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Guides d'ondes quantiques bidimensionnels

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Résumé

Nous étudions les propriétés spectrales des *guides d'ondes quantiques bidimensionnels* qui constituent un modèle raisonnable pour la dynamique quantique non-relativiste d'une particule dans les films conducteurs déposés sur une surface isolante. Mathématiquement, il s'agit du laplacien Dirichlet dans un voisinage tubulaire d'épaisseur constante construit autour d'une surface non-compacte plongée dans $\mathbb{R}^3$. Sous des hypothèses appropriées sur la décroissance des courbures de la surface à l'infini, nous localisons le spectre essentiel et fournissons des conditions suffisantes variées garantissant l'existence des états liés quantiques dûs à la géométrie. De plus, si la surface de référence est un plan courbé faiblement, nous trouvons le développement asymptotique de l'unique valeur propre correspondante par rapport au paramètre décrivant ce couplage faible. Nous établissons un développement limité d'une valeur propre aussi dans les guides d'ondes bidimensionnels droits mais avec une frontière déformée localement par des bosses et des creux. Cette thèse contient à la fin une étude du spectre d'une variété non-compacte générale qui possède au moins un pôle. Nous nous concentrons sur les variétés à symétrie radiale et les surfaces. Dans ces cas particuliers, nous montrons que le spectre est tout l'axe réel positif en posant certaines conditions supplémentaires sur la décroissance des courbures à l'infini.

Abstract

We study spectral properties of *quantum layers* which represent a reasonable model for the non-relativistic quantum dynamics of a particle in conductive films produced on an insulting surface. Mathematically, one considers the Dirichlet Laplacian in a tubular neighbourhood of constant width built over a non-compact surface embedded in $\mathbb{R}^3$. Under appropriate hypotheses on the decay of surface curvatures at infinity, we localize the essential spectrum and provide miscellaneous sufficient conditions which guarantee the existence of geometrically induced quantum bound states. Furthermore, if the reference surface is a mildly curved plane, we find the asymptotic expansion of the corresponding unique eigenvalue evaluated with respect to a parameter describing this weak coupling. We establish an asymptotic expansion of an eigenvalue also in layers which are straight but one of its boundaries is deformed locally by dents and bulges. This thesis contains eventually an investigation of the spectrum of a general non-compact manifold which possesses at least one pole. We restrict our attention to the manifolds with radial symmetry and surfaces. In these particular cases, we show that the spectrum is all the positive real axis provided we put some additional conditions on the decay of curvatures at infinity.

A mes parents

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On entend souvent dire que la carte de la terre ne comprend plus aucune zone blanche, que notre planète se trouve désormais totalement explorée, fouillée, recensée, et que c'est bien triste parce que la découverte et l'aventure sont devenues impossibles. J'écoute ce genre de discours d'une oreille distraite, car de l'autre oreille j'entends mille rumeurs venues de mon jardin et de mon village, si peu connus l'un et l'autre, si mal explorés, fouillés, recensés l'un et l'autre qu'une vie n'y suffirait pas. Et puis j'ai sous mon bonnet un gros œuf gris et blanc qui constitue à lui seul un continent, mieux une planète, mieux un système solaire dont l'exploration à peine entreprise nous invite au voyage le plus formidable, le plus vertigineux.

Ce voyage, la neurologie nous y invite, mais en même temps, elle le sème d'écueils. Par exemple, le vieillissement. J'ai inauguré mes premières lunettes il y a peu de temps. Or voici qu'on m'annonce des nouvelles concernant mon cerveau tout à fait alarmantes. Ses cellules, me dit-on, ne se renouvellent pas, et elles meurent à raison de dix mille par jour. Et cela depuis ma naissance. Bref mon œuf gris et blanc fond sur ma tête, comme neige au soleil. Einstein disait : "Pour marcher au pas, point n'est besoin de cerveau, la moelle épinière suffit." Est-ce à dire que bientôt je ne marcherai plus qu'au pas ?

Alors là, je me rebiffe. Marcher au pas ? Je l'ai assez fait dans mon enfance. Comme beaucoup de jeunes, j'adorais les clans, les embrigadements, les mots d'ordre. Et puis, *en vieillissant*, j'ai commencé à secouer tout cela. J'ai balancé par-dessus bord les familles et les idéologies. J'ai cessé d'avoir peur de la solitude, de l'indépendance, des risques impliqués nécessairement par l'invention. Et à quarante ans, je me suis mis à écrire des livres, des livres que j'aurais été bien incapable de seulement imaginer quand j'avais vingt ans. Alors je dis : le cerveau tout neuf du bébé, oui. Mais l'apprentissage, l'expérience, la recherche tâtonnante, patiente, étendue sur toute une vie, cela compte aussi. Il y a d'abord le donné, et avec cela, on construit, on se construit.

