamma(\mathcal{G}; \underline{l}^*)$ is an equilateral mandarin graph whose spectral gap equals $\pi E_{0-} = \pi \mu$, which finishes the proof of the theorem. $\square$

The proof above yields the following.

Corollary 3.5.6. *Let $\mathcal{G}$ be a discrete graph and let $\underline{l} \in \mathcal{L}_{\mathcal{G}}$. Assume that $\Gamma(\mathcal{G}; \underline{l})$ is a supremizer of $\mathcal{G}$ and that the spectral gap $k_1(\Gamma(\mathcal{G}; \underline{l}))$ is a simple eigenvalue and let f be the corresponding eigenfunction. Denote $\Gamma_+ := \{x \in \Gamma \mid f(x) > 0\}$, $\Gamma_- := \{x \in \Gamma \mid f(x) < 0\}$ and further denote by β_+, β_- their corresponding first Betti numbers. Then*

1. $\beta_+ + \beta_- \leq 1$.
2. If $\beta_+ + \beta_- = 1$ there exists a choice of lengths $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ such that $\Gamma(\mathcal{G}; \underline{l}^*)$ is an equilateral flower and

$$k_1(\Gamma(\mathcal{G}; \underline{l})) = k_1(\Gamma(\mathcal{G}; \underline{l}^*)) = \beta\pi.$$

3. The number of (non-dummy) vertices at which f vanishes is at most one. Such a vertex may exist only if $\beta_+ + \beta_- = 0$ and if it exists then this vertex is of degree four.

Remark. We note that Γ_- , Γ_+ defined above are open sets and hence not metric graphs in the sense defined so far in the paper. Nevertheless, we can still define their Betti numbers according to the usual definition for topological spaces.

Démonstration. We start from equation (3.41) in the preceding proof. If $\beta_+ + \beta_- > 1$ we get that $k < \pi\beta$, so that the spectral gap of $\Gamma(\mathcal{G}; \underline{l})$ is strictly smaller than the one we can get by turning it into an equilateral flower ($\pi\beta$) which contradicts it being a supremum. Therefore $\beta_+ + \beta_- \leq 1$, which is claim (1).

If $\beta_+ + \beta_- = 1$, then by (3.41), the spectral gap of $\Gamma(\mathcal{G}; \underline{l})$ equals $\pi(\beta - \delta)$. As it cannot be smaller than the one of the equilateral flower we have $\delta = 0$, which means that f does not vanish at vertices (with the exception of the dummy ones) and also that there exists $\underline{l}^* \in \overline{\mathcal{L}}_{\mathcal{G}}$ for which $\Gamma(\mathcal{G}; \underline{l}^*)$ is an equilateral flower, hence showing claim (2).

If $\beta_+ + \beta_- = 0$, then by (3.41), the spectral gap of $\Gamma(\mathcal{G}; \underline{l})$ equals $\pi(\beta + 1 - \delta)$. As it cannot be smaller than the one of the equilateral flower we have $\delta \leq 1$, which means that f vanishes at most on a single (non-dummy) vertex. In addition, if such a vertex exists its degree equals four. $\square$

Another corollary of the proof of Theorem 3.2.4 is the following

Corollary 3.5.7. *Let $\mathcal{G}$ be a discrete graph. Let $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ and assume that $\Gamma := \Gamma(\mathcal{G}; \underline{l})$ decomposes as*

$$\Gamma = \Gamma_+ \cup \Gamma_0 \cup \Gamma_-, \quad (3.42)$$

such that

1. *The subgraphs Γ_+ , Γ_0 and Γ_- are pairwise edge disjoint.*
2. *The subgraphs Γ_+ and Γ_- do not have any vertex in common.*
3. *The vertices of Γ_0 have an odd degree in Γ .*

Then, the spectral gap of Γ cannot be both a simple eigenvalue and a critical value as a function of $\underline{l} \in \mathcal{L}_{\mathcal{G}}$.

Démonstration. Let k denote the spectral gap of Γ and assume that it is a simple eigenvalue and a critical value. Let f be the eigenfunction corresponding to k . Since k is simple, Courant's nodal theorem ([48, 57, 42]) entails that f has exactly two nodal domains. By Lemma 3.5.3 and as the vertices of Γ_0 are of odd degree, we deduce that f vanishes on every edge of Γ_0 . From the decomposition (3.42), it follows that Γ_+ and Γ_- are contained each in a different nodal domain of Γ and also that each is a connected subgraph. Furthermore, Γ_0 does not have any interior vertex as otherwise, it would belong to a third nodal domain. It follows that Γ_0 consists of edges connecting vertices of Γ_+ and Γ_- .

Observe that $f|_{\Gamma_+}$ is a Neumann eigenfunction on Γ_+ . Indeed, it satisfies Neumann conditions at all vertices of $\Gamma_+ \setminus \Gamma_0$ and its derivative vanishes at each edge connected to a vertex in $\Gamma_+ \cap \Gamma_0$. Therefore, $f|_{\Gamma_+}$ should be orthogonal to the constant function on Γ_+ . As $f|_{\Gamma_+}$ is positive everywhere, this is possible only if Γ_+ consists of a single vertex, which we denote by v_+ (it cannot contain more than a single vertex as we have shown it is connected). The same goes for Γ_- (its vertex denoted by v_-) and as we have shown that Γ_0 consists of edges connecting vertices of Γ_+ and Γ_- , we conclude that Γ is a mandarin graph. As all derivatives of f at $v_{\pm}$ vanish and f cannot vanish more than once on edges connecting them we deduce that all those edges are of equal length. Hence, Γ is an equilateral mandarin, whose spectral gap is not a simple eigenvalue and we get a contradiction. $\square$

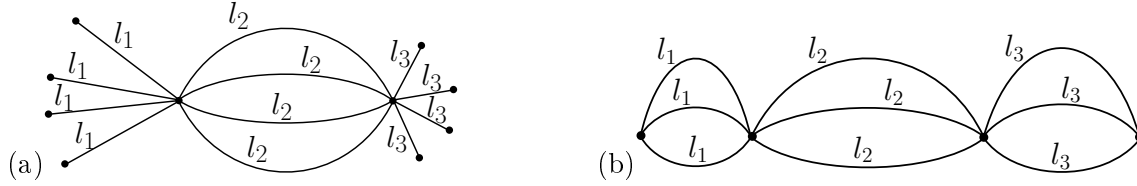


FIGURE 3.3 – Two examples for the standard chain graphs

This corollary applies, among other examples, to graphs having a bridge linking two vertices of odd degrees, or to bipartite and d -regular graphs for some odd d . All of those cannot have a spectral gap which is both simple and a critical value.

Demonstrating examples of the other side, we next show a family of discrete graphs, $\mathcal{G}$, and connected subsets $\mathcal{L}^* \subset \mathcal{L}_{\mathcal{G}}$, such that for all $\underline{l}^* \in \mathcal{L}^*$, $\Gamma(\mathcal{G}; \underline{l}^*)$ satisfies the conditions of Lemma 3.5.3. This provides a collection of graphs whose spectral gap is both simple and a critical value. Those graphs are essentially chains of mandarins glued serially one to the other and with an optional star glued at either side of this chain. We call those standard chains (see Figure 3.3).

Proposition 3.5.8. *Let $n \geq 2$, $M \geq 1$ be integers. Take some M discrete n -mandarin graphs and glue them serially to form a chain of mandarins. At each end of this chain either glue or not an n -star graph at its central vertex. Let $S \in \{0, 1, 2\}$ be the number of star graphs which were glued and assume $M + S \geq 2$. Denote the obtained discrete graph by $\mathcal{G}$. Set $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ to be a vector of edge lengths such that*

1. *All edges belonging to the same mandarin have equal length.*
2. *All edges belonging to the same star graph have equal length, which is in the range $(0, \frac{1}{2n})$.*

Then for all such $\underline{l}^ \in \mathcal{L}_{\mathcal{G}}$, $\Gamma(\mathcal{G}; \underline{l}^*)$ satisfies the conditions of Lemma 3.5.3. Namely*

1. *The spectral gap, $k_1[\Gamma(\mathcal{G}; \underline{l}^*)]$, is a simple eigenvalue.*
2. *The function $\underline{l} \mapsto k_1[\Gamma(\mathcal{G}; \underline{l})]$ has a critical value at $\underline{l} = \underline{l}^*$.*

In addition, the corresponding spectral gap $k = k_1[\Gamma(\mathcal{G}; \underline{l})]$ equal to $n\pi$.

Démonstration. Let $\underline{l}^* \in \mathcal{L}_{\mathcal{G}}$ which satisfies the assumptions of the proposition. Denote $\Gamma := \Gamma(\mathcal{G}; \underline{l}^*)$ and note that we may construct Γ by taking n intervals, $\{\gamma_i\}_{i=1}^n$, of length $\frac{1}{n}$ each, picking $M + 1$ points on each interval which are similarly positioned on each of the intervals, and identifying each set of parallel n points to form a vertex of Γ . We use this decomposition of Γ to describe an eigenfunction which is shown on the sequel to correspond to the spectral gap of Γ . Set $f|_{\gamma_i}(x) = \cos(n\pi x_i)$ on each γ_i . It is easy to check that f satisfies Neumann conditions at all vertices and hence it is a valid eigenfunction and its k -eigenvalue equals $n\pi$. We conclude that the spectral gap obeys, $k_1[\Gamma] \leq n\pi$, and show in the sequel that this is actually an equality and that the spectral gap is a simple eigenvalue.

Let g be an eigenfunction corresponding to the spectral gap $k_1[\Gamma]$. We may assume that all the restrictions $g|_{\gamma_i}$ at mentioned intervals are equal. Otherwise, we symmetrize g by taking

$$\forall 1 \leq i \leq n, \quad \tilde{g}|_{\gamma_i} = \sum_{j=1}^n g|_{\gamma_j}.$$

This symmetrized function $\tilde{g}$ indeed satisfies Neumann conditions at all vertices and we just need to justify that it is different from the zero function. Assume by contradiction that it is the zero

function. In particular $\tilde{g}$ vanishes at all vertices and hence g itself vanishes at all vertices which are not leaves. Necessarily, there exists some edge on which g does not identically vanish. If such an edge, e , is an inner edge we get that $k_1[\Gamma] \geq \frac{\pi}{l_e} > n\pi$, and a contradiction. If this edge is a dangling edge, we get by assumption (2) that $k_1[\Gamma] \geq \frac{\pi}{2l_e} > n\pi$, which is again a contradiction. Hence we continue assuming that g is an eigenfunction with all $\{g|_{\gamma_i}\}_{i=1}^n$ equal to each other. From here we conclude that for all i , $g|_{\gamma_i}$ is an eigenfunction of the interval with Neumann vertex conditions at its both ends. This together with g being an eigenfunction corresponding to the spectral gap implies $g = f$ and $k_1[\Gamma] = n\pi$.

Next, we show the simplicity of $k_1[\Gamma]$. Let g be an eigenfunction of $k_1[\Gamma]$, not assuming it is symmetric this time. Take all parallel edges of some mandarin which is a subgraph of Γ . All those edges have a common length $l < \frac{1}{n}$ and we have $k_1[\Gamma] \cdot l = n\pi l < \pi$ so that $\sin(k_1[\Gamma] \cdot l) \neq 0$. Therefore, the value of g at each and every one of those parallel edges is uniquely given by

$$g|_e = \frac{1}{\sin(k_1[\Gamma] \cdot l)} \{g(u) \sin(k_1[\Gamma] \cdot (l - x)) + g(v) \sin(k_1[\Gamma] \cdot x)\},$$

where u, v are the vertices of this mandarin and e any edge connecting them. A similar argument shows that g is also uniquely determined at the dangling edges. The simplicity of $k_1[\Gamma]$ follows.

Finally, computing the energy, $\mathcal{E}_e = (f')^2 + k^2 f^2$, of f as defined above, we get that it is equal on all edges. By Lemma 3.5.2 we conclude that the function $\underline{l} \mapsto k_1[\Gamma(\mathcal{G}; \underline{l})]$ has a critical value at $\underline{l} = \underline{l}^*$. $\square$

We note that the particular case $n = 2$, $M = 1$, $S = 1$ is dealt with in Lemma 3.8.1. It is stated there that for this particular stower the graphs $\Gamma(\mathcal{G}; \underline{l})$ not only have the spectral gap as a critical value, but they are also maximizers. Furthermore, those graphs are supremizers and thus satisfy the conditions of Theorem 3.2.4. Indeed, this stower has a spectral gap of 2π , which equals the spectral gap of a single cycle, which is merely a one petal flower or a two edge mandarin.

In general, the graphs in the proposition above share the same spectral gap as equilateral n -mandarin graphs. As such they obey the conclusion of Theorem 3.2.4 even though they do not satisfy the requirements of the theorem as they are not necessarily supremizers. For example, the graphs $\Gamma(\mathcal{G}; \underline{l}^*)$ of the proposition above are not supremizers if we take $n \geq 3$. In this case, there is a choice of lengths, $\underline{l}$, for which $\Gamma(\mathcal{G}; \underline{l})$ is a stower graph with $E_p = M \cdot (n - 1)$ and $E_l = S \cdot n$, whose spectral gap is $\frac{\pi}{2}(2M \cdot (n - 1) + S \cdot n)$ and greater than $n\pi$.

3.6 Gluing Graphs

In this section we develop spectral gap inequalities for graphs whose vertex connectivity equals one. Such graphs may be obtained by considering two disjoint graphs and identifying two vertices, one of each graph. We bound the spectral gap of the obtained graph by the sum of spectral gaps of its two subgraphs and provide necessary and sufficient conditions for equality to hold (Proposition 3.6.5). We use this in order to prove sufficient conditions needed for graphs with vertex connectivity one to be supremizers (Theorem 3.2.6).

We fix some notations to use throughout this section. Let Γ be a graph and let v be a vertex of Γ . We say that f satisfies the δ -type conditions at v with parameter θ if

$$\begin{aligned} &f \text{ is continuous at } v \\ &\text{and} \\ &\cos\left(\frac{\theta}{2}\right) \sum_{e \in \mathcal{E}_v} \frac{df}{dx_e}(v) = \sin\left(\frac{\theta}{2}\right) f(v), \end{aligned} \tag{3.43}$$

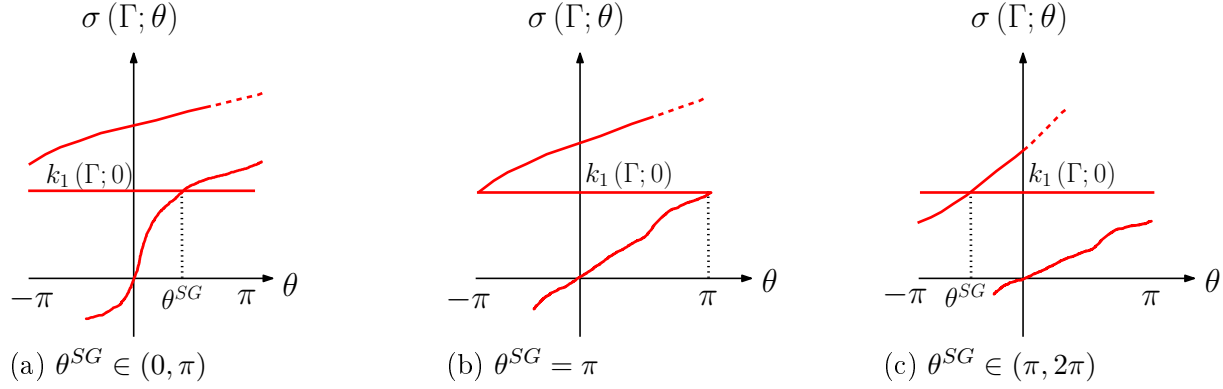


FIGURE 3.4 – Three examples of dispersion relations curves

where $\theta \in (-\pi, \pi]$ (see Definition A.2.1). Note that Neumann conditions are obtained as a special case with $\theta = 0$ and Dirichlet conditions are obtained from $\theta = \pi$. We denote by $k_n(\Gamma; \theta)$ the n^{th} k -eigenvalue of Γ , endowed with the δ -type condition with parameter θ at v and Neumann at all other vertices. The corresponding k -spectrum is denoted by

$$\sigma(\Gamma; \theta) := \cup_n \{k_n(\Gamma; \theta)\}. \quad (3.44)$$

It will be understood in the sequel which vertex v is chosen so that it is not indicated in the notation. In addition, we omit the notation Γ from $k_n(\Gamma; \theta)$ and $\sigma(\Gamma; \theta)$ whenever it is clear which graph we refer to. Similarly, θ is omitted from these notations whenever $\theta = 0$ to comply with the notations used so far. At this point, we refer the reader to Appendix A.2, where we quote some results from [43] on δ -type conditions, that are used throughout this section. The structure of the spectrum as it depends on the parameter θ (for some chosen vertex v) is described in the next lemma, which quotes parts of theorem 3.1.13 from [43], slightly rephrased for our purpose.

Lemma 3.6.1. *Let Γ be a metric graph and let v be a vertex of Γ . There exist a bounded from below discrete set, $\Delta(\Gamma) \subset \mathbb{R}$ and a real smooth function, $K(\Gamma; \cdot) : (-\pi, \infty) \rightarrow \mathbb{R}$ (called “dispersion relation”) such that*

1. *The function $\theta \mapsto K(\Gamma; \theta)$ is strictly increasing.*
2. *For any $\theta \in (-\pi, \pi]$, $\sigma(\Gamma; \theta) = \{K(\Gamma; \theta + 2\pi n)\}_{n=0}^{\infty} \cup \Delta(\Gamma)$.*

Remark. We see from the lemma above that $\Delta(\Gamma) = \cap \sigma(\Gamma; \theta)$. The values of this discrete set, common to all spectra, are often called flat bands.

A particular value of θ which plays a special role is defined below.

Definition 3.6.2. Let Γ be a graph and let v be a vertex of Γ . $\theta^{SG} \in \mathbb{R}$ which satisfies

$$K(\Gamma; \theta^{SG}) = k_1(\Gamma; 0),$$

is called the spectral gap parameter (SGP) of Γ (with respect to v). See Figure 3.4.

In the following we point out some of the SGP properties.

Lemma 3.6.3.

1. *The spectral gap parameter exists and it is unique.*
2. *$\theta^{SG} \in [0, 2\pi]$.*

3. If $\theta^{SG} \neq 2\pi$ then $k_1(\Gamma; 0) \in \Delta(\Gamma)$.

4. If $\theta^{SG} \in (0, \pi]$ then

$$\begin{cases} k_0(\theta) < k_1(0) & \text{for } \theta \in (0, \theta^{SG}) \\ k_0(\theta) = k_1(0) & \text{for } \theta \in [\theta^{SG}, \pi] \\ k_1(\theta - 2\pi) = k_1(0) & \text{for } \theta \in (\pi, 2\pi] \end{cases} \quad (3.45)$$

5. If $\theta^{SG} \in (\pi, 2\pi)$ then

$$\begin{cases} k_0(\theta) < k_1(0) & \text{for } \theta \in [0, \pi] \\ k_1(\theta - 2\pi) < k_1(0) & \text{for } \theta \in (\pi, \theta^{SG}) \\ k_1(\theta - 2\pi) = k_1(0) & \text{for } \theta \in [\theta^{SG}, 2\pi] \end{cases} \quad (3.46)$$

Démonstration. The existence of the spectral gap parameter follows from $K(\Gamma; 0) = 0$ together with $K(\Gamma; \cdot)$ being monotonically increasing. This latter argument also shows the uniqueness of the SGP and that $\theta^{SG} \geq 0$.

We have that $K(\Gamma; 2\pi) = k_n(\Gamma; 0)$ for some n and hence, by continuity and monotonicity of K we get $\theta^{SG} \leq 2\pi$, which shows property (2) above.

If $\theta^{SG} < 2\pi$ we have $k_1(\Gamma; 0) \in \sigma(\Gamma; 0) \cap \sigma(\Gamma; \theta^{SG})$ and by Lemma A.2.5 conclude $k_1(\Gamma; 0) \in \Delta(\Gamma)$, which proves property (3). Finally, properties (4) and (5) are straightforward consequences of the strict monotonicity of K together with the eigenvalue interlacing with respect to the δ -type condition parameter (see Lemma A.2.2). $\square$

The main construction in this section involves scaling two disjoint graphs and gluing them at a vertex to form a new graph, as defined below.

Definition 3.6.4. Let Γ_1, Γ_2 two Neumann graphs of total length 1 each. Let v_i be a vertex of Γ_i ($i = 1, 2$). Let Γ be the graph obtained by the following process

1. Multiply all edge lengths of Γ_1 by some factor $L \in [0, 1]$.
2. Multiply all edge lengths of Γ_2 by a factor of $1 - L$.
3. Identify v_1 and v_2 of the graphs above and endow the new vertex with Neumann vertex conditions.

We call Γ the *gluing* of Γ_1, Γ_2 (with respect to v_1, v_2 and L).

Proposition 3.6.5. Let Γ_1, Γ_2 two connected Neumann graphs of total length 1 each. Let v_i be a vertex of Γ_i ($i = 1, 2$). Let Γ be the gluing of Γ_1, Γ_2 with respect to v_1, v_2 and some value $L \in [0, 1]$. Let $\theta_1^{SG}, \theta_2^{SG}$ be the spectral gap parameters of Γ_1, Γ_2 with respect to v_1, v_2 , correspondingly. Then the following inequality holds

$$k_1(\Gamma) \leq k_1(\Gamma_1) + k_1(\Gamma_2), \quad (3.47)$$

with equality if and only if both conditions below are satisfied

1. $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$
2. $\theta_1^{SG} + \theta_2^{SG} \leq 2\pi$

Additional necessary conditions for equality in (3.47) are

- (a) The spectral gaps of the glued graphs obey $k_1(\Gamma_1) \in \Delta(\Gamma_1)$ and $k_1(\Gamma_2) \in \Delta(\Gamma_2)$.
- (b) The spectral gap of the outcome graph, $k_1(\Gamma)$ is a multiple (i.e. non-simple) eigenvalue.

Démonstration. We start by showing the inequality (3.47).

Let $L \in [0, 1]$. If $L = 0$ ($L = 1$), then $\Gamma = \Gamma_2$ ($\Gamma = \Gamma_1$) and (3.47) obviously holds as a strict inequality and indeed condition (1) is violated if $L = 0$ or $L = 1$. We therefore assume $L \in (0, 1)$. Denote by $\tilde{\Gamma}_1$ the graph obtained by multiplying all edge lengths of Γ_1 by L and by $\tilde{\Gamma}_2$ the graph obtained by multiplying all edge lengths of Γ_2 by $1 - L$. Therefore identifying the vertices v_1, v_2 of Γ_1, Γ_2 gives the graph Γ . Applying Lemma A.2.3 we get

$$k_1(\Gamma) \leq k_2(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2).$$

As the spectrum of $\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2$ is the union of spectra of both graphs, we have that

$$k_0(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) = k_1(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) = 0 \quad \text{and} \quad k_2(\tilde{\Gamma}_1 \cup \tilde{\Gamma}_2) = \min(k_1(\tilde{\Gamma}_1), k_1(\tilde{\Gamma}_2))$$

and conclude

$$k_1(\Gamma) \leq \min(k_1(\tilde{\Gamma}_1), k_1(\tilde{\Gamma}_2)) = \min\left(\frac{k_1(\Gamma_1)}{L}, \frac{k_1(\Gamma_2)}{1-L}\right). \quad (3.48)$$

We consider the right hand side of (3.48) as a function of L . The minimal value of this function is $k_1(\Gamma_1) + k_1(\Gamma_2)$ and it is obtained at $L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)}$, which proves (3.47). In addition, as the minimal value of this function is unique, it also proves that condition (1) is necessary for equality in (3.47) to hold. From now on we assume throughout the proof that condition (1) of the proposition is satisfied, so that $k_1(\tilde{\Gamma}_1) = k_1(\tilde{\Gamma}_2)$.

Next, we examine two ranges of $\theta_1^{SG}, \theta_2^{SG}$ values and show those values make the inequality in (3.47) strict.

1. $\theta_1^{SG} > \pi$ and $\theta_1^{SG} > \pi$.

By (3.46) we have $k_0(\tilde{\Gamma}_i; \pi) < k_1(\tilde{\Gamma}_i; 0)$ for both $i = 1, 2$. Assume first that $k_0(\tilde{\Gamma}_1; \pi) \neq k_0(\tilde{\Gamma}_2; \pi)$ and without loss of generality that $k_0(\tilde{\Gamma}_1; \pi) > k_0(\tilde{\Gamma}_2; \pi)$.

Examine the function

$$h(\theta) := \begin{cases} k_0(\tilde{\Gamma}_1; \theta) - k_1(\tilde{\Gamma}_2; -\theta) & \theta \in [0, \pi) \\ k_0(\tilde{\Gamma}_1; \pi) - k_0(\tilde{\Gamma}_2; \pi) & \theta = \pi \end{cases}. \quad (3.49)$$

By lemma A.2.4 we have that h is a continuous non-decreasing function. In addition $h(0) = -k_1(\tilde{\Gamma}_2; 0) < 0$ and by the assumption $k_0(\tilde{\Gamma}_1; \pi) > k_0(\tilde{\Gamma}_2; \pi)$ we have $h(\pi) > 0$. Hence h vanishes at some value $\tilde{\theta} \in (0, \pi)$, so that we find

$$k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta}). \quad (3.50)$$

Denote by $\tilde{f}_1$ the eigenfunction corresponding to $k_0(\tilde{\Gamma}_1; \tilde{\theta})$ and by $\tilde{f}_2$ the eigenfunction corresponding to $k_1(\tilde{\Gamma}_2; -\tilde{\theta})$. We use $\tilde{f}_1, \tilde{f}_2$ to construct an eigenfunction on the whole of Γ as follows. First, notice that for both $i = 1, 2$, $\tilde{f}_i(v_i) \neq 0$. Assuming otherwise, we obtain that $\tilde{f}_i$ obeys Dirichlet condition at v_i and as $\tilde{\theta} \neq \pi$ we get that $\tilde{f}_i$ obeys Neumann conditions as well at v_i . Since $\tilde{\theta} < \theta_i^{SG}$, the corresponding eigenvalue is strictly lower than the spectral gap. As $\tilde{f}_i(v_i) \neq 0$ for $i = 1, 2$, we may normalize the $\tilde{f}_i$'s so that $\tilde{f}_1(v_1) = \tilde{f}_2(v_2)$. Now form an eigenfunction f on Γ by setting

$$f(x) := \begin{cases} \tilde{f}_1(x) & x \in \tilde{\Gamma}_1, \\ \tilde{f}_2(x) & x \in \tilde{\Gamma}_2. \end{cases} \quad (3.51)$$

where we consider $\tilde{\Gamma}_1, \tilde{\Gamma}_2$ as subgraphs of Γ . The normalization $\tilde{f}_1(v_1) = \tilde{f}_2(v_2)$ gives that f is continuous at the glued vertex v . In addition, its sum of derivatives there equals

$$\sum_{e \in \mathcal{E}_{v_1}} \tilde{f}'_1|_e(v_1) + \sum_{e \in \mathcal{E}_{v_2}} \tilde{f}'_2|_e(v_2) = \tan\left(\frac{\tilde{\theta}}{2}\right) \tilde{f}_1(v_1) + \tan\left(\frac{-\tilde{\theta}}{2}\right) \tilde{f}_2(v_2) = 0. \quad (3.52)$$

We conclude that f is a Neumann eigenfunction on Γ whose eigenvalue equals $k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta})$. However, this eigenvalue is strictly smaller than $k_1(\tilde{\Gamma}_i)$, for both $i = 1, 2$, as shows the following chain of inequalities

$$k_0(\tilde{\Gamma}_1; \tilde{\theta}) \leq k_0(\tilde{\Gamma}_1; \pi) < k_1(\tilde{\Gamma}_1; 0) = k_1(\tilde{\Gamma}_2; 0), \quad (3.53)$$

where the first inequality is due to eigenvalue monotonicity, the second is by (3.46) and the last equality results since our current working assumption is the validity of condition (1), as discussed above. Therefore, we have found an eigenvalue of Γ strictly smaller than both $k_1(\tilde{\Gamma}_i)$, so that there is a strict inequality in (3.48) and therefore strict inequality in (3.47).