Michel Tournier : "Mon œuf et moi"

Table des matières

I PREMIÈRE PARTIE **15**

i Introduction **17**
- i.1 Le présent modèle : *Guide d'ondes quantique bidimensionnel* . . . 17
- i.2 Le modèle général : *Guide d'ondes quantique* . . . 18
- i.3 Sommaire des résultats connus . . . 19
  - i.3.1 Les géométries courbes . . . 19
  - i.3.2 Les diverses géométries . . . 21

ii Présentation des résultats **23**
- ii.1 Définitions et préliminaires . . . 23
  - ii.1.1 La surface de référence . . . 24
  - ii.1.2 L'espace des configurations . . . 25
  - ii.1.3 L'hamiltonien . . . 26
  - ii.1.4 La motivation . . . 27
- ii.2 ad Chapitre iv : La courbure locale . . . 28
- ii.3 ad Chapitre v : La courbure globale . . . 29
- ii.4 ad Chapitre vi : La courbure faible . . . 32
- ii.5 ad Chapitre vii : Les bosses et les creux . . . 33
- ii.6 ad Chapitre viii : Sur le spectre des variétés non-compactes . 37

iii Conclusion **41**

II DEUXIÈME PARTIE **45**

iv La courbure locale **47**
- iv.1 Introduction . . . 49
- iv.2 Formulation of the problem . . . 50
  - iv.2.1 Properties of the reference surface . . . 50
  - iv.2.2 Metric properties of the layer . . . 51
  - iv.2.3 Various expressions of the Hamiltonian . . . 52
  - iv.2.4 Coordinate decoupling . . . 53

iv.3 Spectrum of locally deformed planar layers 54
iv.3.1 The essential spectrum 54
iv.3.2 Existence of Bound States 55
References 59

v La courbure globale **61**
v.1 Introduction 63
v.2 Survey of the Paper 64
v.3 Preliminaries 66
v.3.1 The Surface Geometry 66
v.3.2 The Layer Geometry 67
v.3.3 The Hamiltonian 68
v.4 Essential Spectrum 69
v.5 Discrete Spectrum 70
v.6 Cylindrically Symmetric Layers 74
v.7 A Layer without Bound States 76
References 79

vi La courbure faible **81**
vi.1 Introduction 83
vi.2 The results 84
vi.3 Weakly Coupled Schrödinger Operators in a Planar Layer . . 86
vi.3.1 Birman-Schwinger Analysis 87
vi.3.2 Proof of Lemma vi.4 91
vi.4 Mildly Curved Layers 94
vi.4.1 The Geometry 94
vi.4.2 The Hamiltonian 96
vi.4.3 The Ground State Asymptotics 97
vi.4.4 The Thin Layer Limit 100
References 103

vii Les bosses et les creux **105**
vii.1 Introduction 107
vii.2 Locally deformed layers 109
vii.2.1 The curvilinear coordinates 109
vii.2.2 The straightening transformation 110
vii.2.3 Weak coupling analysis 112
vii.3 An alternative method 117
vii.3.1 The asymptotic expansion 117
vii.3.2 The next-to-leading order 120
vii.3.3 The critical case 121
References 125

viii Sur le spectre des variétés non-compactes **127**
viii.1 Curved Layers 129
viii.1.1 Preliminaries 129
viii.1.2 Essential Spectrum 134
viii.1.3 Cylindrically Symmetric Layers 137
viii.1.4 Addendum. Partial Wave Decomposition 137
viii.2 Curved Strips 139
viii.3 Complete Manifolds 141
viii.3.1 The Laplacian 142
viii.3.2 Radially Symmetric Case 143
viii.3.3 Surfaces 147

Bibliographie **149**

Première partie

Chapitre i

Introduction

L'étude de la relation entre la géométrie et l'analyse spectrale est un domaine important de la physique mathématique. Déjà, d'un point de vue purement mathématique, il est très intéressant de comprendre l'influence de la forme ou de la métrique de l'espace des configurations et des conditions aux bords sur le spectre des opérateurs différentiels définis dans cet espace. D'autre part, on peut essayer de caractériser quelques propriétés intrinsèques d'une variété à l'aide de la connaissance des spectres de ces opérateurs. L'intérêt pour la physique découle bien sûr du fait que de nombreux systèmes de la nature sont décrits par des équations aux dérivées partielles et que l'étude de ces dernières se fait souvent à l'aide de l'analyse spectrale des opérateurs différentiels correspondants. Un exemple classique est donné par l'équation des ondes qui devient l'équation de Helmholtz dans la situation stationnaire et on s'intéresse alors aux propriétés spectrales de l'opérateur laplacien. Si l'espace des configurations est une région tubulaire infinie avec conditions aux bords de Dirichlet ou Neumann, on obtient un modèle raisonnable pour les guides d'ondes acoustiques ou certains guides d'ondes électromagnétiques. Dans le cas quantique, même si l'interprétation des solutions est différente, mathématiquement on arrive à la même équation stationnaire dérivée de l'équation de Schrödinger. On obtient ainsi un modèle pour les *guides d'ondes quantiques* que l'on va préciser par la suite. Cette thèse est une contribution à ce domaine de recherche par l'étude d'une classe des guides d'ondes en mécanique quantique non-relativiste.

i.1 Le présent modèle : *Guide d'ondes quantique bidimensionnel*

Le but de cette thèse est l'analyse spectrale des *guides d'ondes quantiques bidimensionnels* – "quantum layers" en anglais – qui constituent un modèle raisonnable pour la dynamique quantique non-relativiste d'une particule dans les films conducteurs déposés sur une surface isolante. Ces

systèmes mésoscopiques seront nommés au début de la Section i.2 dans laquelle on peut aussi trouver des indications pour notre modèle mathématique considéré :

Définition 1 (Guide d'ondes quantique bidimensionnel).
Laplacien Dirichlet entre deux surfaces non-compactes parallèles.

Cette catégorie des guides d'ondes fournit une généralisation des bandes quantiques [22] en dimension trois et elle n'a pas, à ce jour, été abordée. Notons Ω l'espace des configurations ; par abus de notation, cet espace sera souvent confondu avec le guide d'ondes bidimensionnel. L'intérêt de cette thèse réside probablement en majeure partie dans l'étude du spectre de l'opérateur

$$-\Delta_D^{\Omega} \qquad \text{sur} \qquad L^2(\Omega) \tag{i.1}$$

défini comme l'extension de Friedrichs. La notion des surfaces parallèles, qui comprend aussi une définition exacte de Ω, sera introduite précisément dans la Section ii.1 ; cependant, nous pouvons également voir Ω comme un voisinage d'épaisseur constante construit autour d'une surface de référence Σ dans son espace normal $\mathrm{N}\Sigma$. Nous découvrirons des effets quantiques dûs à la géométrie de la surface de référence dans des conditions variées.

Un autre modèle considéré dans cette thèse est donné par une perturbation locale du guide d'ondes bidimensionnel plat Ω_0 :

Définition 2 (Guide d'ondes quantique bidimensionnel bosselé).
Laplacien Dirichlet entre deux plans parallèles dont un est déformé localement par des bosses et des creux.

Ces guides constituent une généralisation en dimension trois des bandes quantiques droites avec des bosse et des creux [7]. Nous nous intéressons avant tout à la situation où la perturbation est faible. Notons dans le cas présent Ω_λ l'espace des configurations où λ est un paramètre qui régule la petitesse de la déformation $\Omega_\lambda \setminus \Omega_0$. La dynamique quantique est alors encore décrite à l'aide de l'analyse spectrale de l'opérateur (i.1) où il faut seulement remplacer Ω par Ω_λ.

i.2 Le modèle général : *Guide d'ondes quantique*

Voici une description succincte des guides d'ondes quantiques inspirée de l'introduction de l'article [22]. Les développements récents dans le domaine de la physique des semi-conducteurs accompagnés par les progrès rapides des diverses méthodes de fabrication ont permis de produire une grande quantité de petits objets de structure cristalline très pure. Mentionnons certains d'entre eux : les *films fins* produits sur une surface isolante par des techniques épitaxiales, les *sandwichs* obtenus en combinant des films de

différents matériaux de semi-conducteur, les sandwichs de films d'épaisseurs variées que l'on l'appelle *hétérostructures*, et les *fils quantiques* obtenus par bombardement d'ions à partir des films de semi-conducteur convenablement masqués. Par la dernière méthode, on peut créer sur le substratum des graphes divers et on peut pareillement produire des *jonctions*.

De tels systèmes qui, d'un côté sont suffisamment grands pour être expérimentalement réalisables, et en même temps assez petits pour que des effets quantiques soient observables, sont appelés *systèmes mésoscopiques*. Des expériences indiquent une dépendance de leurs propriétés de conductivité eu égard à leur forme, leur courbure ou le changement de la section transverse. Pour plus d'informations sur le plan physique, voir [22, 69] et les références s'y trouvant. Récapitulons les propriétés caractéristiques de ces microstructures : (a) *petite taille* (de dix à cent nm), (b) *grande pureté* (la trajectoire libre moyenne des particules peut être de quelques μm ou même plus grande), (c) *structure cristalline*, (d) *contrainte* (les fonction propres des particules sont habituellement supprimées aux bornes entre différents matériaux de semi-conducteur).