We now assume $k_0(\tilde{\Gamma}_1; \pi) = k_0(\tilde{\Gamma}_2; \pi)$. Denote by $\tilde{f}_1, \tilde{f}_2$ as above the corresponding eigenfunctions. By (3.46) $k_0(\tilde{\Gamma}_i; \pi) < k_1(\tilde{\Gamma}_i; 0)$ for both $i = 1, 2$ and therefore $\tilde{f}_i$ does not obey Neumann conditions at v_i (as otherwise, its eigenvalue would be the spectral gap). Using that the sum of derivatives of $\tilde{f}_i$ at v_i differs from zero, we may normalize both $\tilde{f}_1, \tilde{f}_2$ so that their sums of derivatives are opposite. Now, constructing a function f on Γ as in (3.51) shows just as above (see (3.53) and the argument which follows) that inequality (3.48) is strict in this case as well. We conclude that the inequality in (3.47) is strict if $\theta_1^{SG} > \pi$ and $\theta_1^{SG} > \pi$.

2. $\theta_1^{SG} + \theta_2^{SG} > 2\pi$ and $\{\theta_1^{SG} \leq \pi < \theta_2^{SG} \text{ or } \theta_2^{SG} \leq \pi < \theta_1^{SG}\}$.

Assume without loss of generality that $\theta_1^{SG} < \theta_2^{SG}$. We have the following chain of inequalities

$$k_0(\tilde{\Gamma}_2; \pi) < k_1(\tilde{\Gamma}_2; 0) = k_1(\tilde{\Gamma}_1; 0) = k_0(\tilde{\Gamma}_1; \pi),$$

where the first inequality comes from (3.46) (keeping in mind that $\theta_2^{SG} > \pi$), the first equality is our working assumption (assuming the validity of condition (1)) and the second equality comes from (3.45) (keeping in mind that $\theta_1^{SG} \leq \pi$). Therefore, defining the function h as in (3.49) we find that $h(0) < 0$ and $h(\pi) > 0$. As before we conclude that h vanishes for some value $\tilde{\theta} \in (0, \pi)$ and hence $k_0(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\tilde{\Gamma}_2; -\tilde{\theta})$. Similarly to the previous case, we may use this equality to construct a Neumann eigenfunction on Γ whose eigenvalue equals $k_0(\tilde{\Gamma}_1; \tilde{\theta})$ and to show that strict inequality happens in (3.47) for this case.

Notice that condition (2) of the proposition forms the complement of the two cases examined above. Therefore, we have proven so far that this condition is necessary for the equality in (3.47) to hold. We proceed to show that conditions (1),(2) are sufficient as well. Recall that assuming condition (1) implies $k_1(\tilde{\Gamma}_1; 0) = k_1(\tilde{\Gamma}_2; 0)$. We further assume by contradiction that $k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0)$, and consider the following two cases for the $\theta_1^{SG}, \theta_2^{SG}$ values :

1. $\theta_1^{SG} \leq \pi$ and $\theta_2^{SG} \leq \pi$.

First, we note that by (3.45) we have $k_1(\tilde{\Gamma}_i; 0) = k_0(\tilde{\Gamma}_i; \pi)$ for both $i = 1, 2$.

Let f be the eigenfunction corresponding to $k_1(\Gamma)$. Denote $\tilde{f}_i = f|_{\tilde{\Gamma}_i}$ for $i = 1, 2$. We find that there exists some $\tilde{\theta}$ such that $k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma)$, for some n_1 . We cannot have $\tilde{\theta} = \pi$, as otherwise we get

$$k_{n_1}(\tilde{\Gamma}_1; \pi) = k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0) = k_0(\tilde{\Gamma}_1; \pi)$$

and contradiction. We find that as $\tilde{f}_1$ satisfies the δ -type condition at v_1 with the parameter $\tilde{\theta}$, $\tilde{f}_2$ satisfies the δ -type condition at v_2 with the parameter $-\tilde{\theta}$ (since the total sum of derivatives is zero and see (3.52)). Assume without loss of generality that $\tilde{\theta} > 0$. We get that

$$k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_2; 0), \quad (3.54)$$

which implies either $n_2 = 0$ or $n_2 = 1$. We rule out $n_2 = 0$ as it renders the left hand side of (3.54) negative, while $k_1(\Gamma) > 0$. We also rule out $n_2 = 1$, as by (3.45) the left and right hand sides of (3.54) are equal. Hence, in this case, we get a contradiction to the assumption $k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0)$.

2. $\theta_1^{SG} + \theta_2^{SG} \leq 2\pi$ and $\{\theta_1^{SG} \leq \pi < \theta_2^{SG} \text{ or } \theta_2^{SG} \leq \pi < \theta_1^{SG}\}$.

We repeat the construction of $\tilde{f}_1, \tilde{f}_2$ as in the previous case to get that there exists some $\tilde{\theta} \neq \pi$ such that $k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma)$, for some n_1 and $k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma)$, for some n_2 . Assume without loss of generality $\theta_1^{SG} < \theta_2^{SG}$. Combining

$$k_{n_1}(\tilde{\Gamma}_1; \tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_1; 0)$$

with (3.45) shows that $n_1 = 0$ and $0 < \tilde{\theta} < \theta_1^{SG}$. Similarly, we have for $\tilde{\Gamma}_2$,

$$k_{n_2}(\tilde{\Gamma}_2; -\tilde{\theta}) = k_1(\Gamma) < k_1(\tilde{\Gamma}_2; 0),$$

where the positivity of the left hand side implies $n_2 = 1$. Together with (3.46) we get $-\tilde{\theta} < \theta_2^{SG} - 2\pi$. Combining that with $\tilde{\theta} < \theta_1^{SG}$ gives $\theta_1^{SG} + \theta_2^{SG} > 2\pi$ and contradiction to the assumption in this case.

Thus we have shown that conditions (1),(2) of the proposition are also necessary for equality in (3.47) to hold.

Finally, we show the necessity of conditions (a),(b) of the proposition. We have seen that necessary conditions for equality in (3.47) are $\{\theta_1^{SG} \leq \pi \text{ and } \theta_2^{SG} \leq \pi\}$ or $\{\theta_1^{SG} + \theta_2^{SG} \leq 2\pi \text{ and } \{\theta_1^{SG} \leq \pi < \theta_2^{SG} \text{ or } \theta_2^{SG} \leq \pi < \theta_1^{SG}\}\}$. Under those conditions we have both $\theta_1^{SG} \neq 2\pi$ and $\theta_2^{SG} \neq 2\pi$ and by Lemma 3.6.3,(3) we get $k_1(\tilde{\Gamma}_i) \in \Delta(\tilde{\Gamma}_i)$ for both $i = 1, 2$, which is condition (a). Now, in order show that $k_1(\Gamma)$ is a non-simple eigenvalue we construct two linearly independent eigenfunctions. As $k_1(\tilde{\Gamma}_i) \in \Delta(\tilde{\Gamma}_i)$, by Lemma A.2.5 there exists an eigenfunction corresponding to $k_1(\tilde{\Gamma}_i)$ which vanishes at v_i and its sum of derivatives vanishes there as well. Extend this function to an eigenfunction of Γ , whose eigenvalue is $k_1(\tilde{\Gamma}_i) = k_1(\Gamma)$ by setting it to be equal zero on the complementary subgraph, $\tilde{\Gamma}_{3-i}$. Performing this for both $i = 1$ and $i = 2$ we get two linearly independent eigenfunctions on Γ , which shows the necessity of condition (b). $\square$

We use Proposition 3.6.5 to study the supremizers of graphs whose vertex connectivity equals one. Let $\mathcal{G}$ be such a graph which is obtained by taking two graphs $\mathcal{G}_1, \mathcal{G}_2$ and identifying two of their vertices v_1, v_2 . An immediate guess is that a supremizer of $\mathcal{G}$ may be obtained by taking the supremizers of $\mathcal{G}_1, \mathcal{G}_2$ and identifying their vertices corresponding to v_1, v_2 . This holds under some conditions, as stated in Theorem 3.2.6 and proved below.

Proof of Theorem 3.2.6. We start by formulating the Dirichlet criterion in terms of the SGP, θ^{SG} , used in the conditions of Proposition 3.6.5. Let Γ be a graph which obeys the Dirichlet criterion. This means that $k_0(\Gamma; \pi) = k_1(\Gamma; 0)$ and by Lemma 3.6.3 we deduce $\theta^{SG} \leq \pi$. Hence, condition (3) of Theorem 3.2.6 implies condition (2) of Proposition 3.6.5.

Assuming conditions (1),(3) of the theorem we may now apply Proposition 3.6.5 and get

$$k_1(\Gamma) = k_1(\Gamma_1) + k_1(\Gamma_2). \quad (3.55)$$

Let $\hat{\Gamma}$ be a supremizer of $\mathcal{G}$. In particular, $k_1(\Gamma) \leq k_1(\hat{\Gamma})$. Denote by $\hat{\Gamma}_1, \hat{\Gamma}_2$ the subgraphs of $\hat{\Gamma}$ corresponding to $\mathcal{G}_1, \mathcal{G}_2$ and rescaled such that the total length of each of them equals 1. By Proposition 3.6.5

$$k_1(\hat{\Gamma}) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2). \quad (3.56)$$

Hence we get

$$k_1(\hat{\Gamma}) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2) \leq k_1(\Gamma_1) + k_1(\Gamma_2) = k_1(\Gamma),$$

where the second inequality holds as Γ_1, Γ_2 are supremizers. We therefore get that $k_1(\Gamma) = k_1(\hat{\Gamma})$, so that Γ is a supremizer of $\mathcal{G}$ as $\hat{\Gamma}$ is a supremizer of $\mathcal{G}$ (and possibly $\Gamma = \hat{\Gamma}$).

We now further assume that either for both $i = 1, 2$ Γ_i is the unique supremizer of $\mathcal{G}_i$ or that both Γ_1, Γ_2 obey the strong Dirichlet criterion and any other supremizer violates the Dirichlet criterion. Assume that $\hat{\Gamma}$ is a supremizer of $\mathcal{G}$ so that $k_1(\Gamma) = k_1(\hat{\Gamma})$. From (3.55), (3.56) we get

$$k_1(\Gamma_1) + k_1(\Gamma_2) \leq k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2). \quad (3.57)$$

As Γ_1, Γ_2 are supremizers of $\mathcal{G}_1, \mathcal{G}_2$, we have an equality in (3.57) and get that for both $i = 1, 2$, $k_1(\Gamma_i) = k_1(\hat{\Gamma}_i)$, so that $\hat{\Gamma}_1, \hat{\Gamma}_2$ are supremizers of $\mathcal{G}_1, \mathcal{G}_2$ as well. If both Γ_1, Γ_2 are unique supremizers of $\mathcal{G}_1, \mathcal{G}_2$ then $\Gamma_i = \hat{\Gamma}_i$ for both $i = 1, 2$. Hence, $\hat{\Gamma} = \Gamma$.

We carry on by assuming that both Γ_1, Γ_2 obey the strong Dirichlet criterion and any other supremizer violates the Dirichlet criterion. From Lemma 3.6.3 we deduce that a graph violates the Dirichlet criterion if and only if its spectral gap parameter satisfies $\theta^{SG} \in (\pi, 2\pi]$. If for both $i = 1, 2$, $\hat{\Gamma}_i$ is different than Γ_i , then we have $\theta_1^{SG}, \theta_2^{SG} \in (\pi, 2\pi]$ and by Proposition 3.6.5 we have the strict inequality

$$k_1(\hat{\Gamma}) < k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2), \quad (3.58)$$

which together with

$$k_1(\hat{\Gamma}_1) + k_1(\hat{\Gamma}_2) = k_1(\Gamma_1) + k_1(\Gamma_2) = k_1(\Gamma)$$

contradicts $\hat{\Gamma}$ being a supremizer. From Lemma 3.6.6 which follows this proof we deduce that a graph obeys the strong Dirichlet criterion if and only if its SGP equals π . Therefore, if $\hat{\Gamma}_i = \Gamma_i$ for either $i = 1$ or $i = 2$, say $\hat{\Gamma}_1 = \Gamma_1$, then we have $\theta_1^{SG} = \pi$ and $\theta_2^{SG} \in (\pi, 2\pi]$ and once again we get by Proposition 3.6.5 the inequality (3.58) which contradicts $\hat{\Gamma}$ being a supremizer. $\square$

Lemma 3.6.6. *Let $k \in \Delta(\Gamma)$. Let $n \in \mathbb{N}$ and $\theta \in (-\pi, \pi]$ such that $k = K(\theta + 2n\pi)$. Assume that k has multiplicity $m + 1$ in the spectrum $\sigma(\Gamma; \theta)$. Then, for any $\theta' \neq \theta$, k has a multiplicity m as an eigenvalue in the spectrum $\sigma(\Gamma; \theta')$.*

Démonstration. Since $\Delta(\Gamma)$ is a discrete set, for $k' < k$ sufficiently close to k , k' does not belong to $\Delta(\Gamma)$. Thus, for $\theta' < \theta$ sufficiently close to θ , $K(\theta' + 2n\pi)$ is not in $\Delta(\Gamma)$. We define $a \in \mathbb{N}$ as the unique integer satisfying $K(\theta' + 2n\pi) = k_a(\Gamma, \theta')$ for all $\theta' < \theta$ sufficiently close to θ . Since $K(\cdot + 2n\pi)$ and $k(\Gamma, \cdot)$ are continuous functions of their arguments (see Lemma 3.6.1 and Lemma A.2.4), letting θ' go to θ gives

$$k = k_a(\Gamma, \theta).$$

If $\theta \neq \pi$, we may argue similarly with $\theta' > \theta$ sufficiently close to θ to find that

$$k = k_b(\Gamma, \theta) < k_b(\Gamma, \theta').$$

Notice that since a and b are respectively minimal and maximal integers such that $k = k_a(\Gamma, \theta) = k_b(\Gamma, \theta)$, the multiplicity assumption on k in $\sigma(\Gamma; \theta)$ entails $b = a + m$. As K is strictly increasing and by Lemma A.2.2, we get

$$\forall \theta' \in (-\pi, \theta), \quad k_a(\Gamma; \theta') < k = k_{a+1}(\Gamma; \theta') = \cdots = k_b(\Gamma; \theta') < k_{b+1}(\Gamma; \theta')$$

and

$$\forall \theta' \in (\theta, \pi], \quad k_{a-1}(\Gamma; \theta') < k = k_a(\Gamma; \theta') = \cdots = k_{b-1}(\Gamma; \theta') < k_b(\Gamma; \theta').$$

We conclude from these inequalities that k has multiplicity m in $\sigma(\Gamma; \theta')$ for all $\theta' \neq \theta$.

If $\theta = \pi$, we have

$$\forall \theta' \neq \pi, \quad k = k_b(\Gamma, \pi) < k_{b+1}(\Gamma, \theta'),$$

and once again

$$\forall \theta' \neq \pi, \quad k_a(\Gamma; \theta') < k = k_{a+1}(\Gamma; \theta') = \cdots = k_b(\Gamma; \theta') < k_{b+1}(\Gamma; \theta'),$$

from which the result follows. $\square$

3.7 Symmetrization of dangling edges and loops

Proposition 3.7.1. *Let $\mathcal{G}$ be a graph with $E \geq 3$ edges. Let v be a vertex of $\mathcal{G}$ and e_1, e_2 either two dangling edges or two loops connected to v . Let l_1, l_2 be the lengths of those edges and denote their average by $\ell := \frac{1}{2}(l_1 + l_2)$.*

Denoting $\tilde{\Gamma} := \Gamma(\mathcal{G}; (l_1, l_2, l_3, \dots, l_E))$, $\Gamma := \Gamma(\mathcal{G}; (\ell, \ell, l_3, \dots, l_E))$, we have

$$k_1(\tilde{\Gamma}) \leq k_1(\Gamma). \quad (3.59)$$

Moreover, if either $k_1(\Gamma) = \frac{\pi}{2\ell}$ in the dangling edges case (respectively, $k_1(\Gamma) = \frac{\pi}{\ell}$ in the loops case) or alternatively both the following conditions are satisfied

1. Γ is a supremizer of some graph.
2. $k_1(\tilde{\Gamma})$ is a simple eigenvalue.

then equality above holds if and only if $l_1 = l_2$.

Démonstration. Let f be an eigenfunction of Γ corresponding to $k_1(\Gamma)$. The proof for both cases - dangling edges and loops - is by constructing a test function $\tilde{f}$ on $\tilde{\Gamma}$, whose Rayleigh quotient obeys $\mathcal{R}(\tilde{f}) \leq \mathcal{R}(f) = k_1(\Gamma)^2$, from which (3.59) follows.

We start with the dangling edges case. First, we get a bound on $k_1(\Gamma)$ using a test function,

$$g|_{e_1 \cup e_2} = \cos\left(\frac{\pi x}{2\ell}\right), \quad g|_{\Gamma \setminus (e_1 \cup e_2)} = 0, \quad (3.60)$$

where $e_1 \cup e_2$ is considered as single interval. We have $\mathcal{R}(g) = \left(\frac{\pi}{2\ell}\right)^2$ and hence $k_1(\Gamma) \leq \frac{\pi}{2\ell}$.

Assume that $k_1(\Gamma) = \frac{\pi}{2\ell}$. Let $\tilde{f}$ be the following test function on $\tilde{\Gamma}$.

$$\tilde{f}|_{\tilde{e}_1 \cup \tilde{e}_2} = \cos\left(\frac{\pi x}{2\ell}\right), \quad \tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = \tilde{f}(v),$$

where $\tilde{f}(v)$ in the right equation is determined from the value $\tilde{f}|_{\tilde{e}_1 \cup \tilde{e}_2}$ on the left attains at v . As $\tilde{f}$ is not necessarily orthogonal to the constant function, we actually take $\tilde{f} - \langle \tilde{f} \rangle$ to be the test function, where $\langle \tilde{f} \rangle := \int_{\tilde{\Gamma}} \tilde{f} dx$. By Lemma A.3.1

$$\mathcal{R}(\tilde{f} - \langle \tilde{f} \rangle) = \frac{\left(\frac{\pi}{2\ell}\right)^2 \ell}{\ell + |\tilde{f}(v)|^2 2\ell(1-2\ell)} < \left(\frac{\pi}{2\ell}\right)^2 = (k_1(\Gamma))^2, \quad (3.61)$$

where we use that $l_1 \neq l_2 \Rightarrow \tilde{f}(v) = \cos(\frac{\pi l_1}{2\ell}) \neq 0$ to get the inequality.

Next, assume $k_1(\Gamma) < \frac{\pi}{2\ell}$ and also that $f(v) = 0$. Then f has to identically vanish on both e_1 and e_2 . We may then choose the test function $\tilde{f} = f$ and get $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$, as required.

Finally, assume $k_1(\Gamma) < \frac{\pi}{2\ell}$ and $f(v) \neq 0$. This results with $f|_{e_1} = f|_{e_2}$. Assume without loss of generality that $l_1 < l_2$. We define the test function $\tilde{f}$ on $\tilde{\Gamma}$ as follows.

$$\tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = f|_{\Gamma \setminus (e_1 \cup e_2)}, \quad \tilde{f}|_{\tilde{e}_1} = f|_{e_1(0, l_1)},$$

where $e_1(0, l_1)$ denotes a subset of e_1 in Γ whose origin is v . On $\tilde{e}_2$ we set

$$\tilde{f}|_{\tilde{e}_2}(x) = \begin{cases} f|_{e_2}(x) & x \in (0, \ell) \\ f|_{e_1}(l_1 + l_2 - x) & x \in (\ell, l_2) \end{cases}.$$

This is a valid continuous test function and by construction, $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$.

We have therefore shown inequality (3.59) and also that assuming $k_1(\Gamma) = \frac{\pi}{2\ell}$ assures equivalence between $l_1 = l_2$ and equality in (3.59). It is therefore left to show that under assumptions (1),(2) of the proposition, $l_1 \neq l_2$ implies $k_1(\tilde{\Gamma}) < k_1(\Gamma)$. Assume by contradiction that $l_1 \neq l_2$ and also $k_1(\tilde{\Gamma}) = k_1(\Gamma)$. As Γ is a supremizer of some graph, $\tilde{\Gamma}$ is also a supremizer of the same graph. Since $k_1(\tilde{\Gamma})$ is simple we deduce from Lemma 3.5.5 that its spectral gap is a critical value and by Lemma 3.5.3 we get $|\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v)| = |\frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)|$, where $\tilde{f}$ is the eigenfunction corresponding to $k_1(\tilde{\Gamma})$. If $\tilde{f}(v) = 0$ we get that $\tilde{f}$ has at least three nodal domains (at least one nodal domain on each of $\tilde{e}_1$, $\tilde{e}_2$ and $\tilde{\Gamma} \setminus \{\tilde{e}_1 \cup \tilde{e}_2\}$), which contradicts Courant's nodal theorem ([48, 57, 42]). Assume without loss of generality $\tilde{f}(v) > 0$. As $l_1 \neq l_2$ and as the derivative of $\tilde{f}$ vanishes at the endpoints of $\tilde{e}_1$, $\tilde{e}_2$, we get that at least one of $\tilde{e}_1$, $\tilde{e}_2$ should contain two nodal domains of $\tilde{f}$. In addition, by Courant's bound it is not possible for both derivatives, $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v)$, $\frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$ to be negative as this results with a total of at least three nodal domains. If one derivative is positive and the second is negative, i.e., $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v) = -\frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$, we get that $f|_{\tilde{e}_1 \cup \tilde{e}_2}$ is proportional to $\cos(\frac{\pi}{2\ell}x)$, so that $k_1(\tilde{\Gamma}) = \frac{\pi}{2\ell}$, which is a contradiction, to what we have shown above (see (3.61)). If both derivatives are positive, $\frac{\partial}{\partial x_{\tilde{e}_1}} \tilde{f}(v) = \frac{\partial}{\partial x_{\tilde{e}_2}} \tilde{f}(v)$, then we get contradiction as $\langle \tilde{f} \rangle \neq 0$. Indeed, assuming without loss of generality $l_1 < l_2$, the restriction of $\tilde{f}$ on an interval of length $l_2 - l_1$ at the end of edge $\tilde{e}_2$ is of zero mean, but the $\tilde{f}$'s restriction to the rest of the graph is positive, as $\tilde{f}$ has only two nodal domains and therefore.

We turn to deal with the loops case. Just as above, we start by getting an upper bound on the spectral gap. Choose the following test function on Γ

$$g|_{e_1 \cup e_2} = \cos\left(\frac{\pi x}{\ell}\right) \quad g|_{\Gamma \setminus (e_1 \cup e_2)} = 0, \quad (3.62)$$

where $e_1 \cup e_2$ is considered as single cycle (self intersecting itself at its middle). In this case, $\mathcal{R}(g) = \left(\frac{\pi}{\ell}\right)^2$ so that $k_1(\Gamma) \leq \frac{\pi}{\ell}$.

The proof now splits into three cases exactly as it was for the dangling edges :

1. If $k_1(\Gamma) = \frac{\pi}{\ell}$, we may construct a test function $\tilde{f}$ on $\tilde{\Gamma}$, such that $\mathcal{R}(\tilde{f}) \leq \mathcal{R}(f)$ and with equality only if $l_1 = l_2$.
2. If $k_1(\Gamma) < \frac{\pi}{\ell}$ and $f(v) = 0$, we conclude that f identically vanishes on the edges e_1, e_2 and we may construct a test function $\tilde{f}$ on $\tilde{\Gamma}$, such that $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$.
3. If $k_1(\Gamma) < \frac{\pi}{\ell}$ and $f(v) \neq 0$, we conclude that both $f|_{e_1}$ and $f|_{e_2}$ are symmetric functions and write

$$f|_{e_i} = A_i \cos(k_1(\Gamma) \cdot x),$$

for $x \in \left(-\frac{\ell}{2}, \frac{\ell}{2}\right)$ and $A_i \in \mathbb{R}$. Construct a test function $\tilde{f}$ on $\tilde{\Gamma}$ by setting

$$\tilde{f}|_{\tilde{\Gamma} \setminus (\tilde{e}_1 \cup \tilde{e}_2)} = f|_{\Gamma \setminus (e_1 \cup e_2)},$$

and

$$\tilde{f}|_{\tilde{e}_i}(x) = A_i \cos\left(k_1(\Gamma) \left|x - \frac{l_i - \ell}{2}\right|\right) \quad \text{for } x \in \left(-\frac{l_i}{2}, \frac{l_i}{2}\right).$$

This last relation pictorially means that if $\tilde{e}_1$ is the shorter edge, $\tilde{f}|_{\tilde{e}_1}$ is a symmetric function which equals $f|_{e_1}$ up to a piece of length $\ell - l_1$ around the middle of the edge e_1 which is glued to the middle of the the edge e_2 . Overall, $\tilde{f}$ has zero mean and $\mathcal{R}(\tilde{f}) = \mathcal{R}(f)$, as required.

Just as above, assumptions (1),(2) of the proposition together with assuming $l_1 \neq l_2$ and $k_1(\tilde{\Gamma}) = k_1(\Gamma)$, enables to use Lemmata 3.5.5 and 3.5.3 together with Courant's bound to arrive at a contradiction. $\square$

An immediate generalization of this proposition is the following.

Corollary 3.7.2. *Let $\mathcal{G}$ be a graph with $E \geq 3$ edges. Let $n \geq 2$ be an integer. Let v be a vertex of $\mathcal{G}$ and $e_1, \dots, e_n$ be either n dangling edges or n loops connected to v . Denote by $l_1, \dots, l_n$ the lengths of those edges and by $l_{n+1}, \dots, l_E$ the lengths of all other edges. Defining*

$$\ell := \frac{1}{n} \sum_{i=1}^n l_i,$$

and denoting $\tilde{\Gamma} := \Gamma(\mathcal{G}; (l_1, \dots, l_n, l_{n+1}, \dots, l_E))$, $\Gamma := \Gamma(\mathcal{G}; (\ell, \dots, \ell, l_{n+1}, \dots, l_E))$, we have

$$k_1(\tilde{\Gamma}) \leq k_1(\Gamma). \tag{3.63}$$

Moreover, if either $k_1(\Gamma) = \frac{\pi}{2\ell}$ in the dangling edges case (respectively, $k_1(\Gamma) = \frac{\pi}{\ell}$ in the loops case) or alternatively both the following conditions are satisfied

1. Γ is a supremizer of some graph.
2. $k_1(\tilde{\Gamma})$ is a simple eigenvalue.

then equality above holds if and only if $l_j = \ell$, for all $1 \leq j \leq n$.

Démonstration. Denote by $\vec{L}$ the vector of lengths $(l_1, \dots, l_n)$, and by $k_1(l_1, \dots, l_n)$ the corresponding spectral gap, keeping all the other $E - n$ edge lengths fixed. Assume without loss of generality that $l_1 \geq \dots \geq l_n$. If $l_1 > l_n$, we replace these two lengths by $\frac{1}{2}(l_1 + l_n)$ and get by Proposition 3.7.1 that

$$k_1(l_1, \dots, l_n) \leq k_1\left(\frac{1}{2}(l_1 + l_n), l_2, \dots, l_{n-1}, \frac{1}{2}(l_1 + l_n)\right). \quad (3.64)$$

Repeating this process infinitely many times, we get a sequence of vectors

$$\{\vec{L}^{(m)}\}_{m=1}^{\infty} := \{(l_1^{(m)}, \dots, l_n^{(m)})\}_{m=1}^{\infty}$$

such that

- $l_1^{(m)} \geq \dots \geq l_n^{(m)}$ (up to reordering the lengths),
- $\frac{1}{n} \sum_{i=1}^n l_i^{(m)} = \ell$
- $l_1^{(m)} - l_n^{(m)} \rightarrow 0$ as $m \rightarrow \infty$
- the sequence $\{k_1(\ell_1^{(m)}, \dots, \ell_n^{(m)})\}_{m=1}^{\infty}$ is non-decreasing

From the first three claims we deduce that, $l_j^{(m)} \rightarrow \ell$ as $m \rightarrow \infty$, for any $1 \leq j \leq n$. Therefore, the continuity of eigenvalues with respect to edge lengths (see Appendix (A.1)) gives

$$k_1(l_1^{(m)}, \dots, l_n^{(m)}) \rightarrow k_1(\ell, \dots, \ell) \text{ as } m \rightarrow \infty.$$

As the sequence $\{k_1(\ell_1^{(m)}, \dots, \ell_n^{(m)})\}_{m=1}^{\infty}$ is non-decreasing it follows that

$$k_1(l_1, \dots, l_n) \leq k_1(\ell, \dots, \ell), \quad (3.65)$$

as desired.

We now turn to the strict inequality conditions. In the dangling edge case, if the spectral gap satisfies $k_1(\ell, \dots, \ell) = \frac{\pi}{2\ell}$, then particular eigenfunctions are given by that of the equilateral star with n edges and total length $n\ell$. Among them, we choose one supported only on two edges and repeat the argument given in Proposition 3.7.1 to deduce the strict inequality if $l_i \neq l_j$ for some $i \neq j$. We argue similarly if $k_1(\ell, \dots, \ell) = \frac{\pi}{\ell}$ in the dangling loops case. Alternatively, we may assume by contradiction that there exist $i \neq j$ such that $l_i \neq l_j$ and $k_1(\tilde{\Gamma}) = k_1(\Gamma)$. This together with assumptions (1),(2) enables to proceed exactly as in the proof of Proposition 3.7.1 in order to get a contradiction. $\square$

3.8 Applications of graph gluing and symmetrization

This section applies the techniques of graph gluing and edge symmetrization developed in the previous two sections in order to prove the next few corollaries.

Proof of Corollary 3.2.7. This proof is a direct application of Theorem 3.2.6 once we observe the following

1. The glued vertices, v_1, v_2 become the central vertices of the supremizing stowers.
2. Every equilateral stower obeys the Dirichlet criterion with respect to its internal vertex, assuming the numbers of its petals and leaves obey $E_p + E_l \geq 2$.
3. Denoting the supremizing stowers by Γ_1, Γ_2 , their spectral gaps are

$$k_1(\Gamma_i) = \frac{\pi}{2} \left(2E_p^{(i)} + E_l^{(i)} \right).$$

4. Gluing Γ_1, Γ_2 with the length parameter

$$L = \frac{k_1(\Gamma_1)}{k_1(\Gamma_1) + k_1(\Gamma_2)} = \frac{2E_p^{(1)} + E_l^{(1)}}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}},$$

results with an equilateral stower whose all petals are of length $\frac{2}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}}$ and all dangling edges are of length $\frac{1}{2E_p^{(1)} + E_l^{(1)} + 2E_p^{(2)} + E_l^{(2)}}$.

□

Remark. We note that an equilateral stower obeys the strong Dirichlet criterion. Therefore, by Theorem 3.2.6, if we assume for $\mathcal{G}_1, \mathcal{G}_2$ that all their supremizers other than the stower violate the Dirichlet criterion, we also get uniqueness in Corollary 3.2.7.

Proof of Corollary 3.2.8. We show that equilateral stars and flowers (with $E \geq 2$) satisfy condition (b) of Theorem 3.2.6, when considered as supremizers of the corresponding stowers. This allows to employ Theorem 3.2.6 in order to glue a star with a flower and to show the statement of the Corollary for all stowers with $E_l \geq 2$ and $E_p \geq 2$ (note that when gluing an equilateral flower and equilateral star according to condition (1) of Theorem 3.2.6, the stower obtained is equilateral). The rest of the stowers will be dealt with, at the end of the proof.

Start by noting that Theorem 3.2.2 implies that the statement of the corollary holds for all star graphs, which are stowers with $E_p = 0$, $E_l \geq 2$. The spectral gap of equilateral star is $\frac{E\pi}{2}$ and it remains the same after imposing Dirichlet condition at their central vertex, so that it obeys the Dirichlet criterion. Furthermore the multiplicity of its spectral gap is $E - 1$ and it increases to E after imposing Dirichlet condition, so that it obeys the strong Dirichlet criterion. As equilateral stars are unique maximizers of stars, we conclude that they obey condition (b) of Theorem 3.2.6.

Among the flower graphs, we start with the two-petal and three-petal flowers. An easy calculation reveals that the spectral gap of a flower with two petals equals 2π . Note that this spectral gap is independent of the edge lengths, so that this give a continuous family of (trivial) maximizers. In particular, the equilateral flower with two petals is a non-unique maximizer. Yet, this equilateral two-petal flower is the only maximizer in this family which obeys the Dirichlet criterion and it further obeys the strong Dirichlet criterion, as we show next. Consider a two-petal flower whose edge lengths are $l_1 \neq l_2$ and assume $l_1 > l_2$. Imposing Dirichlet condition at the vertex lowers the spectral gap of the graph from 2π to $\frac{\pi}{l_1}$, so that it does not obey the Dirichlet criterion. The equilateral flower, on the other hand, maintains the spectral gap of 2π even after imposing a Dirichlet condition at its vertex. In addition, its spectral gap with Neumann condition at the vertex is a simple eigenvalue, but once imposing Dirichlet at the vertex, the spectral gap becomes of multiplicity two. By this we have shown that the two-petal flower satisfies condition (b) of Theorem 3.2.6.

Let Γ be a flower with three petals and denote its vertex by v . Let $\tilde{\Gamma}$ be the two petal subgraph which consists of the largest two petals of Γ . Denote the total length of $\tilde{\Gamma}$ by $\tilde{l}$ (so that $\tilde{l} \geq \frac{2}{3}$). Let $\tilde{f}$ be the first non-constant eigenfunction on $\tilde{\Gamma}$. Construct the following test function on Γ

$$f|_{\tilde{\Gamma}} = \tilde{f}, \quad f|_{\Gamma \setminus \tilde{\Gamma}} = \tilde{f}(v).$$

By Lemma A.3.1

$$\mathcal{R}(f - \langle f \rangle) = \frac{\left(\frac{2\pi}{\tilde{l}}\right)^2 \frac{\tilde{l}}{2}}{\frac{\tilde{l}}{2} + |\tilde{f}(v)|^2 \tilde{l} (1 - \tilde{l})} \leq \left(\frac{2\pi}{\tilde{l}}\right)^2 \leq (3\pi)^2,$$

where equality holds if and only if $\tilde{l} = \frac{2}{3}$ and $\tilde{f}(v) = 0$. Conversely, it is easy to show that the spectral gap of the equilateral three-petal flower equals 3π . Hence the equilateral three petal graph is a unique maximizer. In addition, imposing a Dirichlet condition at the vertex maintains a spectral gap of 3π , so that the three-petal equilateral flower obeys the Dirichlet criterion. It further obeys the strong Dirichlet criterion as the multiplicity of its spectral gap is 2 and it increases to 3 after imposing Dirichlet condition at central vertex. Therefore, a three petal flower satisfies condition (b) of Theorem 3.2.6.

From the above, we may glue two flowers of those types (each either with two petals or three petals) and get a four, five or six petal flower. Applying Theorem 3.2.6 shows that the equilateral version of each of these graphs serves as the unique maximizer. Furthermore, it is easy to show that any equilateral flower obeys the strong Dirichlet criterion (as was shown for the two-petal and three-petal flower above). This together with the uniqueness of four, five and six petal flowers implies that they obey condition (b) of Theorem 3.2.6. Repeating this gluing process as many times as needed shows that any equilateral flower is both a unique maximizer (except for $E = 2$) and obeys condition (b) of Theorem 3.2.6 (which holds also for $E = 2$).

By this, we have both proved the corollary for all stars and flowers with $E \geq 2$ and also conclude the validity of the corollary for all stowers with $E_l \geq 2$ and $E_p \geq 2$, as claimed in the beginning of this proof. It is left to treat stowers with either $E_p = 1$ or $E_l = 1$. In order to do that, we state in lemmata 3.8.1, 3.8.2, 3.8.3, 3.8.4 (which follow this proof) that the current corollary is valid for the following small stowers $(E_p, E_l) \in \{(1, 2), (1, 3), (2, 1), (3, 1)\}$ and that in addition, the equilateral versions of those stowers all obey condition (b) of Theorem 3.2.6. Hence, each stower with either $E_p = 1$ or $E_l = 1$ may be obtained by gluing one of those small stowers with an appropriate flower or star and applying Theorem 3.2.6 for such a gluing finishes the proof. $\square$

Remark. We note that the proof above might have been simplified if we were after a weaker result. Namely, using the more elementary methods of Rayleigh quotient calculations one can prove the statement in the Corollary for all stowers except those with $E_p = 1$ or $E_l = 1$ and without the uniqueness part of the result.

Proof of Corollary 3.2.9. Let $\mathcal{G}$ be a graph with E edges out of which E_l are leaves and $E - E_l$ are internal edges. Let $\underline{l} \in \mathcal{L}_{\mathcal{G}}$ and denote $\Gamma := \Gamma(\mathcal{G}; \underline{l})$. Identifying all internal (i.e. non-leaf) vertices of Γ we get a stower graph with E_l leaves and $E - E_l$ petals which we denote by $\tilde{\Gamma}$ and by Lemma A.2.3 we get

$$k_1(\Gamma) \leq k_1(\tilde{\Gamma}).$$

From Corollary 3.2.8 we have

$$k_1(\tilde{\Gamma}) \leq \pi \left((E - E_l) + \frac{E_l}{2} \right) = \pi \left(E - \frac{E_l}{2} \right) \quad (3.66)$$

if $E \geq 2$ and $(E, E_l) \neq (2, 1)$ which are exactly the conditions in this corollary and this proves its first part.

Assuming equality in (3.7) we have equality in (3.66). If further $(E, E_l) \notin \{(2, 0), (3, 2)\}$, we satisfy the uniqueness conditions in Corollary 3.2.8. Namely, we conclude that equality in (3.66) is possible only if $\tilde{\Gamma}$ is equilateral in the stower sense : leaves are of half length than petals. We conclude that Γ is also equilateral in the following sense : all of its leaves are of length $\frac{1}{2E-E_l}$ each and all the rest (inner) edges are of length $\frac{2}{2E-E_l}$ each. We carry on by conditioning on the number of internal (i.e. non-leaf) vertices of Γ and keeping in mind that $k_1(\Gamma) = \pi \left(E - \frac{E_l}{2} \right)$.

If Γ has a single internal vertex then it is a stower graph and we are done. Assume that Γ has at least two internal vertices. Choose two such internal vertices. In the following we described a recursive process which marks some set of edges of the graphs, to be denoted by $\mathcal{E}_0$. Choose a path on Γ connecting v_+ with v_- without going through graph leaves. This is possible as Γ is connected. Choose an arbitrary edge, e , on this path and add it to $\mathcal{E}_0$. Next, if $\Gamma \setminus e$ is connected repeat the step above on $\Gamma \setminus e$. Namely, choose a path on $\Gamma \setminus e$ connecting v_+ and v_- not going through graph leaves (with the exception of v_+, v_- which might have now turned themselves into leaves). Repeat this process until $\Gamma \setminus \mathcal{E}_0$ is a disconnected graph. We may then write $\Gamma = \Gamma_+ \cup \Gamma_- \cup \mathcal{E}_0$, where Γ_+ is a connected subgraph of Γ containing v_+ , and similarly for Γ_- and v_- . Set the following test function on Γ :

$$f(x) = \begin{cases} 1 & x \in \Gamma_+ \\ -1 & x \in \Gamma_- \\ \cos(k_1(\Gamma) \cdot x) & x \in e \text{ s.t. } e \in \mathcal{E}_0. \end{cases}$$

By construction, this test function is continuous. It is easy to verify by (A.18) (alternatively, by an easy extension of Lemma A.3.1) that $\mathcal{R}(f) < k_1(\Gamma)$ if $\Gamma_+ \cup \Gamma_- \neq \emptyset$. As $\mathcal{R}(f) < k_1(\Gamma)$ contradicts the equality in (3.7) we conclude that $\Gamma_+ \cup \Gamma_- = \emptyset$, which implies that $\Gamma = \mathcal{E}_0$ and hence Γ is a mandarin graph. It is actually an equilateral mandarin, as we have shown above. $\square$

The lemmata needed in the proof of Corollary 3.2.8 are now stated. Their proofs involve some technical computations and appear in Appendix A.4.

Lemma 3.8.1. *Let $\mathcal{G}$ be a stower with $E_p = 1$ petal and $E_l = 2$ leaves. Then $\mathcal{G}$ has a continuous family of maximizers whose spectral gap is 2π . Those are all the stowers with both leaf lengths equal and not greater than $\frac{1}{4}$. Furthermore, the equilateral stower obeys condition (b) of Theorem 3.2.6.*

Lemma 3.8.2. *Let $\mathcal{G}$ be a stower graph with $E_p = 1$ petal and $E_l = 3$ leaves. Then the equilateral stower graph is the unique maximizer of $\mathcal{G}$, and the corresponding spectral gap equals $\frac{5\pi}{2}$. Furthermore, the equilateral stower obeys condition (b) of Theorem 3.2.6.*

Lemma 3.8.3. *Let $\mathcal{G}$ be a stower graph with $E_l = 1$ and $E_p = 2$. Then $\mathcal{G}$ has a unique maximizer, which is the equilateral stower graph with spectral gap equal to $\frac{5\pi}{2}$. Furthermore, the equilateral stower obeys condition (b) of Theorem 3.2.6.*

Lemma 3.8.4. *Let $\mathcal{G}$ be a stower graph with $E_l = 1$ and $E_p = 3$. Then $\mathcal{G}$ has a unique maximizer, which is the equilateral stower graph with spectral gap equal to $\frac{7\pi}{2}$. Furthermore, the equilateral stower obeys condition (b) of Theorem 3.2.6.*

The stower with $E_p = E_l = 1$ was not mentioned in the theorem above, as it is not maximized by the equilateral stower. Its unique supremizer is the single loop graph ($E_p = 1, E_l = 0$), as we state in the following in order to complete the picture.

Lemma 3.8.5. *Let $\mathcal{G}$ be a stower graph with one leaf and one petal. Then $\mathcal{G}$ has a unique maximizer, which is the unit circle, with spectral gap equal to 2π .*

3.9 Summary

This work investigates the problem of optimizing a graph's spectral gap in terms of its edge lengths. We start by providing a natural formulation of this problem (Definitions 3.1.1, 3.1.2 and adjacent discussion). Our formalism allows both to state the optimization questions in utmost generality (for all graph topologies and all edge length values) and moreover to determine when such a question is fully answered. For example, this is the case with the infimization problem for which both the optimal bounds and all the possible infimizing topologies are found, with no more room for improvement (see the discussion which follows Theorem 3.2.1). Contrary to the infimization problem, we point out that the supremization problem is not solved in full generality. We show its complete solution for tree graphs and for a family of graphs whose vertex connectivity equals one. In addition, a global upper bound is provided (Corollary 3.2.9), improving the upper bound known so far, by taking into account the number of graph leaves. Furthermore, we provide a set of techniques to tackle the supremization problem. Among those are the gluing graphs approach, the symmetrization of dangling edges and loops and the characterization of local maximizers. Those tools are applicable in the current work and might assist in further exploration of the problem. The techniques and the results of the current work lead to forming a few conjectures regarding the maximization problem.

First, the supremizer graph families known so far are stower graphs (including stars and flowers as particular cases) and mandarin graphs. The spectral gap of these graphs is highly degenerate due to their large symmetry groups. The symmetry groups corresponding to the stower and the mandarin are correspondingly $S_{E_p} \times S_{E_l}$ and S_E , where E is the number of mandarin edges and E_p, E_l numbers of stower petals and leaves. The corresponding spectral gap multiplicity of both a stower and a mandarin is $E - 1$, which is indeed high. In the other extreme of spectral gaps which are simple eigenvalues, we show that those are unlikely to be supremizers. In Theorem 3.2.4 we prove that a supremizer whose spectral gap is simple can never have a spectral gap higher than a mandarin and in some cases than a flower (Corollary 3.5.6). In Proposition 3.6.5 we prove that if a supremizer is obtained by the gluing method then its spectral gap is necessarily a multiple eigenvalue. As high multiplicities of eigenvalues is related to large order symmetry groups (or even to large dimension of their representations), the discussion above leads to the following two conjectures :

1. A supremizer of a graph is obtained by choosing edge lengths which maximize the order of the symmetry group of the resulting graph⁷.
2. A supremizer of a graph is obtained by choosing edge lengths which maximize the multiplicity of the spectral gap.

We note that the conjectures above are not necessarily correlated. We demonstrate this by mandarin chains, which are M copies of n -mandarin graphs glued serially, as presented in Proposition 3.5.8. The symmetry group of those graphs is $(S_n)^M$ whose order is $(n!)^M$. Yet, a mandarin chain with $n \geq 2$, $M \geq 2$ always has a simple spectral gap, as proved in Proposition 3.5.8. Hence, the large order of the symmetry group does not guarantee large multiplicity of the spectral gap. Seeking for supremizers for those graphs, we observe that turning such a graph into an equilateral flower with $m(n-1)$ petals, increases its spectral gap from $n\pi$ to $M(n-1)\pi$. The symmetry group of this flower is $S_{M(n-1)}$, which is of order $(M(n-1))!$. For most values of n, M , the flower's symmetry group is of larger order than that of the mandarin chain, which is correlated to its spectral gap being of higher multiplicity. However, for $n = 3$, $M = 2$, the symmetry group of the flower is of order 24, while that of the mandarin chain is of order 36. This flower possesses a higher spectral gap (3π) than the mandarin chain (4π) despite its lower order symmetry group. On one hand, this example serves in

7. We thank Gregory Berkolaiko for raising this conjecture in a private communication.

the favor of the second conjecture over the first one. On the other hand, we still do not know what is the supremizer in this example and feel that at this stage, both conjectures are equally appealing.

Finally, we state a more explicit conjecture : the supremizer of a certain graph is either a stower graph (in its generalized sense) or a mandarin. These are indeed the only supremizers this work revealed. Given a certain graph, the maximal spectral gap among all stowers which may be obtained from that graph equals $\pi(\beta + \frac{E_l}{2})$, where β is the graph's first Betti number and E_l is the number of its dangling edges. The maximal spectral gap among all possible mandarins has a less explicit expression, and we describe it next. Let $\mathcal{G}$ be a graph and let $\mathcal{G}_1, \mathcal{G}_2$ be two connected subgraphs, sharing neither an edge nor a vertex and such that each vertex of $\mathcal{G}$ belongs to $\mathcal{G}_1 \cup \mathcal{G}_2$. Let $E(\mathcal{G}_1, \mathcal{G}_2)$ be the number of edges connecting a vertex of $\mathcal{G}_1$ to a vertex of $\mathcal{G}_2$. Contracting all edges of $\mathcal{G}_1$ and $\mathcal{G}_2$ we get a mandarin of $E(\mathcal{G}_1, \mathcal{G}_2)$ edges. The maximal spectral gap among all mandarins is therefore given by

$$\pi \cdot \max_{\mathcal{G}_1, \mathcal{G}_2} E(\mathcal{G}_1, \mathcal{G}_2).$$

We note that the expression above is curiously related to the Cheeger constant, but do not further elaborate on that. For the allowed $(\mathcal{G}_1, \mathcal{G}_2)$ partitions among which we maximize we may also write $E(\mathcal{G}_1, \mathcal{G}_2) = \beta + 1 - (\beta_1 + \beta_2)$, where β_i is the first Betti number of $\mathcal{G}_i$. This expression allows for a comparison with the optimal stower spectral gap, $\pi(\beta + \frac{E_l}{2})$. For example it is seen that for a graph with at most one dangling edge, the mandarin achieves a strictly higher spectral gap than the stower (or flower in this case) only if there is a partition where both $\mathcal{G}_1, \mathcal{G}_2$ are tree graphs. On the other hand, if the graph has at least three dangling edges, any mandarin has a lower spectral gap than the optimal stower. Does the conjecture above hold or are there supremizers other than stowers and mandarins? This question remains open.

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Troisième partie

Transformée de Fourier

Chapitre 4

Transformée de Fourier sur les groupes de Lie nilpotents d'indice 2

4.1 Introduction

4.1.1 Definition of 2-steps Lie groups

Let G be a real, simply connected nilpotent Lie group. Denote by $\mathfrak{g}$ its Lie algebra. It is well-known (see [97]) that for such groups, the exponential map

$$\exp : \mathfrak{g} \rightarrow G$$

is a global diffeomorphism from $\mathfrak{g}$ onto G . This map becomes a Lie isomorphism once one endows the Lie algebra $\mathfrak{g}$ with the group law given by the Baker-Campbell-Hausdorff formula, which terminates after a finite number of terms since G is nilpotent. In order to lighten the notation, we will henceforth assume that G is the set $\mathbb{R}^n$ endowed with some group law.

In the sequel, we will restrict our attention to nilpotent groups of step 2, for which all commutators are central. That is, we assume that for any $x, y, z \in \mathbb{R}^n$, we have $[x, [y, z]] = 0$. Let us denote by p the dimension of the center of the group. Then, there exists an integer m , a decomposition $\mathbb{R}^n = \mathbb{R}^m \oplus \mathbb{R}^p$ and a bilinear, antisymmetric map

$$\sigma : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^p$$

such that, for $Z, Z' \in \mathbb{R}^m$ and $s, s' \in \mathbb{R}^p$,

$$(Z, s) \cdot (Z', s') = (Z + Z', s + s' + \frac{1}{2}\sigma(Z, Z')). \quad (4.1)$$

The map σ and the integers m, p are determined by the group law and dimension. Conversely, for any integers m, p and any bilinear, antisymmetric map $\sigma : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^p$, one may define a Lie group of step 2 by the formula (4.1). Now, given $\lambda \in \mathbb{R}^p$, we define the matrix $\mathcal{U}^{(\lambda)} \in \mathcal{M}_m(\mathbb{R})$ as follows. For any $Z, Z' \in \mathbb{R}^m$, there holds

$$\langle \lambda, \sigma(Z, Z') \rangle = \langle Z, \mathcal{U}^{(\lambda)} \cdot Z' \rangle.$$

If $(s_1, \dots, s_p)$ denotes an orthonormal basis of $\mathbb{R}^p$, we also define $\mathcal{U}_k \in \mathcal{M}_m(\mathbb{R})$ by

$$\langle s_k, \sigma(Z, Z') \rangle = \langle Z, \mathcal{U}_k \cdot Z' \rangle.$$

Conversely, the map σ may be defined from $(\mathcal{U}_k)_{1 \leq k \leq p}$ thanks to the equality

$$\sigma(Z, Z') = (\langle Z, \mathcal{U}_k \cdot Z' \rangle)_{1 \leq k \leq p}.$$

Notice that the map $\lambda \mapsto \mathcal{U}^{(\lambda)}$ is linear, with its image spanned by $(\mathcal{U}_k)_{1 \leq k \leq p}$. As $\mathcal{U}^{(\lambda)}$ is an antisymmetric matrix, its rank is an even number. We define the integer d by

$$2d := \max_{\lambda \in \mathbb{R}^p} \text{rank } \mathcal{U}^{(\lambda)}.$$

The set $\tilde{\Lambda} := \{\lambda \in \mathbb{R}^p \mid \text{rank } \mathcal{U}^{(\lambda)} = 2d\}$ is then a non empty Zariski-open subset of $\mathbb{R}^p$ - in particular, it is open and dense in $\mathbb{R}^p$ for the Euclidean topology. Since the map $\lambda \mapsto \mathcal{U}^{(\lambda)}$ is continuous, there exist d continuous functions

$$\eta_j : \mathbb{R}^p \rightarrow \mathbb{R}_+, 1 \leq j \leq d,$$

such that, in a suitable basis (see for instance [105]), $\mathcal{U}^{(\lambda)}$ reduces to the form

$$\begin{bmatrix} 0 & \eta(\lambda) & 0 \\ -\eta(\lambda) & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \in \mathcal{M}_m(\mathbb{R}),$$

where

$$\eta(\lambda) := \text{diag}(\eta_1(\lambda), \dots, \eta_d(\lambda)) \in \mathcal{M}_d(\mathbb{R}).$$

We loosely denote by $(x_1(\lambda), \dots, x_d(\lambda), y_1(\lambda), \dots, y_d(\lambda), r_1(\lambda), \dots, r_t(\lambda))$ such a basis. For readability purposes, we will often shorten the notation to $(x_1, \dots, x_d, y_1, \dots, y_d, r_1, \dots, r_t)$.