Bien que ces systèmes soient très compliqués, on peut toutefois faire des hypothèses simplificatrices tout en préservant leurs propriétés spécifiques. Il est évident de (a) et de (b) que la trajectoire libre moyenne est en général deux ou trois ordres au dessus de la taille de la structure. Par conséquent le mouvement de particules peut être supposé *balistique* dans une approximation raisonnable, c'est-à-dire inviolé par la dispersion sur des impuretés. La simplification la plus importante vient de la propriété (c). Il est bien connu qu'une particule dans un réseau cristallin se déplace comme une particule *libre* avec une certaine masse effective $m^\star$. Une formulation de ce problème dans le cadre mathématique rigoureux peut être trouvé dans le travail [5]. En association avec (d) on voit que la dynamique à l'intérieur de la microstructure peut être modélisée comme une particule libre vivant dans une région spatiale correspondante avec *conditions aux bords de Dirichlet*. Dénotons l'espace des configurations par Ω. Si on néglige les effets dûs au spin, nous pouvons identifier l'hamiltonien de la particule avec le laplacien Dirichlet $-\Delta_D^\Omega$. Pour un ensemble Ω ouvert, cet opérateur est défini comme l'extension de Friedrichs du laplacien libre avec son domaine défini au départ sur $C_0^\infty(\Omega)$ – *cf.* [77, Sec. XIII. 15] ou [17, Chap. 6]. On a posé $\hbar^2/(2m^\star)$ égal à 1 car les valeurs de ces constantes physiques n'importent pas ici.

i.3 Sommaire des résultats connus

i.3.1 Les géométries courbes

Parmi les plus beaux résultats n'ayant pas de contreparties classiques, il y a l'*effet de localisation dû à la courbure* qui peut produire des états liés dans les guides d'ondes quantiques courbés. De tels états peuvent gêner

la propagation des ondes dans ces guides. On a en fait prédit cet effet depuis longtemps, lors des tentatives formelles de justification de la quantification sur les variétés générales [61, 56, 14, 15, 84], et c'est P. Exner et P. Šeba [40] qui ont mis en évidence ce phénomène rigoureusement. Les auteurs ont démontré à l'aide du principe de mini-max l'existence d'états liés dans les bandes infinies courbées dans le plan sous la condition que la courbure décroît rapidement à l'infini et que l'épaisseur soit constante et suffisamment petite.

Ce résultat était très étonnant parce que de telles régions n'ont aucune trajectoire classique fermée, à l'exception de quelquesunes dont l'ensemble des contitions initiales est de mesure nulle dans l'espace des phases. En substance, rien ne peut empêcher une particule classique de s'échapper à l'infini dans la bande. Dans ces systèmes, les états liés ne résultent pas de l'image "traditionnelle" où un potentiel attractif crée des régions classiquement permises et interdites, mais ici les conditions aux bords sur les frontières courbées donnent effectivement une interaction attractive. Les états liés dûs à la courbure fournissent en même temps un exemple qui montre que l'intuition basée sur les concepts semi-classiques peut s'avérer parfois trompeuse lorsque l'on traite des systèmes quantiques.

Une caractéristique du résultat initial de P. Exner et P. Šeba était que leur preuve de l'existence d'états liés ne marchait que pour les bandes suffisamment fines. Dans [40], ils précisent aussi les épaisseurs pour lesquelles leur preuve fonctionne. Ces bornes critiques sont également étudiées dans [21], tandis que [29] affaiblit substantiellement les hypothèses sur la décroissance de la courbure. Un progrès considérable a été réalisé par J. Goldstone et R. L. Jaffe [49] qui ont utilisé une fonction d'essai et effectué ainsi une démonstration variationnelle de l'existence d'états liés dans ces bandes courbées. Leur preuve n'exige pas que la bande soit fine dans le sens de [40]. En même temps, ils proposent une généralisation de leur résultat aux tubes de dimension trois.

Néanmoins il y avait toujours une question ouverte : dans les postulats de tous ces travaux a dû être inclus la condition que les frontières de ces guide d'ondes quantiques doivent être au moins quatre fois différentiables. En même temps, les états liés dans le guide d'ondes de la forme en L déterminés explicitement dans [41] ont suggéré que cette dernière condition est d'origine purement technique. L'énergie de l'état lié y est calculée et a été vérifiée expérimentalement dans les guides d'ondes électromagnétiques plats [9]. Un autre exemple de ce type sont les tubes de la forme en V [4, 10]. Un affaiblissement essentiel de l'hypothèse sur la régularité des frontières des bandes dans le plan a été réalisé dans [78], où la courbure de référence n'est pas supposée différentiable, afin de démontrer l'existence d'états liés.