4.1.2 A few examples

A prime example of a 2-step Lie group is given for $d \geq 1$ by the Heisenberg group $\mathbb{H}^d$, which is the set $\mathbb{R}^{2d} \times \mathbb{R}$ endowed with the group law

$$(Z, s) \cdot (Z', s') = (Z + Z', s + s' + \frac{1}{2}\sigma_c(Z, Z')),$$

where σ_c is the canonical symplectic form on $\mathbb{R}^d \times \mathbb{R}^d$. For $x, y, x', y' \in \mathbb{R}^d$,

$$\sigma_c((x, y), (x', y')) = \langle y, x' \rangle - \langle y', x \rangle,$$

where $\langle \cdot, \cdot \rangle$ denotes the usual scalar product on $\mathbb{R}^d$. Regarding the choice of suitable bases, let $(x_1, \dots, x_d, y_1, \dots, y_d)$ be a basis of $\mathbb{R}^{2d}$ in which the matrix of σ_c assumes the form

$$\begin{bmatrix} 0 & I_d \\ -I_d & 0 \end{bmatrix} \in \mathcal{M}_{2d}(\mathbb{R}).$$

For strictly positive λ , we choose $(x_1, \dots, x_d, y_1, \dots, y_d)$ as a basis of $\mathbb{R}^{2d}$, while for λ strictly negative this choice becomes $(y_1, \dots, y_d, x_1, \dots, x_d)$. Hence, for any nonzero λ , we have, as desired,

$$\mathcal{U}^{(\lambda)} = \begin{bmatrix} 0 & |\lambda|I_d \\ -|\lambda|I_d & 0 \end{bmatrix} \in \mathcal{M}_{2d}(\mathbb{R}).$$

Let us point out that even on this simple example, the eigenvectors as functions of λ are discontinuous around 0. We present here another example. Given the matrices

$$J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \text{ and } S = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \in \mathcal{M}_2(\mathbb{R}),$$

we define for λ in $\mathbb{R}^2$, the matrix

$$\mathcal{U}^{(\lambda)} = \begin{bmatrix} \lambda_1 J & \lambda_2 S \\ -\lambda_2 S & -\lambda_1 J \end{bmatrix} \in \mathcal{M}_4(\mathbb{R}).$$

On $\mathbb{R}^4 \times \mathbb{R}^2$, we consider the group law generated by the matrices $\mathcal{U}^{(\lambda)}$. That is, for $Z, Z' \in \mathbb{R}^4$ and $s, s' \in \mathbb{R}^2$, we have

$$(Z, s) \cdot (Z', s') := \left(Z + Z', s_1 + s'_1 + \frac{1}{2} \left\langle Z, \begin{bmatrix} J & 0 \\ 0 & -J \end{bmatrix} Z' \right\rangle, s_2 + s'_2 + \frac{1}{2} \left\langle Z, \begin{bmatrix} 0 & S \\ -S & 0 \end{bmatrix} Z' \right\rangle \right).$$

The positive eigenvalues of $\mathcal{U}^{(\lambda)}$ are

$$\eta_{\pm}(\lambda) = ||\lambda_1| \pm |\lambda_2||.$$

In particular, $\eta_{-}(\lambda)$ vanishes on the straight lines $\{\lambda \in \mathbb{R}^2, |\lambda_1| = |\lambda_2|\}$ whereas $\eta_{+}(\lambda)$ remains strictly positive for any nonzero λ .

4.1.3 Definition of the Fourier transform

We now turn to the practical aspects of the theory we aim at. Given $(v_1, \dots, v_m)$ any basis of $\mathbb{R}^m$ and $(s_1, \dots, s_p)$ the canonical basis of $\mathbb{R}^p$, a basis of g is given by $\{V_i, 1 \leq i \leq m\} \cup \{S_k, 1 \leq k \leq p\}$, with

$$V_i := \partial_{v_i} - \frac{1}{2} \sum_{k=1}^m (\mathcal{U}_k \cdot Z)_i \partial_{s_k} = \partial_{v_i} - \frac{1}{2} \sum_{k,j=1}^m (\mathcal{U}_k)_{ij} Z_j \partial_{s_k},$$

$$S_k = \partial_{s_k}.$$

Choosing for $(v_1, \dots, v_m)$ a basis $(x_1(\lambda), \dots, r_t(\lambda))$, the family $(V_i)_{1 \leq i \leq m}$ decomposes as

$$X_j = X_j(\lambda) = \partial_{x_j(\lambda)} + \frac{1}{2} \eta_j(\lambda, \nabla_s) y_j(\lambda) \quad \text{for } 1 \leq j \leq d,$$

$$Y_j = Y_j(\lambda) = \partial_{y_j(\lambda)} - \frac{1}{2} \eta_j(\lambda, \nabla_s) x_j(\lambda) \quad \text{for } 1 \leq j \leq d,$$

$$R_l = R_l(\lambda) = \partial_{r_l(\lambda)} \quad \text{for } 1 \leq l \leq t,$$

where the vector field $\eta_j(\lambda, \nabla_s)$ is defined by

$$\eta_j(\lambda, \nabla_s) := \frac{\eta_j(\lambda)}{|\lambda|} \frac{\lambda}{|\lambda|} \cdot \nabla_s$$

whenever $\eta_j(\lambda)$ is nonzero and $\eta_j(\lambda, \nabla_s) = 0$ otherwise. Hence, for each λ in $\mathbb{R}^p$, we have a family of vector fields $(\eta_j(\lambda, \nabla_s))_{1 \leq j \leq d}$ acting on $\mathbb{R}^p$. In particular, for all λ in $\mathbb{R}^p$, $\eta_j(\lambda, \nabla_s)$ satisfies

$$\eta_j(\lambda, \nabla_s) \left(e^{i\langle \lambda, \cdot \rangle} \right) (s) = i \eta_j(\lambda) e^{i\langle \lambda, s \rangle},$$

thus justifying the slight abuse of notation. We emphasize here the fact that the X_j and the Y_j are indeed vector fields, not mere pseudodifferential operators as one may be tempted to think. For each value of the parameter λ in $\mathbb{R}^p$, we have chosen a basis of $\mathbb{R}^m$ in which $\mathcal{U}^{(\lambda)}$ has an antidiagonal structure. This basis in turn simplifies as much as possible the expressions of the

vector fields $(V_i)_{1 \leq i \leq m}$, hence helping us in the upcoming computations. We define similarly the right-invariant vector fields $\tilde{V}_i$ for $1 \leq i \leq m$ by

$$\tilde{V}_i := \partial_{v_i} + \frac{1}{2} \sum_{k=1}^m (\mathcal{U}_k \cdot Z)_i \partial_{s_k}.$$

In the basis $(x_1(\lambda), \dots, r_t(\lambda))$ defined above, the family $(\tilde{V}_i)_{1 \leq i \leq m}$ decomposes as

$$\begin{aligned} \tilde{X}_j &= \tilde{X}_j(\lambda) = \partial_{x_j(\lambda)} - \frac{1}{2} \eta_j(\lambda, \nabla_s) y_j(\lambda) \text{ for } 1 \leq j \leq d, \\ \tilde{Y}_j &= \tilde{Y}_j(\lambda) = \partial_{y_j(\lambda)} + \frac{1}{2} \eta_j(\lambda, \nabla_s) x_j(\lambda) \text{ for } 1 \leq j \leq d, \\ \tilde{R}_l &= R_l \text{ for } 1 \leq l \leq t. \end{aligned}$$

For (λ, ν, w) in $\tilde{\Lambda} \times \mathbb{R}^t \times \mathbb{R}^n$ with $w = (x, y, r, s)$, we define the irreducible unitary representations of $\mathbb{R}^n$ on $L^2(\mathbb{R}^d)$

$$(u_w^{\lambda, \nu} \phi)(\xi) := e^{-i\langle \nu, r \rangle} e^{-i\langle \lambda, s + [\xi + \frac{x}{2}, y] \rangle} \phi(\xi + x). \quad (4.2)$$

Definition 4.1.1. With the notations from above, the Fourier transform of the function f in $L^1(\mathbb{R}^n)$ at the point (λ, ν) in $\tilde{\Lambda} \times \mathbb{R}^t$ is a unitary operator acting on $L^2(\mathbb{R}^n)$ with

$$\mathcal{F}^g(f)(\lambda, \nu) := \int_{\mathbb{R}^n} f(w) u_w^{\lambda, \nu} dw.$$

Thinking of this operator as an infinite matrix, we look at its coefficients in a suitable basis. For n, m in $\mathbb{N}^d$ and $(\lambda, \nu) \in \tilde{\Lambda} \times \mathbb{R}^t$, we let

$$\widetilde{\mathcal{F}}_g(f)(n, m, \lambda, \nu) := (\mathcal{F}^g(f)(\lambda, \nu) H_{m, \eta(\lambda)} | H_{n, \eta(\lambda)})_{L^2(\mathbb{R}^d)}.$$

Expanding out the scalar product, we notice the operator equality

$$\widetilde{\mathcal{F}}_g(f)(n, m, \lambda, \nu) = \mathcal{F}_{\mathbb{R}^t}(\mathcal{F}_g(f)(n, m, \lambda))(\nu) = \mathcal{F}_g(\mathcal{F}_{\mathbb{R}^t}(f)(\nu))(n, m, \lambda),$$

where $\mathcal{F}_{\mathbb{R}^t}$ denotes the standard Fourier transform on the commutative group $(\mathbb{R}^t, +)$ and

$$\mathcal{F}_g(f)(n, m, \lambda) := \int_{(\mathbb{R}^d)^3 \times \mathbb{R}^p} f(x, y, s) e^{-i\langle \lambda, s \rangle} e^{-i\langle \eta(\lambda), (\xi + \frac{x}{2}), y \rangle} H_{m, \eta(\lambda)}(\xi + x) H_{n, \eta(\lambda)}(\xi) d\xi dx dy ds.$$

The action of the Fourier transform $\mathcal{F}_{\mathbb{R}^t}$ is already well-known and commutes with that of $\mathcal{F}_g$.

Henceforth, we will assume that t is equal to 0 and will not mention ν anymore.

We will focus solely on the properties of $\mathcal{F}_g$. Performing an obvious change of variable inside the integral leads to the more symmetric form

$$\mathcal{F}_g(f)(n, m, \lambda) = \int_{\mathbb{R}^d \times \mathbb{R}^n} f(w) e^{-i\langle \lambda, s \rangle} e^{-i\langle \eta(\lambda), \xi, y \rangle} H_{m, \eta(\lambda)}\left(\xi + \frac{x}{2}\right) H_{n, \eta(\lambda)}\left(\xi - \frac{x}{2}\right) d\xi dw.$$

Denoting $\hat{w} = (n, m, \lambda)$ and letting

$$\mathcal{W}(\hat{w}, x, y) := \int_{\mathbb{R}^d} e^{-i\langle \eta(\lambda), \xi, y \rangle} H_{m, \eta(\lambda)}\left(\xi + \frac{x}{2}\right) H_{n, \eta(\lambda)}\left(\xi - \frac{x}{2}\right) d\xi,$$

we see that

$$\mathcal{F}_g(f)(n, m, \lambda) = \int_{\mathbb{R}^n} \overline{e^{i\langle \lambda, s \rangle} \mathcal{W}(\hat{w}, x, y)} f(w) dw.$$

If one thinks of the family of functions $(\mathcal{W}(\hat{w}, \cdot, \cdot))_{\hat{w} \in \mathbb{N}^{2d} \times \tilde{\Lambda}}$ as a non commutative replacement of the characters on $\mathbb{R}^m$, then the latter formula is very similar to that of the usual Fourier transform on $\mathbb{R}^n$.

4.1.4 The frequency space

Let us now describe what should be $\hat{g}$, the frequency space of g . Since $\mathcal{F}_g(f)(n, m, \lambda)$ has been defined for f in $L^1(\mathbb{R}^n)$, n, m in $\mathbb{N}^d$ and λ in $\tilde{\Lambda}$, the set

$$\tilde{g}_E := \mathbb{N}^d \times \mathbb{N}^d \times \tilde{\Lambda}$$

is a natural choice. Endowing $\tilde{g}_E$ with the distance

$$\rho_E((n, m, \lambda), (n', m', \lambda'))^2 := |\eta(\lambda) \cdot (n + m) - \eta(\lambda') \cdot (n' + m')|^2 + |(n - m) - (n' - m')|^2 + |\lambda - \lambda'|^2$$

allows to account for the different types of decay (see Section 4.4 for more details). Hence, the metric space $(\tilde{g}_E, \rho_E)$ seems to be a reasonable candidate for the Fourier space of g . However, it fails to be complete : for instance, denoting

$$\Lambda_0 := \mathbb{R}^p \setminus \tilde{\Lambda},$$

points of the type $(0, 0, \lambda_0)$ in $\mathbb{N}^{2d} \times \Lambda_0$ belong to the completion of $(\tilde{g}_E, \rho_E)$. While it is possible to directly describe the completion of $(\tilde{g}_E, \rho_E)$, writing exactly how we extend both $\tilde{g}_E$ and ρ_E is tedious. It is comparatively easier to look first at a *Euclidean* isometric embedding of $(\tilde{g}_E, \rho_E)$. The set underlying the metric space, denoted by $\tilde{g}$, will be an embedding of $\tilde{g}_E$ into, say, $\mathbb{R}^n$. The distance, however, will simply be a restriction of a standard Euclidean distance $|\cdot|$ on $\tilde{g}$. The main idea is that we reduce to a well-known distance, at the cost of a more intricate Fourier space.

We now make precise the ideas above. For λ in $\tilde{\Lambda}$ and j between 1 and d , we define

$$g_j(\lambda) = ((\eta_j(\lambda) \cdot \mathbb{N}) \times \mathbb{Z})_+ := \left\{ (a_j, b_j) \in \mathbb{R}_+ \times \mathbb{Z} \mid \frac{a_j \pm \eta_j(\lambda)b_j}{2} \in \eta_j(\lambda) \cdot \mathbb{N} \right\}$$

and

$$g(\lambda) := \left\{ (a, b) \in (\mathbb{R}_+)^d \times \mathbb{Z}^d \mid \frac{a \pm \eta(\lambda) \cdot b}{2} \in \eta(\lambda) \cdot \mathbb{N}^d \right\} = \prod_{j=1}^d g_j(\lambda).$$

A way to think about the set $g_j(\lambda)$ is the following. For any b_j in $\mathbb{Z}$ and λ in $\tilde{\Lambda}$, we have

$$\{a_j \in \mathbb{R}_+ \mid (a_j, b_j) \in g_j(\lambda)\} = \{(2n + |b_j|)\eta_j(\lambda) \mid n \in \mathbb{N}\}.$$

Otherwise said, given b_j and λ , the admissible a_j 's form a half-infinite comb of width $2\eta_j(\lambda)$ starting at $\eta_j(\lambda)|b_j|$. The set $\tilde{g}$ is now defined by

$$\tilde{g} := \bigsqcup_{\lambda \in \tilde{\Lambda}} g(\lambda) \times \{\lambda\}.$$

As previously explained, we endow $\tilde{g}$ with the distance inherited from the Euclidean distance on $\mathbb{R}^d \times \mathbb{Z}^d \times \mathbb{R}^p$. The isometry between $\tilde{g}_E$ and $\tilde{g}$ is given by

$$i_E : \begin{cases} \tilde{g}_E & \longrightarrow & \tilde{g} \\ (n, m, \lambda) & \longmapsto & (\eta(\lambda) \cdot (n + m), n - m, \lambda). \end{cases}$$

Of course, as $\tilde{g}_E$ was not complete, $\tilde{g}$ is not either. We finally describe the completion of $(\tilde{g}, |\cdot|)$. Consider a sequence $(\lambda_p)_p \subset \tilde{\Lambda}$ converging to λ_0 in Λ_0 at which η_j vanishes. At least formally, we expect the constraint defining $g_j(\cdot)$ to become vacuous and hence, it seems natural to let

$$g_j(\lambda_0) = ((0 \cdot \mathbb{N}) \times \mathbb{Z})_+ := \mathbb{R}_+ \times \mathbb{Z}.$$

We then define as before, for λ in $\mathbb{R}^p$,

$$g(\lambda) := \prod_{j=1}^d g_j(\lambda).$$

With this convention, we expect the completion of $\tilde{g}$ for $|\cdot|$ to be

$$\hat{g} := \bigsqcup_{\lambda \in \mathbb{R}^p} g(\lambda) \times \{\lambda\}.$$

This is indeed true, as shown by Proposition 4.3.1.

4.2 Description of the results

The main goal of this paper is to establish a familiar Fourier theory on stratified nilpotent Lie groups of step 2. We begin from the well-known representation-theoretic Fourier transform, whose main properties are recalled in Appendix B.2. In particular, this Fourier transform is an intertwining operator for the subelliptic laplacian, acting on functions on g and a rescaled version of the quantum harmonic oscillator, acting on functions on $\mathbb{R}^d$. Since rescaled Hermite functions form an eigenbasis of $L^2(\mathbb{R}^d)$ for the quantum harmonic oscillator, it is natural to expand the representation-theoretic Fourier transform on a rescaled Hermite basis. This idea, borrowed from [86], leads to the definition of a frequency space $\tilde{g}$. This frequency space being noncomplete, we describe its completion $\hat{g}$ and prove some of its properties in Section 4.3.

In Section 4.4, we prove that the so-called 'Fourier kernel' $\mathcal{W}$ does possess a continuous extension from $\tilde{g}$ to $\hat{g}$. Moreover, we give an explicit expression of the kernel at the boundary points of $\hat{g}$ as a power series involving some combinatorial quantities $F_{\ell_1, \ell_2}(b_j)$. These quantities bear some resemblance with the well-known (alternate) Vandermonde convolution in the combinatorics literature (see [100] for more details).

In Section 4.5, we prove a lemma on functions approximating a Dirac mass in their last variable. As a consequence, we are able to define the Fourier transform of functions independent of the central variable, much as we may define the Fourier transform of functions on $\mathbb{R}^n$ independent of one variable.

In Section 4.6, we give an integral representation formula for the Fourier kernel at the boundary, which may be of independent interest. Finding this formula relies on several space-frequency properties of the original Fourier kernel $\mathcal{W}$ akin to the familiar derivation-multiplication duality in the torus or the whole space for the usual, commutative Fourier transform.

The interested reader will find in Appendix B.1 some standard computations and definitions involving the Hermite functions.

4.3 Topology and measure theory on $\hat{g}$

4.3.1 The completion of the frequency space.

We begin by giving some foundation to the theory, by proving that the completion of the natural frequency space $\tilde{g}$ for the distance $|\cdot|$ is indeed what it ought to be.

Proposition 4.3.1. *The closure of $\tilde{g}$ in $(\mathbb{R}_+)^d \times \mathbb{Z}^d \times \mathbb{R}^p$ for the distance $|\cdot|$ is equal to $\hat{g}$.*

Proof. Let $(a(q), b(q), \lambda(q))_{q \in \mathbb{N}}$ be a Cauchy sequence in $\tilde{g}$. As $\tilde{g}$ is a subset of $(\mathbb{R}_+)^d \times \mathbb{Z}^d \times \mathbb{R}^p$, which is complete for the distance $|\cdot|$, there exists $(a, b, \lambda) \in (\mathbb{R}_+)^d \times \mathbb{Z}^d \times \mathbb{R}^p$ such that

$$(a(q), b(q), \lambda(q)) \longrightarrow (a, b, \lambda) \in (\mathbb{R}_+)^d \times \mathbb{Z}^d \times \mathbb{R}^p \text{ as } q \rightarrow \infty.$$

To simplify the exposition of the proof, we look separately at each component $g_j(\lambda)$ for j between 1 and d and distinguish between two cases.

- Assume that $\eta_j(\lambda)$ is nonzero. Then, there exists a strictly positive c such that for all q in $\mathbb{N}$, we have $\eta_j(\lambda(q)) \geq c$. Hence, the two sequences of integers

$$\left(\frac{\eta_j(\lambda(q))^{-1} a_j(q) \pm b_j(q)}{2} \right)_{q \in \mathbb{N}}$$

are also Cauchy sequences. Thus, they are constant for large enough q . Passing to the limit in the equations above give

$$\frac{\eta_j(\lambda)^{-1} a_j \pm b_j}{2} \in \mathbb{N},$$

which exactly says that (a_j, b_j) belongs to $g_j(\lambda)$.

- Assume now that $\eta_j(\lambda) = 0$. Since $(b_j(q))_{q \in \mathbb{N}}$ is a Cauchy sequence of integers, we immediately get $b \in \mathbb{Z}$. On the other hand, as $(a(q))_{q \in \mathbb{N}}$ is a Cauchy sequence in $\mathbb{R}_+$, we have $a \in \mathbb{R}_+$. Thus, we again have $(a, b) \in g_j(\lambda)$, this time in the extended sense.

Up to now, we have shown that $\hat{g}$ contains the closure of $\tilde{g}$ for the Euclidean distance. Conversely, let (a, b, λ_0) be in $\hat{g} \setminus \tilde{g}$ (in particular, λ_0 does not lie in Λ_0). Denote

$$J(\lambda_0) := \{1 \leq j \leq d \mid \eta_j(\lambda_0) = 0\}.$$

Since $\tilde{\Lambda}$ is dense in $\mathbb{R}^p$, there exists a sequence $(\lambda(q))_{q \in \mathbb{N}} \subset \tilde{\Lambda}$ with

$$\lambda(q) \rightarrow \lambda_0 \text{ as } q \rightarrow \infty.$$

Regarding b , we simply let $b(q) = b$ for all q in $\mathbb{N}$. We again distinguish between two cases to define the sequence $(a_j(q))_{q \in \mathbb{N}}$.

- If j is not in $J(\lambda_0)$, there exists $h_j^- \in \mathbb{N}$ such that

$$\frac{a_j - \eta_j(\lambda_0)|b_j|}{2} = h_j^- \eta_j(\lambda_0).$$

Defining for q in $\mathbb{N}$

$$a_j(q) := \eta_j(\lambda(q))(2h_j^- + |b_j|),$$

we see that, for any q in $\mathbb{N}$,

$$\frac{a_j(q) - \eta_j(\lambda(q))|b_j|}{2} \in \eta_j(\lambda(q)) \cdot \mathbb{N}.$$

Hence, for any q in $\mathbb{N}$, we have $(a_j(q), b_j, \lambda(q)) \in g_j(\lambda(q))$ and moreover, as $q \rightarrow \infty$,

$$a_j(q) \rightarrow \eta_j(\lambda_0)(2h_j^- + |b_j|) = a_j.$$

- If j belongs to $J(\lambda_0)$, we use a similar strategy. Let $(h_j^-(q))_{q \in \mathbb{N}}$ be a sequence of integers tending to infinity such that $2h_j^-(q)\eta_j(\lambda(q)) \rightarrow a_j$ as $q \rightarrow \infty$. Similarly to the first case, we define, for q in $\mathbb{N}$,

$$a_j(q) := \eta_j(\lambda(q))(2h_j^-(q) + b_j).$$

In the particular case where $a_j = 0$, we do not want to let $h_j^-(q) \equiv 0$ for all $q \in \mathbb{N}$, so as to ensure that $2h_j^-(q) + b_j \geq 0$ for q big enough. Of course, we have

$$(a_j(q), b_j) \in g_j(\lambda(q))$$

for q big enough and

$$a_j(q) \rightarrow a_j \text{ as } q \rightarrow \infty.$$

Gathering what we did for each coordinate, we have found a sequence $(a(q), b, \lambda(q))_{q \in \mathbb{N}} \subset \tilde{g}$ converging to (a, b, λ) for $|\cdot|$. This closes the proof. $\square$

As a consequence of Proposition 4.3.1, $\hat{g}$ is a closed subset of $(\mathbb{R}_+)^d \times \mathbb{Z}^d \times \mathbb{R}^p$ for the standard Euclidean distance. Hence, it is trivially locally compact.

4.3.2 A measure on $\hat{g}$

Owing to the fibered-looking structure of $\hat{g}$, it seems reasonable to define a measure on it through its disintegration on each $g(\lambda)$ for λ in $\mathbb{R}^p$. In turn, defining a measure on each $g_j(\lambda)$ for j between 1 and d immediately gives rise to a measure on $g(\lambda)$, simply by taking the tensor product. Finally, denoting

$$g_{j,b_j}(\lambda) := \{a_j \in \mathbb{R}_+ \mid (a_j, b_j) \in g_j(\lambda)\},$$

we have the decomposition

$$g_j(\lambda) := \bigsqcup_{b_j \in \mathbb{Z}} g_{j,b_j}(\lambda) \times \{b_j\}.$$

We now construct a measure $d\hat{w}$ on $\hat{g}$ following a bottom-up procedure, starting from the $g_{j,b_j}(\lambda)$ and ending with $\hat{g}$. Let j be an integer between 1 and d and λ be in $\mathbb{R}^p$ such that $\eta_j(\lambda)$ is nonzero. Given $b_j \in \mathbb{Z}$ and θ in $\mathcal{C}_c(g_{j,b_j}(\lambda))$, the measure $d\mu_{j,b_j}^\lambda$ on $g_{j,b_j}(\lambda)$ is defined by the equality

$$\int_{g_{j,b_j}(\lambda)} \theta(a_j) d\mu_{j,b_j}^\lambda(a_j) := 2\eta_j(\lambda) \sum_{a_j \in g_{j,b_j}(\lambda)} \theta(a_j).$$

That is, in this case, $d\mu_{j,b_j}^\lambda$ is simply a rescaled version of the counting measure on the discrete set $g_{j,b_j}(\lambda)$. If η_j vanishes at λ , we simply let $d\mu_{j,b_j}^\lambda$ be the Lebesgue measure on $g_{j,b_j}(\lambda)$, which is none other than $\mathbb{R}_+$. Now, the measure $d\mu_j^\lambda$ is defined as the integration of the family $(d\mu_{j,b_j}^\lambda)_{b_j \in \mathbb{Z}}$ with respect to the counting measure on $\mathbb{Z}$. That is, given $\theta \in \mathcal{C}_c(g_j(\lambda))$, we have

$$\int_{g_j(\lambda)} \theta(a_j, b_j) d\mu_j^\lambda(a_j, b_j) := \sum_{b_j \in \mathbb{Z}} \int_{g_{j,b_j}(\lambda)} \theta(a_j, b_j) d\mu_{j,b_j}^\lambda(a_j).$$

On $g(\lambda)$, we define the measure $d\mu^\lambda$ as the tensor product of the $d\mu_j^\lambda$, that is

$$d\mu^\lambda := \bigotimes_{j=1}^d d\mu_j^\lambda.$$

Then, the measure $d\hat{w}$ on $\hat{g}$ is the integration of the family $(d\mu^\lambda)_{\lambda \in \mathbb{R}^p}$ with respect to the Lebesgue measure on $\mathbb{R}^p$. That is, for θ in $\mathcal{C}_c(\hat{g})$, we have

$$\int_{\hat{g}} \theta(\hat{w}) d\hat{w} := \int_{\mathbb{R}^p} \left(\int_{g(\lambda)} \theta(a, b, \lambda) d\mu^\lambda(a, b) \right) d\lambda.$$

In the case of the Heisenberg group $\mathbb{H}^d$, since all the η_j for j between 1 and d are equal to $|\cdot|$, the description of the frequency is simpler than in the general case. Indeed, the fiber over a nonzero λ writes

$$\mathbb{H}^d(\lambda) = \left\{ (a, b) \in \mathbb{R}_+^d \times \mathbb{Z}^d \mid \frac{a \pm |\lambda|b}{2} \in |\lambda| \cdot \mathbb{N}^d \right\}.$$

In particular, it is independant of λ as long as λ is nonzero. Hence, the frequency space over all nonzero λ 's tensorizes as

$$\tilde{\mathbb{H}}^d = \mathbb{H}^d(1) \times \mathbb{R} \setminus \{0\}.$$

Over the point 0, the fiber is

$$\mathbb{H}^d(0) = (\mathbb{R}_+ \times \mathbb{Z})^d.$$

Finally, for any nonzero λ , the discrete set $\mathbb{H}^d(\lambda)$ is endowed with the counting measure. On $\mathbb{H}^d(0)$, it becomes the tensor product of the Lebesgue measure on $(\mathbb{R}_+)^d$ and the counting measure on $\mathbb{Z}^d$. We now turn to the other explicit example of a 2-step group we provided in the introduction, which we denote by G . We will only sketch the main elements of its frequency space without delving into unnecessary details. If λ is in $\mathbb{R}^2$ and is such that $|\lambda_1|$ does not equal $|\lambda_2|$, the fibers of the frequency space of G over λ are

$$g_-(\lambda) = \left\{ (a_-, b_-) \in \mathbb{R}_+ \times \mathbb{Z} \mid \frac{a_- \pm ||\lambda_1| - |\lambda_2||b_-}{2} \in ||\lambda_1| + |\lambda_2|| \cdot \mathbb{N} \right\}$$

and

$$g_+(\lambda) = \left\{ (a_+, b_+) \in \mathbb{R}_+ \times \mathbb{Z} \mid \frac{a_+ \pm ||\lambda_1| + |\lambda_2||b_+}{2} \in ||\lambda_1| + |\lambda_2|| \cdot \mathbb{N} \right\}.$$

For such λ 's, the discrete fibers are again endowed with the counting measure. The degeneracy of the fibers and the measures around a nonzero λ for which $|\lambda_1|$ and $|\lambda_2|$ are equal are left to the interested reader, along with the case of the point 0. The relevance of these successive definitions is summarized by the following proposition.

Proposition 4.3.2. *The measure field $\lambda \mapsto d\mu^\lambda$ is weak-* continuous on $\mathbb{R}^p$.*

The proof of this proposition is immediate once we have the next lemma at hand; for this reason, we will only prove the lemma.

Lemma 4.3.1. *Let λ_0 in Λ_0 with, for instance, $\eta_j(\lambda_0) = 0$. Let $b_j \in \mathbb{Z}$. Then, if $\lambda \rightarrow \lambda_0$, we have*

$$d\mu_{j,b_j}^\lambda \rightharpoonup^* d\mu_{j,b_j}^{\lambda_0}$$

in the weak sense of measures.

Proof. Let θ be in $\mathcal{C}_c(\mathbb{R}_+)$. By definition of $d\mu_{j,b_j}^\lambda$, we have

$$\int_{\mathbb{R}_+} \theta(a_j) d\mu_{j,b_j}^\lambda(a_j) = 2\eta_j(\lambda) \sum_{n \in \mathbb{N}} \theta(\eta_j(\lambda)(2n + |b_j|)).$$

Thanks to the continuity of θ and the obvious fact that $\eta_j(\lambda)|b_j| \rightarrow 0$ as $\lambda \rightarrow \lambda_0$, we have

$$\int_{\mathbb{R}_+} \theta(a_j) d\mu_{j,b_j}^\lambda(a_j) = 2\eta_j(\lambda) \sum_{n \in \mathbb{N}} \theta(2\eta_j(\lambda)n) + o(1).$$

Since θ is continuous and compactly supported, the above sum is nothing else than a Riemann sum. Hence, as λ tends to λ_0 , we have

$$\lim_{\lambda \rightarrow \lambda_0} 2\eta_j(\lambda) \sum_{n \in \mathbb{N}} \theta(2\eta_j(\lambda)n) = \int_{\mathbb{R}_+} \theta(a_j) da_j = \langle d\mu_{j,b_j}^{\lambda_0}, \theta \rangle.$$

□

4.4 A study of the Fourier kernel.

Let us define the Fourier kernel

$$\Theta : (\hat{w}, w) \mapsto e^{i\langle \lambda, s \rangle} \mathcal{W}(\hat{w}, x, y).$$

In this section we study closely the properties of Θ . We begin by proving some identities linking its regularity in the spatial variables with its decay in the Fourier variables. These identities are the justification of the 'regularity implies decay' motto, common in (commutative) Fourier analysis. Since the computations performed in this section rely on properties of the (rescaled) Hermite functions, we temporarily parametrize $\tilde{g}$ by $\tilde{g}_E$. Explicitly, we let, for (a, b, λ) in $\tilde{g}$,

$$n := \frac{\eta(\lambda)^{-1} \cdot a - b}{2} \quad \text{and} \quad m := \frac{\eta(\lambda)^{-1} \cdot a + b}{2}.$$

4.4.1 Regularity and decay of Θ

Applying the vector fields X_j and Y_j to Θ , we get

$$X_j(\Theta)(\hat{w}, w) = e^{i\langle \lambda, s \rangle} \left(\partial_{x_j} \mathcal{W} + \frac{1}{2} i \eta_j(\lambda) y_j \mathcal{W} \right) (\hat{w}, x, y)$$

and

$$Y_j(\Theta)(\hat{w}, w) = e^{i\langle \lambda, s \rangle} \left(\partial_{y_j} \mathcal{W} - \frac{1}{2} i \eta_j(\lambda) x_j \mathcal{W} \right) (\hat{w}, x, y).$$

After some computations, we find that

$$\left(\partial_{x_j} \mathcal{W} + \frac{1}{2} i \eta_j(\lambda) y_j \mathcal{W} \right) (\hat{w}, x, y) = - \int_{\mathbb{R}^d} e^{i\langle \eta(\lambda) \cdot \xi, y \rangle} H_{m, \eta(\lambda)} \left(\xi + \frac{x}{2} \right) \partial_{\xi_j} \left(H_{n, \eta(\lambda)} \left(\xi - \frac{x}{2} \right) \right) d\xi.$$

Similarly,

$$\begin{aligned} \left(\partial_{y_j} \mathcal{W} - \frac{1}{2} i \eta_j(\lambda) x_j \mathcal{W} \right) (\hat{w}, x, y) \\ = i \eta_j(\lambda) \int_{\mathbb{R}^d} e^{i\langle \eta(\lambda) \cdot \xi, y \rangle} H_{m, \eta(\lambda)} \left(\xi + \frac{x}{2} \right) \left(\xi_j - \frac{1}{2} x_j \right) \left(H_{n, \eta(\lambda)} \left(\xi - \frac{x}{2} \right) \right) d\xi. \end{aligned}$$

In particular, owing to Equation (B.5), we have

$$(X_j^2 + Y_j^2)(\Theta)(\hat{w}, w) = (-2n_j + 1)\eta_j(\lambda)\Theta(\hat{w}, w). \quad (4.3)$$

Arguing similarly for the right-invariant vector fields, we readily get

$$(\tilde{X}_j^2 + \tilde{Y}_j^2)(\Theta)(\hat{w}, w) = (-2m_j + 1)\eta_j(\lambda)\Theta(\hat{w}, w).$$

Subtracting the two lines gives

$$(X_j^2 + Y_j^2 - \tilde{X}_j^2 - \tilde{Y}_j^2)(\Theta)(\hat{w}, w) = 2\eta_j(\lambda)(m_j - n_j)\Theta(\hat{w}, w).$$

On the other hand, direct computations give

$$X_j^2 - \tilde{X}_j^2 = -2 \sum_k (\mathcal{U}_k \cdot Z)_j \partial_{x_j} \partial_{s_k},$$

whence

$$(X_j^2 - \tilde{X}_j^2)(\Theta)(\hat{w}, w) = -2i(\mathcal{U}^{(\lambda)} \cdot Z)_j \partial_{x_j} \Theta(\hat{w}, w) = -2i\eta_j(\lambda)y_j \partial_{x_j} \Theta(\hat{w}, w).$$

Similarly,

$$(Y_j^2 - \tilde{Y}_j^2)(\Theta)(\hat{w}, w) = 2i\eta_j(\lambda)x_j \partial_{y_j} \Theta(\hat{w}, w).$$

Denoting $\mathcal{T}_j := x_j \partial_{y_j} - y_j \partial_{x_j}$, we have shown the equality

$$2\eta_j(\lambda)(m_j - n_j)\Theta(\hat{w}, w) = 2i\eta_j(\lambda)\mathcal{T}_j(\Theta)(\hat{w}, w),$$

which becomes

$$(m_j - n_j)\mathcal{W}(\hat{w}, w) = i\mathcal{T}_j(\mathcal{W})(\hat{w}, w). \quad (4.4)$$

Finally, it is clear that

$$\nabla_s(\Theta)(\hat{w}, w) = i\lambda\Theta(\hat{w}, w). \quad (4.5)$$

Equations (4.3), (4.4) and (4.5) justify the choice of the distance ρ_E on $\tilde{g}_E$. Together, they account for all decay aspects of Θ in the variable $\hat{w}$.

4.4.2 Continuous extension of $\mathcal{W}$ to $\hat{g}$

To study the continuity of $\mathcal{W}$, first write

$$\mathcal{W}(\hat{w}, x, y) = e^{\frac{i}{2}\langle \eta(\lambda) \cdot x, y \rangle} \widetilde{\mathcal{W}}(\hat{w}, x, y).$$

The new function $\widetilde{\mathcal{W}}$ is a tensor product, as $\mathcal{W}$ was. Denoting

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) := \int_{\mathbb{R}} e^{i\eta_j(\lambda)\xi_j y_j} H_{m_j, \eta_j(\lambda)}(\xi_j + x_j) H_{n_j, \eta_j(\lambda)}(\xi_j) d\xi_j.$$

we only have to exhibit a continuous extension of $\widetilde{\mathcal{W}}_j$ to (bounded sets of) $\hat{g}$. Let us begin with a series expansions for $\widetilde{\mathcal{W}}_j$.

Proposition 4.4.1. *For any $\lambda \in \mathbb{R}^p$, $(a_j, b_j) \in g_j(\lambda)$ and $x_j, y_j \in \mathbb{R}$, we have*

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) = \sum_{\ell_1, \ell_2=0}^{\infty} \eta_j(\lambda)^{\frac{\ell_1+\ell_2}{2}} \frac{(iy_j)^{\ell_1} x_j^{\ell_2}}{\ell_1! \ell_2!} \left(M_j^{\ell_1} H_{m_j} \mid H_{n_j}^{(\ell_2)} \right)_{L^2(\mathbb{R})}.$$

Since we are interested in bounded subsets of $\tilde{g}$, let us define, for $r > 0$,

$$\mathcal{B}_j(r) := \{(a_j, b_j, \lambda, x_j, y_j) \in g_j(\lambda) \times \{\lambda\} \times \mathbb{R}^2 \text{ s.t. } |a_j| + |b_j|^2 + |\lambda|^2 + |x_j|^2 + |y_j|^2 \leq r^2\}.$$

We will, in addition, need to bound locally the function η_j . Define

$$C_{\eta_j} := \sup_{|\lambda|=1} \eta_j(\lambda),$$

which is finite thanks to the continuity of η_j . The homogeneity of η_j entails for all $\lambda \in \mathbb{R}^p$ the bound

$$\eta_j(\lambda) \leq C_{\eta_j} |\lambda|.$$

The proof of Proposition 4.4.1 requires the following lemma.

Lemma 4.4.1. *For any $r > 0$, the function*

$$(a_j, b_j, \lambda, x_j, y_j) \mapsto \sum_{\ell_1, \ell_2=0}^{\infty} \frac{\eta_j(\lambda)^{\frac{\ell_1+\ell_2}{2}} |y_j|^{\ell_1} |x_j|^{\ell_2}}{\ell_1! \ell_2!} \|H_{m_j}^{(\ell_2)}\|_{L^2(\mathbb{R})} \|M_j^{\ell_1} H_{n_j}\|_{L^2(\mathbb{R})}$$

is well-defined and the underlying series converges normally, as a function of $(a_j, b_j, \lambda, x_j, y_j)$, on $\mathcal{B}_j(r)$.

Proof. Arguing by induction (see the details in the Appendix, Lemma B.1.1), we get the bounds

$$\|M_j^{\ell_1} H_{n_j}\|_{L^2(\mathbb{R})} \leq (2n_j + 2\ell_1)^{\frac{\ell_1}{2}}$$

and

$$\|H_{m_j}^{(\ell_2)}\|_{L^2(\mathbb{R})} \leq (2m_j + 2\ell_2)^{\frac{\ell_2}{2}}.$$

Thus,

$$\frac{\eta_j(\lambda)^{\frac{\ell_1}{2}} |y_j|^{\ell_1}}{\ell_1!} \|M_j^{\ell_1} H_{n_j}\|_{L^2(\mathbb{R})} \leq \frac{r^{\ell_1}}{\ell_1!} (2r + 2C_{\eta_j} r \ell_1)^{\frac{\ell_1}{2}} \leq \frac{(2C_{\eta_j} r^{\frac{3}{2}})^{\ell_1}}{\ell_1!} (1 + \ell_1)^{\frac{\ell_1}{2}}.$$

Similarly,

$$\frac{\eta_j(\lambda)^{\frac{\ell_2}{2}} |x_j|^{\ell_2}}{\ell_2!} \|H_{m_j}^{(\ell_2)}\|_{L^2(\mathbb{R})} \leq \frac{r^{\ell_2}}{\ell_2!} (2r + 2C_{\eta_j} r \ell_2)^{\frac{\ell_2}{2}} \leq \frac{(2C_{\eta_j} r^{\frac{3}{2}})^{\ell_2}}{\ell_2!} (1 + \ell_2)^{\frac{\ell_2}{2}}.$$

Owing to the Stirling equivalent, we have

$$\sum_{\ell_1, \ell_2=0}^{\infty} \frac{(2C_{\eta_j} r^{\frac{3}{2}})^{\ell_1+\ell_2}}{\ell_1! \ell_2!} (1 + \ell_1)^{\frac{\ell_1}{2}} (1 + \ell_2)^{\frac{\ell_2}{2}} < \infty,$$

thereby proving the desired convergence. $\square$

We now return to the proof of Proposition 4.4.1.

Proof. [Proof of Proposition 4.4.1] We begin by expanding the exponential in its power series. We have

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) = \int_{\mathbb{R}} \sum_{\ell_1=0}^{\infty} \frac{(i\eta_j(\lambda)\xi_j y_j)^{\ell_1}}{\ell_1!} H_{m_j, \eta_j(\lambda)}(\xi_j + x_j) H_{n_j, \eta_j(\lambda)}(\xi_j) d\xi_j.$$

Since H_{m_j} is an entire function, we may expand it as

$$H_{m_j, \eta_j(\lambda)}(\xi_j + x_j) = \sum_{\ell_2=0}^{\infty} \frac{(\eta_j(\lambda)^{\frac{1}{2}} x_j)^{\ell_2}}{\ell_2!} \left(H_{m_j}^{(\ell_2)} \right)_{\eta_j(\lambda)}(\xi_j)$$

and get

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) = \int_{\mathbb{R}} \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \frac{\eta_j(\lambda)^{\frac{\ell_1+\ell_2}{2}} (iy_j)^{\ell_1} x_j^{\ell_2}}{\ell_1! \ell_2!} \left(H_{m_j}^{(\ell_2)} \right)_{\eta_j(\lambda)}(\xi_j) (M_j^{\ell_1} H_{n_j, \eta_j(\lambda)})(\xi_j) d\xi_j.$$

Rescaling the integration variable, we also have

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) = \int_{\mathbb{R}} \sum_{\ell_1=0}^{\infty} \sum_{\ell_2=0}^{\infty} \frac{\eta_j(\lambda)^{\frac{\ell_1+\ell_2}{2}} (iy_j)^{\ell_1} x_j^{\ell_2}}{\ell_1! \ell_2!} H_{m_j}^{(\ell_2)}(\xi_j) (M_j^{\ell_1} H_{n_j})(\xi_j) d\xi_j.$$

Thanks to the lemma, Fubini's theorem applies and allows us to exchange the integrals with the sums. The series expansion of $\widetilde{\mathcal{W}}_j$ is now justified. $\square$

For $(\ell_1, \ell_2) \in \mathbb{N}^2$ and $1 \leq j \leq d$, let

$$\mathcal{H}_{\ell_1, \ell_2, j} := \begin{cases} \bigsqcup_{\lambda \in \widetilde{\Lambda}} g_j(\lambda) \times \{\lambda\} & \longrightarrow \mathbb{R} \\ (a_j, b_j, \lambda) & \longmapsto \eta_j(\lambda)^{\frac{\ell_1+\ell_2}{2}} \left(M^{\ell_1} H_{m_j} \mid H_{n_j}^{(\ell_2)} \right)_{L^2(\mathbb{R})}. \end{cases}$$

With the above series expansion for $\widetilde{\mathcal{W}}_j$ at hand, we study the $(\mathcal{H}_{\ell_1, \ell_2, j})_{\ell_1, \ell_2 \in \mathbb{N}}$. Defining for $k \in \mathbb{Z}$

$$F_{\ell_1, \ell_2}(k) := \sum_{\ell'_1=0}^{\ell_1} \sum_{\ell'_2=0}^{\ell_2} (-1)^{\ell_2-\ell'_2} \binom{\ell_1}{\ell'_1} \binom{\ell_2}{\ell'_2} \mathbf{1}_{\{2(\ell'_1+\ell'_2)=k+\ell_1+\ell_2\}},$$

we prove the following.

Proposition 4.4.2. *For any $\ell_1, \ell_2 \in \mathbb{N}$, the function $\mathcal{H}_{\ell_1, \ell_2, j}$ is continuous on $\bigsqcup_{\lambda \in \widetilde{\Lambda}} g_j(\lambda) \times \{\lambda\}$. Moreover, given $\lambda_0 \in \eta_j^{-1}(\{0\})$, if*

$$(a_j, b_j, \lambda) \rightarrow (a_j, b_j, \lambda_0) \in \mathbb{R}_+ \times \mathbb{Z} \times \eta_j^{-1}(\{0\}),$$

then

$$\mathcal{H}_{\ell_1, \ell_2, j}(a_j, b_j, \lambda) \longrightarrow \left(\frac{a_j}{4} \right)^{\frac{\ell_1+\ell_2}{2}} F_{\ell_1, \ell_2}(b_j).$$

In order to handle points close to the zero set of η_j , we will need the following lemma. We refer the reader to Appendix B.1 for the definition of the creation and annihilation operators C_j and A_j .

Lemma 4.4.2. *Given $\ell \in \mathbb{N}$, assume that $\eta_j(\lambda) \rightarrow 0$ and $\eta_j(\lambda)n_j \rightarrow \frac{a_j}{2} \in \mathbb{R}_+$. Then*

$$\left\| \eta_j(\lambda)^{\frac{\ell}{2}} \left(\frac{A_j \pm C_j}{2} \right)^{\ell} H_{n_j} - \left(\frac{a_j}{4} \right)^{\frac{\ell}{2}} \sum_{\ell'=0}^{\ell} (\pm 1)^{\ell'} \binom{\ell}{\ell'} H_{n_j+2\ell'-\ell} \right\|_{L^2(\mathbb{R})} \longrightarrow 0.$$

Proof. Let us define

$$\begin{aligned}\mathcal{R}_{\ell,n_j,1}^{\pm} &:= \eta_j(\lambda)^{\frac{\ell}{2}} (A_j \pm C_j)^{\ell} H_{n_j}, \\ \mathcal{R}_{\ell,n_j,2}^{\pm} &:= a_j^{\frac{\ell}{2}} \sum_{\ell'=0}^{\ell} (\pm 1)^{\ell'} \binom{\ell}{\ell'} H_{n_j+2\ell'-\ell}.\end{aligned}$$

We obviously have $\mathcal{R}_{0,n_j,1}^{\pm} = \mathcal{R}_{0,n_j,2}^{\pm} = H_{n_j}$ and thus, $\|\mathcal{R}_{0,n_j,1}^{\pm} - \mathcal{R}_{0,n_j,2}^{\pm}\|_{L^2(\mathbb{R})} = 0$. By definition, we also have

$$\sqrt{\eta_j(\lambda)}(A_j \pm C_j)\mathcal{R}_{\ell,n_j,1}^{\pm} = \mathcal{R}_{\ell+1,n_j,1}^{\pm}.$$

It remains to study the effect of $\sqrt{\eta_j(\lambda)}(A_j \pm C_j)$ on $\mathcal{R}_{\ell,n_j,2}^{\pm}$ to conclude. Recalling Equations (B.1) and (B.2) in the Appendix along with our assumptions on $\eta_j(\lambda)$ and n_j , we have

$$\sqrt{\eta_j(\lambda)}A_j H_{n_j+2\ell'-\ell} = \sqrt{\eta_j(\lambda)} \left(\sqrt{2(n_j+2\ell'-\ell)} H_{n_j+2\ell'-\ell-1} \right) = (\sqrt{a_j} + o(1)) H_{n_j+2\ell'-\ell-1}$$

and

$$\sqrt{\eta_j(\lambda)}C_j H_{n_j+2\ell'-\ell} = \sqrt{\eta_j(\lambda)} \left(\sqrt{2(n_j+2\ell'-\ell+1)} H_{n_j+2\ell'-\ell+1} \right) = (\sqrt{a_j} + o(1)) H_{n_j+2\ell'-\ell+1}.$$

In particular, we have

$$\begin{aligned}& \left\| \sqrt{\eta_j(\lambda)}(A_j \pm C_j)(\mathcal{R}_{\ell,n_j,1}^{\pm} - \mathcal{R}_{\ell,n_j,2}^{\pm}) \right\|_{L^2(\mathbb{R})} \\ & \leq (\sqrt{a_j} + o(1)) \left(\|\mathcal{R}_{\ell,n_j-1,1}^{\pm} - \mathcal{R}_{\ell,n_j-1,2}^{\pm}\|_{L^2(\mathbb{R})} + \|\mathcal{R}_{\ell,n_j+1,1}^{\pm} - \mathcal{R}_{\ell,n_j+1,2}^{\pm}\|_{L^2(\mathbb{R})} \right). \quad (4.6)\end{aligned}$$

Hence,

$$\sqrt{\eta_j(\lambda)}(A_j \pm C_j)\mathcal{R}_{\ell,n_j,2}^{\pm} = a_j^{\frac{\ell+1}{2}} \sum_{\ell'=0}^{\ell} (\pm 1)^{\ell'} \binom{\ell}{\ell'} (H_{n_j+2\ell'-\ell-1} \pm H_{n_j+2\ell'-\ell+1}) + o(1)_{L^2(\mathbb{R})}.$$

Shifting the index of summation in the second sum and using Pascal's rule gives

$$\sum_{\ell'=0}^{\ell} (\pm 1)^{\ell'} \binom{\ell}{\ell'} (H_{n_j+2\ell'-\ell-1} \pm H_{n_j+2\ell'-\ell+1}) = \sum_{\ell'=0}^{\ell+1} (\pm 1)^{\ell'} \binom{\ell+1}{\ell'} H_{n_j+2\ell'-\ell-1},$$

showing, as desired, that

$$\sqrt{\eta_j(\lambda)}(A_j \pm C_j)\mathcal{R}_{\ell,n_j,2}^{\pm} = \mathcal{R}_{\ell+1,n_j,2}^{\pm} + o(1)_{L^2(\mathbb{R})}.$$

Arguing by induction on ℓ and using (4.6), the lemma is proved. $\square$

Proof. [Proof of Proposition 4.4.2] The continuity of $\mathcal{H}_{\ell_1,\ell_2,j}$ on $\bigsqcup_{\lambda \in \tilde{\Lambda}} g_j(\lambda) \times \{\lambda\}$ is easily established. Indeed, if (a'_j, b'_j, λ') is sufficiently close to (a_j, b_j, λ) (depending on the values of $a_j, b_j, \eta_j(\lambda)$) and $\eta_j(\lambda) \neq 0$, the fact that n_j, m_j, n'_j, m'_j are integers forces $n_j = n'_j$ and $m_j = m'_j$. The continuity of $\mathcal{H}_{\ell_1,\ell_2,j}$ at the point (a_j, b_j, λ) follows from that of η_j on $\tilde{\Lambda}$. We now turn to points belonging

to the boundary of $\bigsqcup_{\lambda \in \tilde{\Lambda}} g_j(\lambda) \times \{\lambda\}$. As a corollary of Lemma 4.4.2, for any $1 \leq j \leq d$ and $(\ell_1, \ell_2, b_j) \in \mathbb{N}^2 \times \mathbb{Z}$, we have

$$\mathcal{H}_{\ell_1, \ell_2, j}(a_j, b_j, \lambda) = \left(\frac{a_j}{4}\right)^{\frac{\ell_1 + \ell_2}{2}} \times \sum_{\ell'_1=0}^{\ell_1} \sum_{\ell'_2=0}^{\ell_2} (-1)^{\ell'_2} \binom{\ell_1}{\ell'_1} \binom{\ell_2}{\ell'_2} \left(H_{n_j + \ell_1 - 2\ell'_1} \mid H_{n_j + b_j + \ell_2 - 2\ell'_2} \right)_{L^2(\mathbb{R})} + o(1)$$

as $\eta_j(\lambda) \rightarrow 0$ with $\eta_j(\lambda)n_j \rightarrow \frac{a_j}{2} \in \mathbb{R}_+$. Performing the change of index $\ell'_2 \leftarrow \ell_2 - \ell'_2$ and recalling that the Hermite functions form an orthonormal family of $L^2(\mathbb{R})$, we get

$$\mathcal{H}_{\ell_1, \ell_2, j}(a_j, b_j, \lambda) \longrightarrow \left(\frac{a_j}{4}\right)^{\frac{\ell_1 + \ell_2}{2}} F_{\ell_1, \ell_2}(b_j)$$

as $\eta_j(\lambda) \rightarrow 0$ with $\eta_j(\lambda)n_j \rightarrow \frac{a_j}{2} \in \mathbb{R}_+$. □

An immediate corollary of Proposition 4.4.2 and Lemma 4.4.1 is that, as

$$(a_j, b_j, \lambda) \rightarrow (a_j, b_j, \lambda_0) \in g_j(\lambda) \times \eta_j^{-1}(\{0\}),$$

we have

$$\widetilde{\mathcal{W}}_j(a_j, b_j, \lambda, x_j, y_j) \longrightarrow \sum_{\ell_1, \ell_2=0}^{\infty} \left(\frac{a_j}{4}\right)^{\frac{\ell_1 + \ell_2}{2}} F_{\ell_1, \ell_2}(b_j) \frac{(iy_j)^{\ell_1} x_j^{\ell_2}}{\ell_1! \ell_2!}.$$

4.5 The case of functions independant of the central variable.

The goal of this section is to define properly what the Fourier transform of a function independant of the central variable should be. We begin by a convergence lemma for functions integrated against approximate Dirac masses around some boundary point $\lambda \in \Lambda_0$.

Lemma 4.5.1. *Let $\chi : \mathbb{R}^p \rightarrow \mathbb{R}^p$ be compactly supported and integrable, with*

$$\int_{\mathbb{R}^p} \chi(\lambda) d\lambda = 1.$$

Let $\lambda_0 \in \mathbb{R}^p$. Let θ be in $\mathcal{C}_c(\hat{g})$. Then, as $\varepsilon \rightarrow 0$,

$$I_\varepsilon := \int_{\mathbb{R}^n} \frac{1}{\varepsilon^p} \chi\left(\frac{\lambda - \lambda_0}{\varepsilon}\right) \theta(\hat{w}) d\hat{w} \longrightarrow \langle d\mu^{\lambda_0}, \theta(\cdot, \cdot, \lambda_0) \rangle.$$

Proof. With an obvious change of variable, we have

$$I_\varepsilon = \int_{\mathbb{R}^p} \chi(\lambda) \left(\int_{g(\lambda_0 + \varepsilon\lambda)} \theta(a, b, \lambda_0 + \varepsilon\lambda) d\mu^{\lambda_0 + \varepsilon\lambda}(a, b) \right) d\lambda.$$

Since θ is continuous and compactly supported (hence, uniformly continuous), we have

$$\|\theta(\cdot, \cdot, \lambda_0 + \varepsilon\cdot) - \theta(\cdot, \cdot, \lambda_0)\|_{L^\infty(\hat{g})} \longrightarrow 0$$

as $\varepsilon \rightarrow 0$. Therefore, from the weak- $*$ continuity of the map $\lambda \mapsto d\mu^\lambda$, for any $\lambda \in \mathbb{R}^p$ there holds

$$\int_{g(\lambda_0 + \varepsilon\lambda)} \theta(a, b, \lambda_0 + \varepsilon\lambda) d\mu^{\lambda_0 + \varepsilon\lambda}(a, b) \longrightarrow \int_{g(\lambda_0)} \theta(a, b, \lambda_0) d\mu^{\lambda_0}(a, b)$$

as $\varepsilon \rightarrow 0$. Thanks to the compactness of the supports of both θ and χ , we may apply the dominated convergence theorem to get that, as $\varepsilon \rightarrow 0$,

$$I_\varepsilon \longrightarrow \int_{\mathbb{R}^p} \chi(\lambda) \left(\int_{g(\lambda_0)} \theta(a, b, \lambda_0) d\mu^{\lambda_0}(a, b) \right) d\lambda = \int_{g(\lambda_0)} \theta(a, b, \lambda_0) d\mu^{\lambda_0}(a, b).$$

□

Remark. The conclusion of the above theorem remains true if one replaces the compactness of the support of θ by the assumptions

$$\sup_{\lambda \in \mathbb{R}^p} \int_{g(\lambda)} |\theta(a, b, \lambda)| d\mu^\lambda(a, b) < \infty$$

and

$$\limsup_{R \rightarrow \infty} \sup_{\lambda \in \mathbb{R}^p} \int_{g(\lambda)} |\theta(a, b, \lambda)| \mathbf{1}_{\{|a|^2 + |b|^2 \geq R^2\}} d\mu^\lambda(a, b) = 0.$$

An example of admissible function is given for $\alpha > d$ by

$$\theta_\alpha : (a, b, \lambda) \mapsto (1 + |a|^2 + |b|^2)^{-\alpha}.$$

For $f \in L^1(\mathbb{R}^{2d})$ and $(a, b, \lambda) \in \hat{g}$, we define

$$\mathcal{G}_g^\lambda(f)(a, b) = \int_{\mathbb{R}^{2d}} \overline{\mathcal{W}}(a, b, \lambda, Z) f(Z) dZ.$$

Theorem 4.5.1. Let $\lambda_0 \in \Lambda_0$. Let $\chi \in \mathcal{S}(\mathbb{R}^p)$ be such that $\chi(0) = 1$ and $\mathcal{F}_{\mathbb{R}^p}(\chi)$ is compactly supported. Then, for any $f \in L^1(\mathbb{R}^{2d})$, we have

$$\mathcal{F}_g(f \otimes e^{i\langle \lambda_0, \cdot \rangle} \chi(\varepsilon \cdot)) \rightharpoonup^* (2\pi)^p \mathcal{G}_g^{\lambda_0}(f) d\mu^{\lambda_0} \quad (4.7)$$

as $\varepsilon \rightarrow 0$, in the weak sense of measures.

Proof. Let $\theta \in \mathcal{C}_c(\hat{g})$. By definition of the Fourier transform, we have

$$\int_{\hat{g}} \mathcal{F}_g(f \otimes e^{i\langle \lambda_0, \cdot \rangle} \chi(\varepsilon \cdot))(\hat{w}) \theta(\hat{w}) d\hat{w} = \int_{\mathbb{R}^p} \varepsilon^{-p} \hat{\chi}(\varepsilon^{-1}(\lambda - \lambda_0)) \left(\int_{g(\lambda)} (G\theta)(a, b, \lambda) d\mu^\lambda(a, b) \right) d\lambda,$$

where we abbreviated $\mathcal{F}_{\mathbb{R}^p}(\chi)$ into $\hat{\chi}$ for the sake of readability and defined the function G by

$$G(a, b, \lambda) := \int_{\mathbb{R}^n} f(Z) \overline{\mathcal{W}}(a, b, \lambda, Z) dZ.$$

The assumptions on χ entail in particular that

$$\int_{\mathbb{R}^p} \hat{\chi}(\lambda) d\lambda = (2\pi)^p.$$

Since f belongs to $L^1(\mathbb{R}^{2d})$, G is continuous and hence, the product function $G\theta$ lies in $\mathcal{C}_c(\hat{g})$. Applying Lemma 4.5.1 to $G\theta$ yields, as $\varepsilon \rightarrow 0$,

$$\int_{\hat{g}} \mathcal{F}_g(f \otimes e^{i\langle \lambda_0, \cdot \rangle} \chi(\varepsilon \cdot))(\hat{w}) \theta(\hat{w}) d\hat{w} \longrightarrow (2\pi)^p \int_{g(\lambda_0)} G(a, b, \lambda_0) \theta(a, b, \lambda_0) d\mu^{\lambda_0}(a, b),$$

It only remains to notice that, by definition,

$$G(a, b, \lambda_0) = \mathcal{G}_g^{\lambda_0}(f)(a, b).$$

□

4.6 Computing the kernel at the boundary.

4.6.1 Preliminary identities

Given $(a_j, x_j, y_j, b_j) \in \mathbb{R}_+ \times \mathbb{R}^2 \times \mathbb{Z}$, we let

$$\mathcal{K}(a_j, x_j, y_j, b_j) := \sum_{\ell_1, \ell_2=0}^{\infty} \left(\frac{a_j}{4}\right)^{\frac{\ell_1+\ell_2}{2}} F_{\ell_1, \ell_2}(b_j) \frac{(iy_j)^{\ell_1} x_j^{\ell_2}}{\ell_1! \ell_2!}.$$

Our aim is to find a closed form for the above sum. To this aim, we list a few identities satisfied by this function, which will eventually help us in computing an integral form for $\mathcal{K}$.

Proposition 4.6.1. *For $a_j \in \mathbb{R}_+$, $x_j, y_j, x'_j, y'_j \in \mathbb{R}$ and $b_j \in \mathbb{Z}$, there holds*

1. $\mathcal{K}(0, x_j, y_j, b_j) = \delta_{0, b_j}$,
2. $\mathcal{K}(a_j, x_j, -y_j, b_j) = \overline{\mathcal{K}(a_j, x_j, y_j, b_j)}$,
3. $\mathcal{K}(a_j, -x_j, y_j, -b_j) = \mathcal{K}(a_j, x_j, y_j, b_j)$,
4. $\mathcal{K}(a_j, x_j, -y_j, -b_j) = (-1)^{b_j} \mathcal{K}(a_j, x_j, y_j, b_j)$,
5. $-\Delta_{x_j, y_j} \mathcal{K}(a_j, x_j, y_j, b_j) = a_j \mathcal{K}(a_j, x_j, y_j, b_j)$,
6. $b_j \mathcal{K}(a_j, x_j, y_j, b_j) = i(x_j \partial_{y_j} - y_j \partial_{x_j}) \mathcal{K}(a_j, x_j, y_j, b_j)$,
- 7.

$$\mathcal{K}(a_j, x_j + x'_j, y_j + y'_j, b_j) = \sum_{b'_j \in \mathbb{Z}} \mathcal{K}(a_j, x_j, y_j, b_j - b'_j) \mathcal{K}(a_j, x'_j, y'_j, b'_j).$$

8. $\frac{b_j^2}{a_j} \mathcal{K}(a_j, x_j, y_j, b_j) =$

$$(|x_j|^2 + |y_j|^2) \mathcal{K}(a_j, x_j, y_j, b_j) + a_j \partial_{a_j}^2 \mathcal{K}(a_j, x_j, y_j, b_j) + 2\partial_{a_j} \mathcal{K}(a_j, x_j, y_j, b_j).$$

We begin by proving the easiest ones and postpone the last two.

Proof. [Proof of Identities (1) – (4)] Identity (1) stems from

$$F_{0,0}(b_j) = \delta_{0, b_j},$$

which is obvious. Identity (2) follows directly from the definition. Thanks to the relation

$$F_{\ell_1, \ell_2}(-b_j) = (-1)^{\ell_2} F_{\ell_1, \ell_2}(b_j),$$

Identity (3) ensues. Finally, since $F_{\ell_1, \ell_2}(b_j) = 0$ for $b_j + \ell_1 + \ell_2$ odd, we also have

$$F_{\ell_1, \ell_2}(-b_j) = (-1)^{b_j + \ell_1} F_{\ell_1, \ell_2}(b_j),$$

which in turn implies Identity (4). □

Proof. [Proof of Identities (5) and (6)] To prove Identity (5), notice that as a consequence of Equation (4.3), for $(\hat{w}, w) \in \tilde{g} \times \mathbb{R}^n$,

$$(-2n_j + 1)\eta_j(\lambda)\Theta(\hat{w}, w) = e^{i\langle \lambda, s \rangle} \left(\left(\partial_{x_j} + \frac{1}{2}\eta_j(\lambda)y_j \right)^2 + \left(\partial_{y_j} - \frac{1}{2}\eta_j(\lambda)x_j \right)^2 \right) \mathcal{W}(\hat{w}, x, y).$$

Hence, simplifying the complex exponentials gives

$$(-2n_j + 1)\eta_j(\lambda)\mathcal{W}(\hat{w}, x, y) = \left(\left(\partial_{x_j} + \frac{1}{2}\eta_j(\lambda)y_j \right)^2 + \left(\partial_{y_j} - \frac{1}{2}\eta_j(\lambda)x_j \right)^2 \right) \mathcal{W}(\hat{w}, x, y).$$

Using the fact that $\mathcal{W}$ is a tensor product to look only at $\widetilde{\mathcal{W}}_j$, we get Identity (5) in the limit

$$(a_j, b_j, \lambda) \rightarrow (a_j, b_j, \lambda_0) \in \mathbb{R}_+ \times \mathbb{Z} \times \eta_j^{-1}(\{0\}).$$

Finally, passing to the limit in Equation (4.4) yields

$$b_j \mathcal{K}(a_j, x_j, y_j, b_j) = i(x_j \partial_{y_j} - y_j \partial_{x_j}) \mathcal{K}(a_j, x_j, y_j, b_j), \quad (4.8)$$

which is exactly Identity (6). $\square$

Before proving Identity (7), we state and prove an analogue lemma for the function $\mathcal{W}$.

Lemma 4.6.1. *For any $Z, Z' \in \mathbb{R}^{2d}$, $\lambda \in \tilde{\Lambda}$, $(a, b) \in g(\lambda)$, the following convolution property holds.*

$$e^{-\frac{i}{2}\langle \lambda, \sigma(Z, Z') \rangle} \mathcal{W}(a, b, \lambda, Z + Z') = \sum_{b' \in \mathbb{Z}^d} \mathcal{W}(a - \eta(\lambda) \cdot b', b - b', \lambda, Z) \mathcal{W}(a + \eta(\lambda) \cdot (b - b'), b', \lambda, Z').$$

Proof. Let f_1, f_2 be in $\mathcal{S}(\mathbb{R}^{2d})$, let α be in $\mathcal{S}(\mathbb{R}^p)$. For $(Z, s) \in \mathbb{R}^n$, the definition of the convolution product gives

$$((f_1 \otimes \alpha) \star (f_2 \otimes \alpha))(Z, s) = \int_{\mathbb{R}^n} f_1(Z - Z') f_2(Z') \alpha \left(s - s' - \frac{1}{2} \sigma(Z', Z) \right) \alpha(s') dZ' ds'.$$

Taking the usual Fourier transform with respect to the central variable s gives

$$\mathcal{F}_{\mathbb{R}^p}((f_1 \otimes \alpha) \star (f_2 \otimes \alpha))(Z, \lambda) = \hat{\alpha}(\lambda)^2 \int_{\mathbb{R}^{2d}} e^{\frac{i}{2}\langle \lambda, \sigma(Z, Z') \rangle} f_1(Z - Z') f_2(Z') dZ'.$$

Now, integrating against the function $\overline{\mathcal{W}}(\hat{w}, \cdot)$, we get

$$\mathcal{F}_g((f_1 \otimes \alpha) \star (f_2 \otimes \alpha))(\hat{w}) = \hat{\alpha}(\lambda)^2 \int_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} e^{\frac{i}{2}\langle \lambda, \sigma(Z, Z') \rangle} \overline{\mathcal{W}}(\hat{w}, Z) f_1(Z - Z') f_2(Z') dZ' dZ.$$

Since σ is antisymmetric, a simple change of variable gives

$$\mathcal{F}_g((f_1 \otimes \alpha) \star (f_2 \otimes \alpha))(\hat{w}) = \hat{\alpha}(\lambda)^2 \int_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} e^{\frac{i}{2}\langle \lambda, \sigma(Z, Z') \rangle} \overline{\mathcal{W}}(\hat{w}, Z + Z') f_1(Z) f_2(Z') dZ' dZ. \quad (4.9)$$

Let us now compute the Fourier transform in a different way. Applying formula (B.6) in the Appendix, we have

$$\mathcal{F}_g((f_1 \otimes \alpha) \star (f_2 \otimes \alpha))(\hat{w}) = (\mathcal{F}_g(f_1 \otimes \alpha) \cdot \mathcal{F}_g(f_2 \otimes \alpha))(\hat{w}).$$

Expanding out the operator product and parametrizing it by $\tilde{g}_E$, we get, for $(n, m, \lambda) \in \mathbb{N}^{2d} \times \tilde{\Lambda}$,

$$(\mathcal{F}_g(f_1 \otimes \alpha) \cdot \mathcal{F}_g(f_2 \otimes \alpha))(n, m, \lambda) = \sum_{\ell \in \mathbb{N}^d} \mathcal{F}_g(f_1 \otimes \alpha)(n, \ell, \lambda) \mathcal{F}_g(f_2 \otimes \alpha)(\ell, m, \lambda).$$

Extending the definition of the Fourier transform by setting

$$\mathcal{F}_g(f_1 \otimes \alpha)(n, \ell, \lambda) = \mathcal{F}_g(f_2 \otimes \alpha)(\ell, m, \lambda) = 0$$

whenever a component of ℓ is strictly negative, we also have

$$(\mathcal{F}_g(f_1 \otimes \alpha) \cdot \mathcal{F}_g(f_2 \otimes \alpha))(n, m, \lambda) = \sum_{\ell \in \mathbb{Z}^d} \mathcal{F}_g(f_1 \otimes \alpha)(n, \ell, \lambda) \mathcal{F}_g(f_2 \otimes \alpha)(\ell, m, \lambda).$$

Reverting to a parametrization by $\tilde{g}$, we get, for $(a, b, \lambda) \in \tilde{g}$,

$$\begin{aligned} (\mathcal{F}_g(f_1 \otimes \alpha) \cdot \mathcal{F}_g(f_2 \otimes \alpha))(a, b, \lambda) = \\ \sum_{b' \in \mathbb{Z}^d} \mathcal{F}_g(f_1 \otimes \alpha)(a - \eta(\lambda) \cdot b', b - b', \lambda) \mathcal{F}_g(f_2 \otimes \alpha)(a + \eta(\lambda) \cdot (b - b'), b', \lambda). \end{aligned}$$

Now, by definition of the Fourier transform $\mathcal{F}_g$, the general term of the above sum equals

$$\hat{\alpha}(\lambda)^2 \int_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} \overline{\mathcal{W}}(a - \eta(\lambda) \cdot b', b - b', \lambda, Z) \overline{\mathcal{W}}(a + \eta(\lambda) \cdot (b - b'), b', \lambda, Z') f_1(Z) f_2(Z') dZ dZ'.$$

Furthermore, since g_1 and g_2 lie in $\mathcal{S}(\mathbb{R}^{2d})$, we may exchange the integral on $\mathbb{R}^{2d} \times \mathbb{R}^{2d}$ with the sum on $\mathbb{Z}^d$ to get

$$\begin{aligned} (\mathcal{F}_g(f_1 \otimes \alpha) \cdot \mathcal{F}_g(f_2 \otimes \alpha))(a, b, \lambda) = \\ \hat{\alpha}(\lambda)^2 \int_{\mathbb{R}^{2d} \times \mathbb{R}^{2d}} \sum_{\ell \in \mathbb{Z}^d} \overline{\mathcal{W}}(a - \eta(\lambda) \cdot b', b - b', \lambda, Z) \overline{\mathcal{W}}(a + \eta(\lambda) \cdot (b - b'), b', \lambda, Z') f_1(Z) f_2(Z') dZ dZ'. \end{aligned} \tag{4.10}$$

Having equality between the right-hand sides of (4.9) and (4.10) for any f_1, f_2, α in their respective Schwartz classes, the lemma follows, up to a complex conjugation on both sides. $\square$

We may now prove Identity (7).

Proof. [Proof of Identity (7)] Since $\mathcal{W}$ writes as a tensor product in the basis $(x_1, \dots, x_d, y_1, \dots, y_d)$, Lemma 4.6.1 gives, looking at the variables $(a_j, b_j, x_j, y_j) \in \mathbb{R}_+ \times \mathbb{Z} \times \mathbb{R}^2$,

$$\begin{aligned} e^{-\frac{i}{2}\eta_j(\lambda)x_j y'_j} \mathcal{W}_j(a_j, b_j, \lambda, x_j + x'_j, y_j + y'_j) = \\ \sum_{b'_j \in \mathbb{Z}} \mathcal{W}_j(a_j - \eta_j(\lambda)b'_j, b_j - b'_j, \lambda, x_j, y_j) \mathcal{W}_j(a_j + \eta_j(\lambda)(b_j - b'_j), b'_j, \lambda, x'_j, y'_j). \end{aligned}$$

Then, if $\lambda \rightarrow \lambda_0 \in \eta_j^{-1}(\{0\})$, we obtain as desired

$$\mathcal{K}(a_j, x_j + x'_j, y_j + y'_j, b_j) = \sum_{b'_j \in \mathbb{Z}} \mathcal{K}(a_j, x_j, y_j, b_j - b'_j) \mathcal{K}(a_j, x'_j, y'_j, b'_j).$$

$\square$

Identity (8) is much more intricate to prove and requires several intermediate steps. We begin with a lemma describing the effect of a multiplication operator on the kernel $\mathcal{W}$. To this end, define the operator $\hat{\Delta}_j$ as follows. For $\theta \in \mathcal{C}(\tilde{g})$ and $\hat{w}_j = (a_j, b_j, \lambda) \in g_j(\lambda) \times \tilde{\Lambda}$,

$$\begin{aligned} (-\hat{\Delta}_j \theta)(\hat{w}_j) &:= \eta_j(\lambda)^{-2} (2(a_j + \eta_j(\lambda)) \theta(\hat{w}_j) \\ &\quad - \left(\sqrt{a_j^2 - \eta_j(\lambda)^2 b_j^2} \right) \theta(\hat{w}_j^-) - \left(\sqrt{(a_j + 2\eta_j(\lambda))^2 - \eta_j(\lambda)^2 b_j^2} \right) \theta(\hat{w}_j^+)), \end{aligned}$$

where

$$\hat{w}_j^\pm := (a_j \pm 2\eta_j(\lambda), b_j, \lambda).$$

Lemma 4.6.2. *For $\hat{w}_j = (a_j, b_j, \lambda) \in g_j(\lambda) \times \tilde{\Lambda}$ and $Z_j = (x_j, y_j) \in \mathbb{R}^2$, we have*

$$|Z_j|^2 \mathcal{W}_j(\hat{w}_j, Z_j) = (-\hat{\Delta}_j \mathcal{W}_j)(\hat{w}_j, Z_j).$$

Proof. We temporarily parametrize the space $\tilde{g}$ by $\tilde{g}_E$. Let us denote

$$\begin{aligned} n_j &:= \frac{\eta_j(\lambda)^{-1} a_j - b_j}{2}, \\ m_j &:= \frac{\eta_j(\lambda)^{-1} a_j + b_j}{2}. \end{aligned}$$

From the obvious identity

$$y_j^2 e^{i\eta_j(\lambda)\xi_j y_j} = -\eta_j(\lambda)^{-2} \left(e^{i\eta_j(\lambda)y_j} \right)'' (\xi_j)$$

and integration by parts, we first have

$$\begin{aligned} |Z_j|^2 \mathcal{W}_j(\hat{w}_j, Z_j) &= \\ \eta_j(\lambda)^{-2} \int_{\mathbb{R}} e^{i\eta_j(\lambda)\xi_j y_j} \left(-\frac{d^2}{d\xi_j^2} + \eta_j(\lambda)^2 x_j^2 \right) &\left(H_{m_j, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \right) d\xi_j. \end{aligned}$$

Writing

$$x_j^2 = \left(\xi_j + \frac{x_j}{2} \right)^2 + \left(\xi_j - \frac{x_j}{2} \right)^2 - 2 \left(\xi_j + \frac{x_j}{2} \right) \left(\xi_j - \frac{x_j}{2} \right),$$

we get, thanks to Equation (B.5),

$$\begin{aligned} &\left(-\frac{d^2}{d\xi_j^2} + \eta_j(\lambda)^2 x_j^2 \right) \left(H_{m_j, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \right) \\ &= 2\eta_j(\lambda)(n_j + m_j + 1) H_{m_j, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \\ &\quad - 2 \left(M_j H_{m_j, \eta_j(\lambda)} \right) \left(\xi_j + \frac{x_j}{2} \right) \left(M_j H_{n_j, \eta_j(\lambda)} \right) \left(\xi_j - \frac{x_j}{2} \right) \\ &\quad - 2 \left(H_{m_j, \eta_j(\lambda)} \right)' \left(\xi_j + \frac{x_j}{2} \right) \left(H_{n_j, \eta_j(\lambda)} \right)' \left(\xi_j - \frac{x_j}{2} \right). \end{aligned}$$

Using Equations (B.3) and (B.4) yields

$$\begin{aligned}
& \eta_j(\lambda)^{-1} \left(-\frac{d^2}{d\xi_j^2} + \eta_j(\lambda)^2 x_j^2 \right) \left(H_{m_j, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \right) \\
&= 2(n_j + m_j + 1) H_{m_j, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \\
&\quad - 2\sqrt{n_j m_j} H_{m_j-1, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j-1, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right) \\
&\quad - 2\sqrt{(n_j+1)(m_j+1)} H_{m_j+1, \eta_j(\lambda)} \left(\xi_j + \frac{x_j}{2} \right) H_{n_j+1, \eta_j(\lambda)} \left(\xi_j - \frac{x_j}{2} \right).
\end{aligned}$$

The result follows by reverting to the variables (a_j, b_j, λ) . $\square$

The next lemma describes the behaviour of the operator $-\hat{\Delta}$ as $\eta_j(\lambda) \rightarrow 0$.

Lemma 4.6.3. *Let $\theta : \mathbb{R}_+^* \times \mathbb{Z} \rightarrow \mathbb{R}$ be a $\mathcal{C}^2$ function of its first argument. Then, as $\lambda \rightarrow \lambda_0 \in \Lambda_0$ with $\eta_j(\lambda_0) = 0$, we have, for $(a_j, b_j) \in \mathbb{R}_+^* \times \mathbb{Z}$,*

$$(-\hat{\Delta}_j \theta)(a_j, b_j) \longrightarrow (-\hat{\Delta}_j^0 \theta)(a_j, b_j) := -4a_j \partial_{a_j a_j}^2 \theta(a_j, b_j) - 4\partial_{a_j} \theta(a_j, b_j) + \frac{b_j^2}{a_j} \theta(a_j, b_j).$$

Proof. Since $-\hat{\Delta}_j$ looks like a finite difference operator, it seems only natural to perform Taylor expansions for θ around $\hat{w}_j$ when $\eta_j(\lambda)$ is small. At second order in the parameter $\eta_j(\lambda)$, we have

$$\theta(a_j + 2\eta_j(\lambda), b_j) = \theta(a_j, b_j) + 2\eta_j(\lambda) \partial_{a_j} \theta(a_j, b_j) + \frac{1}{2} (2\eta_j(\lambda))^2 \partial_{a_j a_j}^2 \theta(a_j, b_j) + o(\eta_j(\lambda)^2),$$

$$\theta(a_j - 2\eta_j(\lambda), b_j) = \theta(a_j, b_j) - 2\eta_j(\lambda) \partial_{a_j} \theta(a_j, b_j) + \frac{1}{2} (2\eta_j(\lambda))^2 \partial_{a_j a_j}^2 \theta(a_j, b_j) + o(\eta_j(\lambda)^2),$$

$$\sqrt{a_j^2 - \eta_j(\lambda)^2 b_j^2} = a_j - \frac{1}{2} \frac{\eta_j(\lambda)^2 b_j^2}{a_j} + o(\eta_j(\lambda)^2),$$

$$\sqrt{(a_j + 2\eta_j(\lambda))^2 - \eta_j(\lambda)^2 b_j^2} = a_j + 2\eta_j(\lambda) - \frac{1}{2} \frac{\eta_j(\lambda)^2 b_j^2}{a_j} + o(\eta_j(\lambda)^2).$$

Plugging these equalities in the definition of $-\hat{\Delta}_j$ gives the result. $\square$

We now have the required tools to prove the last Identity of Proposition 4.6.1.

Proof. [Proof of Identity (8)] To circumvent the difficulty of a discrete-to-continuous limit, we argue by duality. Let $\lambda_0 \in \Lambda_0$ with $\eta_j(\lambda_0) = 0$. Let $\psi : \mathbb{R}_+^* \rightarrow \mathbb{R}$ be smooth and compactly supported. For $b_j \in \mathbb{Z}$, $\lambda \in \tilde{\Lambda}$ and $Z_j \in \mathbb{R}^2$, let

$$\mathcal{A}_j(b_j, \lambda, Z_j) := \int_{\mathbb{R}_+} \mathcal{W}_j(a_j, b_j, \lambda, Z_j) \psi(a_j) d\mu_{j, b_j}^\lambda(a_j).$$

Thanks to Lemma 4.6.2, we have

$$|Z_j|^2 \mathcal{A}_j(b_j, \lambda, Z_j) = \int_{\mathbb{R}_+} (-\hat{\Delta}_j \mathcal{W}_j)(a_j, b_j, \lambda, Z_j) \psi(a_j) d\mu_{j, b_j}^\lambda(a_j).$$

Denoting by ${}^t\hat{\Delta}_j$ and ${}^t\hat{\Delta}_j^0$ the adjoints of $\hat{\Delta}_j$ and $\hat{\Delta}_j^0$ respectively for the L^2 inner product, we get

$$|Z_j|^2 \mathcal{A}_j(b_j, \lambda, Z_j) = \int_{\mathbb{R}_+} \mathcal{W}_j(a_j, b_j, \lambda, Z_j) (-{}^t\hat{\Delta}_j \psi)(a_j) d\mu_{j,b_j}^\lambda(a_j).$$

As an immediate corollary of Lemma 4.6.3, for smooth $\theta : \mathbb{R}_+^* \rightarrow \mathbb{R}$ with compact support, we have the convergence

$${}^t\hat{\Delta}_j \theta \rightarrow {}^t\hat{\Delta}_j^0 \theta \text{ in } \mathcal{C}^0(\mathbb{R}_+^*, \mathbb{R})$$

as $\lambda \rightarrow \lambda_0$. Hence, applying this convergence to ψ gives, as $\lambda \rightarrow \lambda_0$,

$$\int_{\mathbb{R}_+} \mathcal{W}_j(a_j, b_j, \lambda, Z_j) (-{}^t\hat{\Delta}_j \psi)(a_j) d\mu_{j,b_j}^\lambda(a_j) \rightarrow \int_{\mathbb{R}_+} \mathcal{W}_j(a_j, b_j, \lambda_0, Z_j) (-{}^t\hat{\Delta}_j^0 \psi)(a_j) da_j.$$

By definition of $-{}^t\hat{\Delta}_j^0$, we get, as $\lambda \rightarrow \lambda_0$,

$$|Z_j|^2 \mathcal{A}_j(b_j, \lambda, Z_j) \rightarrow \int_{\mathbb{R}_+} (-\hat{\Delta}_j^0 \mathcal{K})(a_j, b_j, \lambda_0, Z_j) \psi(a_j) da_j.$$

On the other hand, recalling the definition of $\mathcal{A}_j$ yields

$$|Z_j|^2 \mathcal{A}_j(b_j, \lambda, Z_j) \rightarrow \int_{\mathbb{R}_+} |Z_j|^2 \mathcal{K}(a_j, b_j, \lambda_0, Z_j) \psi(a_j) da_j.$$

Since the reasoning above applies to all smooth and compactly supported $\psi : \mathbb{R}_+^* \rightarrow \mathbb{R}$, the last Identity is proved. $\square$

4.6.2 Another expression for $\mathcal{K}$

The form of Identity (7), of convolution type, motivates us to look at the Fourier synthesis of $\mathcal{K}$ in its last variable. For $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$, let

$$\tilde{\mathcal{K}}(a, x, y, z) := \sum_{b_j \in \mathbb{Z}} \mathcal{K}(a, x, y, b_j) e^{ib_j z}.$$

The function $\tilde{\mathcal{K}}$ is well defined, since for any (a, x, y) in a bounded set $\mathcal{B}$ and any $N \in \mathbb{N}$, we have

$$\sup_{b_j \in \mathbb{Z}} \sup_{(a, x, y) \in \mathcal{B}} (1 + |b_j|^N) |\mathcal{K}(a, x, y, b_j)| < \infty.$$

Applying Identity (7) to $\tilde{\mathcal{K}}$ gives, for $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$,

$$\tilde{\mathcal{K}}(a, x + x', y + y', z) = \tilde{\mathcal{K}}(a, x, y, z) \tilde{\mathcal{K}}(a, x', y', z).$$

From the definition of $\tilde{\mathcal{K}}$ and Identity (1), we infer

$$\tilde{\mathcal{K}}(a, 0, z) = \sum_{b_j \in \mathbb{Z}} \delta_{0,b_j} e^{ib_j z} \equiv 1.$$

Hence, for each $(a, z) \in \mathbb{R}_+ \times \mathbb{R}$, the function $(x, y) \mapsto \tilde{\mathcal{K}}(a, x, y, z)$ is a non trivial, continuous group morphism from $\mathbb{R}^2$ to $\mathbb{R}$. From the equality

$$\tilde{\mathcal{K}}(a, -x, -y, z) = \overline{\tilde{\mathcal{K}}(a, x, y, z)},$$

which stems from Identities (2) – (4), this function is also a character of $\mathbb{R}^2$. Thus, there exists a function $\Phi : \mathbb{R}_+ \times \mathbb{R} \rightarrow \mathbb{R}^2$ such that, for any $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$, we have

$$\tilde{\mathcal{K}}(a, x, y, z) = e^{i\langle(x,y), \Phi(a,z)\rangle}.$$

Since $\mathcal{K}$ is smooth in all variables and rapidly decaying in b_j , the equality

$$\Phi(a, z) = \overline{\tilde{\mathcal{K}}(a, x, y, z)} \nabla_{x,y} \tilde{\mathcal{K}}(a, x, y, z)$$

entails the smoothness of Φ in (a, z) . Thus, Identity (6) applied to $\tilde{\mathcal{K}}$ implies, viewing $\mathbb{R}^2$ as $\mathbb{C}$,

$$\partial_z \Phi(a, z) = i\Phi(a, z).$$

Solving this differential equation leads to

$$\Phi(a, z) = e^{iz} \Phi(a, 0).$$

Thanks to Identity (5), we get

$$|\Phi(a, z)| = \sqrt{a}.$$

Hence, there exists a map $\phi : \mathbb{R}_+ \rightarrow \mathbb{T}$ such that, for any (a, z) in $\mathbb{R}_+ \times \mathbb{R}$,

$$\Phi(a, z) = \sqrt{a} e^{iz} \phi(a).$$

We now transfer the information given by Identity (8) on $\tilde{\mathcal{K}}$ to find an equation on ϕ . For $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$, we have

$$(|x|^2 + |y|^2) \tilde{\mathcal{K}}(a, x, y, z) + 4a \partial_{aa} \tilde{\mathcal{K}}(a, x, y, z) + 4 \partial_a \tilde{\mathcal{K}}(a, x, y, z) + \frac{1}{a} \partial_{zz}^2 \tilde{\mathcal{K}}(a, x, y, z) = 0.$$

To keep as few terms as possible, we divide the above equation by $\tilde{\mathcal{K}}$ and look at the imaginary part. We have

$$\begin{aligned} \Im \left(\frac{4 \partial_a \tilde{\mathcal{K}}(a, x, y, z)}{\tilde{\mathcal{K}}(a, x, y, z)} \right) &= 4 \left(\frac{\langle(x, y), e^{iz} \phi(a)\rangle}{2\sqrt{a}} + \sqrt{a} \langle(x, y), e^{iz} \phi'(a)\rangle \right), \\ \Im \left(\frac{4a \partial_{aa} \tilde{\mathcal{K}}(a, x, y, z)}{\tilde{\mathcal{K}}(a, x, y, z)} \right) &= 4a \left(-\frac{\langle(x, y), e^{iz} \phi(a)\rangle}{4a^{\frac{3}{2}}} + 2 \frac{\langle(x, y), e^{iz} \phi'(a)\rangle}{2\sqrt{a}} + \sqrt{a} \langle(x, y), e^{iz} \phi''(a)\rangle \right), \\ \Im \left(\frac{\partial_{zz} \tilde{\mathcal{K}}(a, x, y, z)}{a \tilde{\mathcal{K}}(a, x, y, z)} \right) &= -\frac{1}{\sqrt{a}} \langle(x, y), e^{iz} \phi(a)\rangle. \end{aligned}$$

Gathering and simplifying these equalities yields

$$a\phi''(a) + 2\phi'(a) = 0.$$

Hence, there exist two constants $C_1, C_2 \in \mathbb{C}$ such that, for all $a > 0$,

$$\phi(a) = \frac{C_1}{a} + C_2.$$

As ϕ takes its values in unit circle, it is in particular bounded, which forces C_1 to vanish. Hence, ϕ is actually constant and there exists $z_0 \in \mathbb{R}$ such that $\phi(a) \equiv e^{iz_0}$ for all $a \in \mathbb{R}_+$. To compute the value of z_0 , we recall that Identity (2) implies that for all $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$,

$$\tilde{\mathcal{K}}(a, x, -y, z) = \overline{\tilde{\mathcal{K}}(a, x, y, -z)}.$$

Hence, for all $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$,

$$e^{\sqrt{ai}(x \cos(z+z_0) - y \sin(z+z_0))} = e^{-\sqrt{ai}(x \cos(-z+z_0) + y \sin(-z+z_0))} = e^{-\sqrt{ai}(x \cos(z-z_0) - y \sin(z-z_0))}.$$

This is only possible if

$$z_0 \equiv \frac{\pi}{2}[\pi].$$

Thus, there exists $\delta \in \{\pm 1\}$ such that for all $(a, x, y, z) \in \mathbb{R}_+ \times \mathbb{R}^3$,

$$\tilde{\mathcal{K}}(a, x, y, z) = e^{\delta \sqrt{ai}(x \sin z - y \cos z)}.$$

Finally, using the definition of $\tilde{\mathcal{K}}$ for small $y > 0$ and $z = x = 0$ gives

$$\tilde{\mathcal{K}}(a, 0, y, 0) = \sum_{b_j \in \mathbb{Z}} \mathcal{K}(a, 0, y, b_j) = \sum_{b_j \in \mathbb{Z}} \sum_{\ell_1 \in \mathbb{N}} \left(\frac{a}{4}\right)^{\frac{\ell_1}{2}} F_{\ell_1, 0}(b_j) \frac{(iy)^{\ell_1}}{\ell_1!} = 1 + \sqrt{ai}y + \mathcal{O}(y^2).$$

On the other hand, the form of $\tilde{\mathcal{K}}$ entails, again for $y > 0$ small,

$$\tilde{\mathcal{K}}(a, 0, y, 0) = e^{-\delta \sqrt{ai}y} = 1 - \delta \sqrt{ai}y + \mathcal{O}(y^2)$$

and $\delta = -1$. Owing to Fourier inversion for periodic functions on the real line, we have, for all $(a, x, y, b_j) \in \mathbb{R}_+ \times \mathbb{R}^2 \times \mathbb{Z}$,

$$\mathcal{K}(a, x, y, b_j) = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-\sqrt{ai}(x \sin z - y \cos z)} e^{ib_j z} dz. \quad (4.11)$$

Quatrième partie

Annexes

Annexe A

Graphes quantiques

A.1 Eigenvalue continuity with respect to edge lengths

In this section we sketch a proof for the continuity of all the graph's eigenvalues (not only the spectral gap) with respect to the graph's edge lengths. The continuity (and even differentiability) of eigenvalues with respect to edge lengths is proven in [43, 49]. Yet, those proofs deal only with positive edge lengths¹, whereas in the current work we are interested in particular in $\mathcal{L}vec \in \partial\mathcal{L}_G$, when we distinguish between supremizers and maximizers (see definition 3.1.2). We claim that eigenvalue continuity indeed carries over to the zero edge length case. We do not prove this in full rigor, but rather point out the general lines for forming a proof for this statement. We start by introducing the scattering approach for quantum graphs (see also [56, 43]).

A.1.1 The scattering approach to the graph spectrum

Let Γ be a Neumann graph. The eigenvalue equation,

$$-\frac{d^2 f}{dx^2} = k^2 f(x) , \quad (\text{A.1})$$

has a solution on each directed edge e , written as (assuming $k \neq 0$)

$$f_e(x_e) = a_e^{\text{in}} e^{-ikx_e} + a_e^{\text{out}} e^{ikx_e} . \quad (\text{A.2})$$

We may consider the edge $\hat{e}$, which is the same as e , but with a reverse direction (resulting in different parametrization of the coordinate, $x_{\hat{e}} = l_e - x_e$) and write the same function as above in the following form

$$f_{\hat{e}}(x_{\hat{e}}) = a_{\hat{e}}^{\text{in}} e^{-ikx_{\hat{e}}} + a_{\hat{e}}^{\text{out}} e^{ikx_{\hat{e}}} . \quad (\text{A.3})$$

Comparing both expressions above we arrive at

$$a_e^{\text{in}} = e^{ikl_e} a_{\hat{e}}^{\text{out}} \quad \text{and} \quad a_{\hat{e}}^{\text{in}} = e^{ikl_e} a_e^{\text{out}} . \quad (\text{A.4})$$

Fixing a vertex v and using the Neumann vertex conditions to relate solutions f_e for all edges whose origin is v one arrives at

$$\vec{a}_v^{\text{out}} = \sigma^{(v)} \vec{a}_v^{\text{in}} , \quad (\text{A.5})$$

where $\vec{a}_v^{\text{out}}$ and $\vec{a}_v^{\text{in}}$ are vectors of the outgoing and incoming coefficients (a_e^{in} , a_e^{out}) at v and $\sigma^{(v)}$ is a $d_v \times d_v$ unitary matrix, d_v being the degree of the vertex v . The matrix $\sigma^{(v)}$ is called the

1. It is possible that the proof in section 4 of [49], which is based on test functions, may be adapted for the zero edge length case. Nevertheless, we provide here a different argument based on the scattering approach.

vertex-scattering matrix and its entries were first calculated in [61] :

$$\sigma_{e,e'}^{(v)} = \frac{2}{d_v} - \delta_{e,e'} . \quad (\text{A.6})$$

We collect all coefficients a_e^{in} from the whole graph into a vector $\vec{a}$ of size $2E$ such that the first E entries correspond to edges which are the inverses of the last E entries. We can then define the matrix J acting on $\vec{a}$ by requiring that it exchanges a_e^{in} and $a_{\hat{e}}^{\text{in}}$ for all e such that,

$$J = \begin{pmatrix} 0 & \mathbf{I} \\ \mathbf{I} & 0 \end{pmatrix} . \quad (\text{A.7})$$

Then, collecting equations (A.5) for all vertices into one system and using (A.4) we have

$$J e^{-ikL} \vec{a} = \Sigma \vec{a} , \quad (\text{A.8})$$

where Σ is block-diagonalizable with individual $\sigma^{(v)}$ as blocks and

$$L = \text{diag}\{l_1, \dots, l_E, l_1, \dots, l_E\}$$

is a diagonal matrix of edge lengths. This can be rewritten as (note that $J^{-1} = J$),

$$\vec{a} = e^{ikL} J \Sigma \vec{a} , \quad (\text{A.9})$$

and hence all the non zero eigenvalues of the graph are the solutions of

$$\det(\mathbf{I} - U(k)) = 0 , \quad (\text{A.10})$$

where $U(k) := e^{ikL} J \Sigma$.

A.1.2 Continuity of eigenvalues via scattering approach

The scattering approach allows for a reduction in the dimensions of the matrix $U(k)$ by reducing a subgraph into a single composite vertex with some (non-trivial) vertex conditions (see section 3.3 in [56]). We pick a certain edge, e , to be the mentioned subgraph and turn it into a single (composite) vertex by shrinking it to zero length.

The length of this edge, l_e , will show up only in the scattering matrix of this composite vertex and will allow to examine how the eigenvalues depend on this length. We carry on with an explicit computation. Let e be an edge connecting two vertices, v_1, v_2 , of degrees d_1, d_2 . Hence, the new composite vertex, v , would be of degree $d_1 + d_2 - 2$. We calculate a reflection coefficient of this vertex (i.e., an on-diagonal entry of its vertex-scattering matrix). The calculation may be done by summing infinitely many trajectories on the original graph all starting by entering v_1 from some edge e_1 (different than e) and eventually leaving v_1 along the same edge, e_1 (see section 3.3 in [56], for further details).

$$\begin{aligned} \sigma_{e_1, e_1}^{(v)} &= \frac{2 - d_1}{d_1} + \frac{2}{d_1} \cdot e^{ik2l_e} \cdot \frac{2 - d_2}{d_2} \cdot \sum_{n=0}^{\infty} \left(e^{ik2l_e} \frac{2 - d_2}{d_2} \frac{2 - d_1}{d_1} \right)^n \cdot \frac{2}{d_1} \\ &= -1 + \frac{2}{d_1} \left(1 + \frac{4 - 2d_2}{e^{-ik2l_e} d_1 d_2 - (2 - d_1)(2 - d_2)} \right) \xrightarrow{l_e \rightarrow 0} -1 + \frac{2}{d_1 + d_2 - 2} . \end{aligned} \quad (\text{A.11})$$

where the continuity of the expression above in l_e is apparent and allows to take the limit $l_e \rightarrow 0$. We calculate just another entry of the composite vertex scattering matrix - the entry which corresponds to entering at vertex v_1 and leaving at v_2 . The calculation is similar to the one above and gives

$$\begin{aligned} \sigma_{e_1, e_2}^{(v)} &= \frac{2}{d_1} \cdot e^{ikl_e} \cdot \sum_{n=0}^{\infty} \left(e^{ik2l_e} \frac{2-d_2}{d_2} \frac{2-d_1}{d_1} \right)^n \cdot \frac{2}{d_2} \\ &= \frac{4}{e^{-ikl_e} d_1 d_2 - e^{ikl_e} (2-d_1)(2-d_2)} \xrightarrow{l_e \rightarrow 0} \frac{2}{d_1 + d_2 - 2}. \end{aligned} \quad (\text{A.12})$$

There is just another computation which is similar in nature and will not be repeated here. All the rest of the composite vertex scattering matrix entries may be obtained by symmetry. We hence get that the resulting scattering matrix when taking the limit $l_e \rightarrow 0$ is the same as the one obtained by considering Neumann conditions at the composite vertex. As the scattering matrix continuously determines the graph's eigenvalues (see (A.10)) we get the desired continuity result.

A.2 δ -type conditions and interlacing theorems

We present here the so-called δ -type conditions, of which both Neumann and Dirichlet conditions form special cases.

Definition A.2.1. We say that f satisfies the δ -type condition with the coefficient α in $\mathbb{R}$ at vertex v if

— f is continuous at v :

$$f_{e_1}(v) = f_{e_2}(v), \quad (\text{A.13})$$

for all edges e_1, e_2 in $\mathcal{E}_v$, where $\mathcal{E}_v$ is the set of edges incident to v .

— the derivatives of f at v satisfy

$$\sum_{e \in \mathcal{E}_v} \frac{df}{dx_e}(v) = \alpha f(v). \quad (\text{A.14})$$

We consider the following transformations

$$\alpha \mapsto \theta = \arg \left(\frac{i + \alpha}{i - \alpha} \right), \quad (\text{A.15})$$

and

$$\theta \mapsto \alpha = i \frac{1 - \exp(i\theta)}{1 + \exp(i\theta)} = \tan \left(\frac{\theta}{2} \right). \quad (\text{A.16})$$

The transformations (A.15), (A.16) are the inverses one of the other and allow to write the condition (A.14) in the form (3.43), which is the one used throughout the paper. We denote by $k_n(\Gamma; \theta)$ the n^{th} k -eigenvalue of such a graph and possibly omit either Γ or θ from this notation whenever it is clear what they are from the context. Similarly, the spectrum is denoted $\sigma(\Gamma; \theta)$ (see (3.44)).

We quote below some useful results from [43] as lemmata. The following lemma is a slight rephrasing of Theorem 3.1.8 from [43].

Lemma A.2.2. *Let Γ be a compact (not necessarily connected) graph. Let v be a vertex of Γ endowed with the δ -type condition and arbitrary self-adjoint vertex conditions at all other vertices of Γ . If $-\pi < \theta < \theta' \leq \pi$, then*

$$k_n(\theta) \leq k_n(\theta') \leq k_{n+1}(\theta).$$

If the eigenvalue $k_n(\theta')$ is simple and its eigenfunction f is such that either $f(v)$ or $\sum f'(v)$ is non-zero, then the inequalities above are strict,

$$k_n(\theta) < k_n(\theta') < k_{n+1}(\theta).$$

The following lemma is a slight rephrasing of Theorem 3.1.10 from [43].

Lemma A.2.3. *Let Γ be a compact (not necessarily connected) graph. Let v_1 and v_2 be vertices of Γ endowed with the δ -type conditions with corresponding coefficients α_1, α_2 and arbitrary self-adjoint vertex conditions at all other vertices of Γ . Let Γ' be the graph obtained from Γ by gluing the vertices v_1 and v_2 together into a single vertex v , so that $\mathcal{E}_v = \mathcal{E}_{v_1} \cup \mathcal{E}_{v_2}$ and endowed with δ -type condition at v , with the coefficient $\alpha_1 + \alpha_2$.*

Then the eigenvalues of the two graphs satisfy the inequalities

$$k_n(\Gamma) \leq k_n(\Gamma') \leq k_{n+1}(\Gamma).$$

We apply the lemma above in the case $\alpha_1 = -\alpha_2$, for which Γ' satisfies Neumann conditions at v . The following lemma is a rephrasing of part of Lemma 3.1.14 from [43] and the discussion which precedes it.

Lemma A.2.4. *The function k_n is continuous and non-decreasing on $(-\pi, \pi]$ and obeys the following continuity relation*

$$k_n(\pi) = \lim_{\theta \rightarrow -\pi^+} k_{n+1}(\theta).$$

The following lemma contains a statement proved in the course of the proof of Lemma 3.1.15 in [43]. We state here the lemma we need and its proof for completeness.

Lemma A.2.5. *Let Γ be a graph and v a vertex of Γ . Let $\theta_1 \neq \theta_2$ and let k be in $\sigma(\Gamma; \theta_1) \cap \sigma(\Gamma; \theta_2)$. Then there exists an eigenfunction corresponding to k which vanishes at v and its sum of derivatives vanish at v . Therefore, this eigenfunction satisfies the δ -type condition at v for every θ in $(-\pi, \pi]$. Hence k belongs to $\Delta(\Gamma)$.*

Démonstration. Let f_1, f_2 be eigenfunctions corresponding to k in $\sigma(\Gamma; \theta_1)$ and $\sigma(\Gamma; \theta_2)$ respectively, with coefficients θ_1, θ_2 . Assume first that k is a multiple eigenvalue either in $\sigma(\Gamma; \theta_1)$ or in $\sigma(\Gamma; \theta_2)$. Assume without loss of generality that it is in $\sigma(\Gamma; \theta_1)$. Further assume that θ_1 is not equal to π . As the eigenvalue is multiple, we can choose a corresponding eigenfunction which vanishes at v and denote it by f_1 . We deduce from the δ -type condition that the sum of derivatives of f_1 at v vanishes as well and conclude that f_1 satisfies δ -type condition at v for any value of θ . If we assume that θ_1 is equal to π , then we may use the multiplicity of the eigenvalue to choose an eigenfunction f_1 whose sum of derivatives at v vanishes and once again conclude that f_1 satisfies δ -type condition at v for any value of θ . We have shown that the lemma holds if one of the eigenvalues is multiple. Otherwise, assume that k is a simple eigenvalue both in $\sigma(\Gamma; \theta_1)$ and in $\sigma(\Gamma; \theta_2)$. Assume without loss of generality that θ_1 is not equal to π . Let f_1 be an eigenfunction corresponding to k and satisfying the δ -type condition with θ_1 . If f_1 does not vanish at v , then the strict eigenvalue interlacing (Lemma A.2.2) contradicts the fact that k belongs to $\sigma(\Gamma; \theta_1) \cap \sigma(\Gamma; \theta_2)$. Therefore f_1 has to vanish at v along with the sum of its derivatives, due to the δ -type condition. $\square$

A.3 A basic Rayleigh quotient computation

In the current section, we develop a basic but useful bound on the Rayleigh quotient, which is used throughout the paper. We define the mean of a function on a graph as

$$\langle f \rangle := \int_{\Gamma} f \, dx, \quad (\text{A.17})$$

and observe that

$$\mathcal{R}(f - \langle f \rangle) = \frac{\int_{\Gamma} |f'|^2 \, dx}{\int_{\Gamma} f^2 \, dx - \langle f \rangle^2}, \quad (\text{A.18})$$

which is useful as the test functions for which the Rayleigh quotient is computed ought to be of zero mean.

Lemma A.3.1. *Let Γ be a graph of length 1. Assume that $\Gamma = \Gamma_1 \cup \Gamma_2$ where $\Gamma_{1,2}$ are subgraphs of Γ such that $\Gamma_1 \cap \Gamma_2$ is a single vertex, denoted by v . Choose an eigenfunction f on Γ_1 corresponding to $k_1(\Gamma_1)$ and extend it to Γ_2 by the constant $f(v)$. The resulting test function on Γ , denoted $\tilde{f}$, satisfies*

$$\mathcal{R}(\tilde{f} - \langle \tilde{f} \rangle) = \frac{k_1(\Gamma_1)^2 \left(\int_{\Gamma_1} f^2 \, dx \right)}{\left(\int_{\Gamma_1} f^2 \, dx \right) + |f(v)|^2 l_2 (1 - l_2)}, \quad (\text{A.19})$$

where l_2 denotes the total length of Γ_2 .

Démonstration. We compute the mean and the L^2 norm of $\tilde{f}$:

$$\langle \tilde{f} \rangle = \int_{\Gamma_2} f(v) \, dx = f(v) l_2$$

and

$$\int_{\Gamma} |\tilde{f}|^2 \, dx = \left(\int_{\Gamma_1} f^2 \, dx \right) + \int_{\Gamma_2} |f(v)|^2 \, dx = \left(\int_{\Gamma_1} f^2 \, dx \right) + |f(v)|^2 l_2.$$

As $\tilde{f}$ is constant on Γ_2 and f is an eigenfunction on Γ_1 , we have

$$\int_{\Gamma} |\tilde{f}'(x)|^2 \, dx = \int_{\Gamma_1} |f'(x)|^2 \, dx = k_1(\Gamma_1)^2 \left(\int_{\Gamma_1} f^2 \, dx \right).$$

Plugging the above in (A.18) gives the desired result. $\square$

An immediate corollary of Lemma A.3.1 is the following.

Corollary A.3.2. *With the notations above we have $k_1(\Gamma) \leq k_1(\Gamma_1)$. This inequality is strict if there exists an eigenfunction of $k_1(\Gamma_1)$ not vanishing at v .*

In the decomposition discussed above, $\Gamma = \Gamma_1 \cup \Gamma_2$, we call Γ_1 the *main subgraph* of Γ and Γ_2 the *attached subgraph*. Note that when the main subgraph is a single loop, we may rotate its eigenfunction so that it achieves its maximal value at v . We exploit this in the sequel when applying Lemma A.3.1, since this choice leads to a low value of the Rayleigh quotient.

A.4 Proofs for small stowers (Lemmata 3.8.1-3.8.5)

In this more technical Appendix, we extensively use Lemma A.3.1. Namely, we consider the decomposition $\Gamma = \Gamma_1 \cup \Gamma_2$ and refer to $\Gamma_{1,2}$ as either the main or the attached subgraph of Γ (see Appendix A.3).

Proof of Lemma 3.8.1. Let us denote by l_1, l_2 and l_p the lengths of the two leaves and the petal, respectively and by v the vertex of degree three. Denote by $k_1(l_1, l_2, l_p)$ the spectral gap corresponding to these edge lengths. First, if $l_1 + l_2 > \frac{1}{2}$, we use the interval made of the two leaves as the main subgraph and the petal as the attached subgraph. We thus get, in this case, the inequality $k_1(l_1, l_2, l_p) < 2\pi$. Now, if $l_1 + l_2 \leq \frac{1}{2}$ and $l_1 = l_2$, explicit calculations show that the spectral gap is equal to 2π . Applying the symmetrization principle on the leaves (Proposition 3.7.1) shows that whenever $l_1 + l_2 \leq \frac{1}{2}$ and $l_1 \neq l_2$, we have $k_1(l_1, l_2, l_p) \leq 2\pi$. We further wish to prove that this inequality is strict and do so by checking the assumptions in Proposition 3.7.1. Assumption (1) is valid as we have shown above that the stower with $l_1 = l_2 \leq \frac{1}{4}$ is a supremizer. We now check assumption (2) - that whenever $0 \leq l_1 < l_2$ and $l_1 + l_2 \leq \frac{1}{2}$ the corresponding spectral gap is simple. In turn, thanks to Proposition 3.7.1, we will get the strict inequality $k_1(l_1, l_2, l_p) < 2\pi$ for $l_1 \neq l_2$ and $l_1 + l_2 \leq \frac{1}{2}$. Assume by contradiction that there exist $0 \leq l_1 < l_2$ with $l_1 + l_2 \leq \frac{1}{2}$ such that the spectral gap $k_1(l_1, l_2, l_p)$ is not simple. Thanks to the multiplicity, we may choose an eigenfunction vanishing at v . Since $l_1 < \frac{1}{4}$, such an eigenfunction has to vanish on the whole edge e_1 for otherwise, the spectral gap would satisfy $k_1(l_1, l_2, l_p) \geq \frac{\pi}{2l_1} > 2\pi$. Furthermore, the eigenfunction does not identically vanish neither on e_2 (again, this would contradict the bound on k_1) nor on e_p (because of the Neumann condition at v). Thus, there exist two integers α, β with α odd such that $k_1(l_1, l_2, l_p) = \frac{\alpha\pi}{2l_2} = \frac{\beta\pi}{l_p}$. From the bound on $k_1(l_1, l_2, l_p)$ and the conditions on the lengths, we get $\alpha = \beta = 1$. But as $k_1(l_1, l_2, l_p) = \frac{\pi}{2l_2}$ and $l_1 \neq l_2$, all eigenfunctions should vanish at v . Using again multiplicity, we may choose another eigenfunction which vanishes at v and at another point on e_2 , call it w . But this contradicts the equality $k_1(l_1, l_2, l_p) = \frac{\pi}{2l_2}$, hence the simplicity. We have therefore found a continuous family of maximizers - all stowers with $l_1 = l_2 \leq \frac{1}{4}$. It is easy to check that among all those, only the equilateral stower satisfies the Dirichlet criterion. In addition, the multiplicity of the spectral gap increases from two to three when imposing the Dirichlet condition at the central vertex, which is exactly the strong Dirichlet criterion. Hence, the equilateral stower satisfies condition (b) of Theorem 3.2.6. $\square$

Proof of Lemma 3.8.2. Denote by Γ the metric graph corresponding to $\mathcal{G}$, whose length of the petal is l_p and lengths of the leaves are l_1, l_2, l_3 (so that $l_p + l_1 + l_2 + l_3 = 1$). Assume for instance that $l_1 \geq l_2 \geq l_3$ and denote $\ell := \frac{l_1 + l_2 + l_3}{3}$. Using the three leaves as a main subgraph and the petal as an attached subgraph, we get the inequality

$$k_1(\Gamma) \leq \frac{\pi}{2\ell}.$$

On the other hand, using the petal and the longest two leaves as a main subgraph and the shortest leaf as an attached subgraph, we use Lemma 3.8.1 to get

$$k_1(\Gamma) \leq \frac{2\pi}{1 - l_3}.$$

Combining these two inequalities,

$$k_1(\Gamma) \leq \min\left(\frac{\pi}{2\ell}, \frac{2\pi}{1-l_3}\right) \leq \min\left(\frac{\pi}{2\ell}, \frac{2\pi}{1-\ell}\right).$$

This immediately yields, for any choice of l_l ,

$$k_1(\Gamma) \leq \frac{5\pi}{2},$$

with equality possible only if $\ell = \frac{1}{5}$ and $l_3 = \ell$. These two conditions together imply $l_1 = l_2 = l_3 = \frac{1}{5}$ and $l_p = \frac{2}{5}$. Conversely, for this specific choice of lengths, it is straightforward to point out the eigenfunction whose k -eigenvalue equals $\frac{5\pi}{2}$. Furthermore, it is also easy to check that in this case, the spectral gap indeed equals $\frac{5\pi}{2}$, with multiplicity three. Furthermore, imposing the Dirichlet condition at the central vertex increases the multiplicity of the spectral gap from three to four. Hence, the equilateral stower satisfies the strong Dirichlet criterion and is a unique supremizer, which proves that the equilateral stower satisfies condition (b) of Theorem 3.2.6. $\square$

Proof of Lemma 3.8.3. Let us denote by l_1, l_2 and l_l the lengths of the two petals and the leaf, respectively. Denote $\ell := \frac{l_1+l_2}{2}$. From Proposition 3.7.1, we have the inequality $k_1(l_1, l_2, l_l) \leq k_1(\ell, \ell, l_l)$. We now focus on the case where $l_1 = l_2 = \ell$. Let v be the central vertex of the stower. Using the two petals as a main subgraph and the leaf as an attached subgraph, we get

$$k_1(\ell, \ell, l_l) \leq \frac{2\pi}{1-l_l}.$$

Thus, for $0 \leq l_l \leq \frac{1}{5}$, we have $k_1(\ell, \ell, l_l) \leq \frac{5\pi}{2}$, with equality possible only if $l_l = \frac{1}{5}$. Now, using the leaf as a main subgraph and the two loops as an attached subgraph, we get

$$k_1(\ell, \ell, l_l) \leq \frac{\pi}{2l_l\sqrt{3-l_l}}.$$

In particular, we have $k_1(\ell, \ell, l_l) < \frac{5\pi}{2}$ for $0.26 \leq l_l \leq 1$. To cover the remaining values of l_l , we construct the following test function. Take the function $x \mapsto \cos(\frac{\pi x}{l_l})$ on the leaf, so that it vanishes at v . On each petal, take the function $x \mapsto \frac{l_l}{1-l_l} \sin(\frac{2\pi x}{1-l_l})$. Denoting the resulting function by h , we have

$$\mathcal{R}(h) = \pi^2 \frac{(1-l_l)^3 + 16l_l^3}{4l_l^2(1-l_l)^2}.$$

In particular, we have $k_1(\ell, \ell, l_l) \leq \frac{5\pi}{2}$ for $\frac{1}{5} \leq l_l \leq \frac{2}{5}$, with equality possible only if $l_l = \frac{1}{5}$. Gathering the information given by these three test functions, we conclude that for all l_l values we have $k_1(\ell, \ell, l_l) \leq \frac{5\pi}{2}$, with equality possible only if $l_l = \frac{1}{5}$.

Moreover, it is easy to show that $k_1(\frac{2}{5}, \frac{2}{5}, \frac{1}{5}) = \frac{5\pi}{2}$ with multiplicity two. This multiplicity increases to three when imposing the Dirichlet condition at the central vertex, so that the equilateral stower satisfies the strong Dirichlet criterion. It only remains to show that if $l_l = \frac{1}{5}$ and $l_1 \neq l_2$, we have $k_1(l_1, l_2, l_l) < \frac{5\pi}{2}$. This is obtained by applying Corollary A.3.2 to the two loops as the main subgraph and the leaf as the attached subgraph. Thus, the equilateral stower is a unique maximizer and satisfies in particular condition (b) of Theorem 3.2.6. $\square$

Proof of Lemma 3.8.4. Denote by l_1, l_2, l_3 and l_l the lengths of the three petals and the leaf. Assume without loss of generality that $l_1 \geq l_2 \geq l_3$ and define $\ell := \frac{l_1 + l_2 + l_3}{3}$. Using the three petals as a main subgraph and the leaf as an attached subgraph, we have $k_1(l_1, l_2, l_3, l_p) \leq \frac{\pi}{2\ell}$. Moreover, equality is possible only if $l_1 = l_2 = l_3 = \ell$. Using the longest two petals and the leaf as a main subgraph and the shortest petal as an attached subgraph we further have

$$k_1(l_1, l_2, l_3, l_l) \leq \frac{5\pi}{2(1 - l_3)} \leq \frac{5\pi}{2(1 - \ell)}.$$

Combining the two bounds we got on k_1 , it follows that $k_1(l_1, l_2, l_3, l_p) \leq \frac{7\pi}{2}$, with an equality possible only if $\ell = \frac{2}{7}$ and $l_3 = \ell$. These two equalities together entail that $l_1 = l_2 = l_3 = \frac{2}{7}$ and $l_l = \frac{1}{7}$. With this choice of lengths, it is easy to show that the spectral gap equals $\frac{7\pi}{2}$ and of multiplicity three. This multiplicity increases to four when imposing the Dirichlet condition at the central vertex, which means that the equilateral stower satisfies the strong Dirichlet criterion. As the equilateral stower is a unique supremizer, it also satisfies condition (b) of Theorem 3.2.6. $\square$

Proof of Lemma 3.8.5. Let $\ell \in [0, 1]$ be the length of the leaf and $1 - \ell$ the length of the petal. Using the leaf as a main subgraph and the petal as an attached subgraph, we get

$$k_1(\ell, 1 - \ell) \leq \frac{2\pi}{2\ell\sqrt{3 - 2\ell}}.$$

In particular, we have $k_1(\ell, 1 - \ell) \leq 2\pi$ as long as $2\ell\sqrt{3 - 2\ell} \geq 1$. This is satisfied for $\ell \geq \frac{1}{3}$, and in this case the inequality is strict. Next, we refer to the scattering approach described in Appendix A and more precisely to equation (A.10), whose zeros are the graph's eigenvalues. This equation is equivalent, in our case, to $F(k, \ell) = 0$, where

$$F(k, \ell) := 2 \cos(k\ell) \sin\left(k \frac{1 - \ell}{2}\right) + \sin(k\ell) \cos\left(k \frac{1 - \ell}{2}\right). \quad (\text{A.20})$$

Substituting $k = 2\pi$, and using basic trigonometric identities, we get

$$F(2\pi, \ell) = 2 \cos(2\pi\ell) \sin(\pi(1 - \ell)) + \sin(2\pi\ell) \cos(\pi(1 - \ell)) \quad (\text{A.21})$$

$$= 2 \sin(\pi\ell) (\cos(2\pi\ell) - \cos^2(\pi\ell)) = 2 \sin(\pi\ell) (\cos^2(\pi\ell) - 1). \quad (\text{A.22})$$

We notice that $F(k, \ell) > 0$ for small positive values of k and that $F(2\pi, \ell) < 0$ for $\ell \in (0, \frac{1}{3}]$. As F is continuous in k , we deduce that there exists some $k < 2\pi$ such that $F(k, \ell) = 0$. This means that for $\ell \in (0, \frac{1}{3}]$, the spectral gap is strictly below 2π . As we have seen above that this is also the case for $\ell > \frac{1}{3}$ and since the spectral gap is 2π for $\ell = 0$ (single cycle graph), the result follows. $\square$

Annexe B

Transformée de Fourier

B.1 Standard computations on the Hermite functions.

In this appendix, we recall the definition of the Hermite functions along with their most useful properties. The computations may be found e.g. in [99]. For x in $\mathbb{R}^d$, the first Hermite function H_0 is defined on $\mathbb{R}^d$ by

$$H_0(x) := \pi^{-\frac{d}{4}} e^{-\frac{|x|^2}{2}}.$$

Let M_j be the multiplication operator with respect to the j -th variable, defined for $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and x in $\mathbb{R}^d$ by

$$(M_j f)(x) := x_j f(x).$$

Defining the creation operator C_j by

$$C_j := -\partial_j + M_j,$$

the Hermite functions family is defined, for n in $\mathbb{N}^d$ by

$$H_n := \frac{1}{\sqrt{2^{|n|} n!}} C^n H_0,$$

where, as usual,

$$C^n := \prod_{j=1}^d C_j^{n_j}, \quad |n| := \sum_{j=1}^d n_j \quad \text{and} \quad n! := \prod_{j=1}^d n_j!.$$

We also define the annihilation operator A_j by

$$A_j := \partial_j + M_j$$

and notice that A_j is the (formal) adjoint of C_j for the usual inner product on $L^2(\mathbb{R}^d)$. It is a standard fact that the family $(H_n)_{n \in \mathbb{N}^d}$ is an orthonormal basis of $L^2(\mathbb{R}^d)$ and in particular that for any (n, m) in $\mathbb{N}^{2d}$,

$$(H_n | H_m)_{L^2(\mathbb{R}^d)} := \int_{\mathbb{R}^d} H_n(x) H_m(x) dx = \begin{cases} 1 & \text{if } n = m, \\ 0 & \text{otherwise.} \end{cases}$$

Furthermore, the very definition of the Hermite functions entails that for any n in $\mathbb{N}^d$ and j between 1 and d , there holds

$$C_j H_n = \sqrt{2(n_j + 1)} H_{n + \delta_j} \tag{B.1}$$

and by duality, we get

$$A_j H_n = \sqrt{2n_j} H_{n-\delta_j}, \quad (\text{B.2})$$

where $n \pm \delta_j := (n_1, \dots, n_j \pm 1, \dots, n_d)$. Adding and subtracting these two equalities gives, for n in $\mathbb{N}^d$ and j between 1 and d ,

$$M_j H_n = \frac{\sqrt{2}}{2} (\sqrt{n_j} H_{n-\delta_j} + \sqrt{n_j+1} H_{n-\delta_j}) \quad (\text{B.3})$$

$$\partial_j H_n = \frac{\sqrt{2}}{2} (\sqrt{n_j} H_{n-\delta_j} - \sqrt{n_j+1} H_{n-\delta_j}). \quad (\text{B.4})$$

Also, combining the action of C_j and A_j gives, for n in $\mathbb{N}^d$ and j between 1 and d ,

$$-\Delta_{\text{osc},j} H_n := (-\partial_j^2 + M_j^2) H_n = (C_j A_j + \text{Id}) H_n = (2n_j + 1) H_n.$$

Now, if η belongs to $(\mathbb{R}_+^*)^d$ and n lies in $\mathbb{N}^d$, we define the rescaled Hermite function $H_{n,\eta}$ by

$$H_{n,\eta} := |\eta|^{\frac{d}{4}} H_n(|\eta|^{\frac{d}{4}} \cdot).$$

These functions satisfy identities similar to those of the usual Hermite functions. In particular, they also form an orthonormal basis of $L^2(\mathbb{R}^d)$ and for n in $\mathbb{N}^d$, η in $(\mathbb{R}_+^*)^d$, we have

$$(-\partial_j^2 + \eta_j^2 M_j^2) H_{n,\eta} = \eta_j (2n_j + 1) H_{n,\eta}. \quad (\text{B.5})$$

We also state and prove here a technical lemma on the growth of the L^2 norms of Hermite functions to which multiple derivatives or multiplication operators are applied.

Lemma B.1.1. *For n, ℓ in $\mathbb{N}$, we have*

$$\|H_n^{(\ell)}\|_{L^2(\mathbb{R})} \leq (2n + 2\ell)^{\frac{\ell}{2}} \quad \text{and} \quad \|M^\ell H_n\|_{L^2(\mathbb{R})} \leq (2n + 2\ell)^{\frac{\ell}{2}}.$$

Démonstration. The proof is a simple induction on ℓ in $\mathbb{N}$. For $\ell = 0$ both inequalities are obvious, for the Hermite functions are an orthonormal family of $L^2(\mathbb{R})$. Given ℓ in $\mathbb{N}$, assume the inequalities to be true for ℓ and all $n \in \mathbb{N}$. Owing to Equation (B.3) and the induction assumption, we have, for n in $\mathbb{N}$,

$$\begin{aligned} \|M^{\ell+1} H_n\|_{L^2(\mathbb{R})} &\leq \frac{1}{\sqrt{2}} \left(\sqrt{n} \|M^\ell H_{n-1}\|_{L^2(\mathbb{R})} + \sqrt{n+1} \|M^\ell H_{n+1}\|_{L^2(\mathbb{R})} \right) \\ &\leq \frac{1}{\sqrt{2}} \left(\sqrt{n} (2n + 2\ell - 2)^{\frac{\ell}{2}} + \sqrt{n+1} (2n + 2\ell + 2)^{\frac{\ell}{2}} \right) \\ &\leq \frac{1}{\sqrt{2}} \left(\sqrt{n+\ell+1} (2n + 2\ell + 2)^{\frac{\ell}{2}} + \sqrt{n+\ell+1} (2n + 2\ell + 2)^{\frac{\ell}{2}} \right) \\ &= (2n + 2(\ell + 1))^{\frac{\ell+1}{2}}. \end{aligned}$$

The proof for multiple applications of the derivative is similar. □

B.2 The representation-theoretic Fourier transform.

We collect here some standard results about the Fourier transform as defined through unitary irreducible representations. We refer the reader to [87], [88], [90], [91], [93], [94], [95], [96], [98], [101], [102], [103] and [104] for further details. We begin with a familiar continuity statement on $L^1(\mathbb{R}^d)$. Recall that the Fourier transform has been defined on page 98.

Theorem B.2.1. *The Fourier transformation is continuous in all its variables, in the following sense.*

— For any λ in $\tilde{\Lambda}$ and ν in $\mathbb{R}^t$, the map

$$\mathcal{F}^g(\cdot)(\lambda, \nu) : L^1(\mathbb{R}^d) \longrightarrow \mathcal{L}(L^2(\mathbb{R}^d))$$

is linear and continuous, with norm bounded by 1.

— For any $\phi \in L^2(\mathbb{R}^d)$ and $f \in L^1(\mathbb{R}^d)$, the map

$$\mathcal{F}^g(f)(\cdot, \cdot)(\phi) : \tilde{\Lambda} \times \mathbb{R}^t \longrightarrow L^2(\mathbb{R}^d)$$

is continuous.

We go on with the analogues of the Plancherel and inversion formula in $L^2(\mathbb{R}^d)$. Let $\|\cdot\|_{HS(L^2(\mathbb{R}^d))}$ be the usual Hilbert-Schmidt norm on operators acting on $L^2(\mathbb{R}^d)$ and

$$\text{Pf}(\lambda) := \prod_{j=1}^d \eta_j(\lambda)$$

be the (absolute value of the) pfaffian of the matrix $\mathcal{U}^{(\lambda)}$. With these notations, the Fourier transform $\mathcal{F}^g(\cdot)$ extends, up to a multiplicative constant, to an isometry from $L^2(\mathbb{R}^d)$ to the two-parameter families

$$(A(\lambda, \nu))_{(\lambda, \nu) \in \tilde{\Lambda} \times \mathbb{R}^t}$$

of Hilbert-Schmidt operators, endowed with the norm

$$\|A\| := \left(\int_{\tilde{\Lambda} \times \mathbb{R}^t} \|A(\lambda, \nu)\|_{HS(L^2(\mathbb{R}^d))}^2 \text{Pf}(\lambda) d\lambda d\nu \right)^{\frac{1}{2}}.$$

More precisely, we have the following theorem.

Theorem B.2.2. *There exists a constant κ depending only on the choice of the group such that, for any f in $L^2(\mathbb{R}^d)$, there holds*

$$\int_{\mathbb{R}^n} |f(w)|^2 dw = \kappa \int_{\tilde{\Lambda} \times \mathbb{R}^t} \|\mathcal{F}^g(f)(\lambda, \nu)\|_{HS(L^2(\mathbb{R}^d))}^2 \text{Pf}(\lambda) d\lambda d\nu.$$

On the Heisenberg group $\mathbb{H}^d$, the pfaffian is simply $\text{Pf}(\lambda) = |\lambda|^d$ and the value of κ is known, namely

$$\kappa(\mathbb{H}^d) = \frac{2^{d-1}}{\pi^{d+1}}.$$

In this context, the inversion formula reads, for f in $L^1(\mathbb{R}^d)$ and almost every w in $\mathbb{R}^n$,

$$f(w) = \kappa \int_{\tilde{\Lambda} \times \mathbb{R}^p} \text{tr}((u_w^{\lambda, \nu})^* \mathcal{F}^g(f)(\lambda, \nu)) \text{Pf}(\lambda) d\lambda d\nu,$$

with the same constant κ . Finally, the Fourier transform exchanges as usual convolution and product, in the following sense. The convolution operator $*$: $L^1(\mathbb{R}^d) \times L^1(\mathbb{R}^d) \rightarrow L^1(\mathbb{R}^d)$ is defined as follows. For any f_1, f_2 in $L^1(\mathbb{R}^d)$ and (Z, s) in $\mathbb{R}^n$,

$$(f_1 * f_2)(Z, s) := \int_{\mathbb{R}^n} f_1((Z, s) \cdot (-Z', -s')) f_2(Z', s') dZ' ds'.$$

The convolution-product intertwining through the Fourier transform may now be stated.

Theorem B.2.3. *For any f_1, f_2 in $L^1(\mathbb{R}^d)$ and (λ, ν) in $\tilde{\Lambda} \times \mathbb{R}^t$, we have, denoting by $\cdot$ the operator composition on $\mathcal{L}(L^2(\mathbb{R}^d))$,*

$$\mathcal{F}^g(f_1 * f_2)(\lambda, \nu) = \mathcal{F}^g(f_1)(\lambda, \nu) \cdot \mathcal{F}^g(f_2)(\lambda, \nu). \quad (\text{B.6})$$

Finally, as in the classical commutative theory, the Fourier transform allows us to diagonalize the action of the subelliptic laplacian on g , whose definition we recall. If $V := (V_1, \dots, V_m)$ is an orthonormal family such that $V \cup \{\partial_{s_k}, 1 \leq k \leq p\}$ is a basis of g , the subelliptic laplacian with respect to the family V is, by definition,

$$\Delta_g := \sum_{j=1}^m V_j^2.$$

One may prove that this definition is independant of V provided it satisfies the two stated conditions. For λ in Λ , f in $\mathcal{C}^\infty(\mathbb{R}^d)$ and x in $\mathbb{R}^d$, define also the rescaled harmonic oscillator

$$(-\Delta_{\text{osc}, \eta(\lambda)} f)(x) := (-\Delta + |\eta(\lambda) \cdot x|^2) f(x).$$

Above, Δ is the standard laplacian acting on smooth functions on $\mathbb{R}^d$. We may now state how the Fourier transform diagonalizes the action of the laplacian.

Theorem B.2.4. *Let f in $\mathcal{C}_c^\infty(\mathbb{R}^n)$. Let (λ, ν) in $\tilde{\Lambda} \times \mathbb{R}^t$. Then, for ϕ in $\mathcal{C}_c^\infty(\mathbb{R}^d)$, there holds*

$$\mathcal{F}^g(-\Delta_g f)(\lambda, \nu)(\phi) = \mathcal{F}^g(f)(\lambda, \nu) (-\Delta_{\text{osc}, \eta(\lambda)} \phi + |\nu|^2 \phi).$$

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