L'article [22] de P. Duclos et P. Exner a été consacré à une revue et à un développement plus profond des idées formulées dans les travaux mentionnés ci-dessus. En particulier, en utilisant une méthode connue de la théorie des

opérateurs de Schrödinger [58, 73], ils ont établi une borne supérieure du nombre d'états liés dans les tubes suffisamment fins.

La méthode numérique introduite dans [68] pour les tubes avec une région courbée en arc de cercle, permet d'observer la dépendance des solutions de la courbure et de l'angle de flexion.

Le problème de diffusion dans les guides d'ondes quantiques où l'on s'intéresse particulièrement aux résonances dues à la courbure a été étudié théoriquement dans [24, 23] et numériquement dans [68].

i.3.2 Les diverses géométries

Il y a aussi d'autres formes possibles des guides d'ondes quantiques qui présentent le comportement analogue. Par exemple, un embranchement croisé de quatre bandes droites est traité dans [4] avec la même technique que les tubes de la forme en V mentionnés ci-dessus ; voir aussi [80] pour les résultats numériques.

Une preuve variationnelle analogue à celle de [49] peut être utilisée pour démontrer l'existence d'états liés dans une bande droite avec une bosse extérieure arbitrairement petite. De plus, si la perturbation est faible, on obtient également le même résultat pour les déformations plus compliquées comprenant des creux intérieurs mais tels que les bosses prédominent [7]. On y trouve alors un développement asymptotique de la valeur propre correspondante effectué par rapport au volume de la perturbation.

Une autre sorte de guides d'ondes quantiques est étudié dans [42]. On considère une paire de bandes droites parallèles dans le plan qui sont couplées latéralement par une fenêtre. On utilise aussi une preuve variationnelle afin de démontrer l'existence d'au moins un état lié pour n'importe quelle largeur de la fenêtre. Les états liés et les problèmes de diffusion sont ensuite discutés en détail à l'aide d'une méthode numérique. Dans [44, 45], on trouve quelques estimations de la valeur propre sous la condition que la fenêtre est petite. Le développement asymptotique exact de la valeur propre a été calculé dans [74].

Ce dernier modèle peut être reconsidéré de manière équivalente comme un guide d'ondes droit contenant une barrière d'épaisseur zéro qui est parallèle aux frontières de la bande. Cette barrière est tout à fait imperméable (on utilise les conditions de Dirichlet) partout sauf en un intervalle borné où elle est remplacée par une lacune transparente. Considérons maintenant une généralisation immédiate en prenant une barrière semi-perméable que l'on peut modéliser à l'aide de la distribution de Dirac avec un couplage variable. L'analyse spectrale et de diffusion de ce système a été effectuée dans les travaux [37, 38, 64, 63] et a conduit à différents effets. En particulier, on observe que les solutions numériques s'approchent des résultats de [42] aussitôt que la fonction de couplage tend vers l'infini en dehors d'un intervalle borné où elle est posée égale à zéro.

Une caractéristique commune observée dans toutes les géométries ouvertes (Ω est non-compacte) mentionnées ci-dessus est l'apparition d'états liés avec des valeurs propres au-dessous du spectre essentiel. Ces états apparaissent grâce à un certain potentiel effectif qui vient d'une déformation du guide d'ondes droit initial, ou d'un couplage entre deux ou plus de ces guides ou d'une interaction ponctuelle. On observe aussi que les valeurs propres dépendent continûment du paramètre de déformation.

Parmi les autres géométries intensivement examinées, il y a les tubes droits contenant une ou plusieurs interactions de Dirac ponctuelles [32, 31, 39], les bandes courbées en présence d'un champ électrique [30], les bandes qui sont bosselées aléatoirement [59], et finalement les guides d'ondes quantiques avec conditions aux bords autres que celles de Dirichlet [27, 18, 3, 72, 65, 28, 79, 66]. Citons aussi des systèmes de guides d'ondes où Ω est un espace euclidien $\mathbb{R}^n$ et où le mouvement de la particule est gouverné par la présence d'un potentiel, d'obstacles ou d'un champ magnétique [35, 36, 43, 33, 34, 62].

Chapitre ii

Présentation des résultats

L'organisation de cette thèse est la suivante. Dans cette partie, nous donnons un résumé détaillé des résultats obtenus qui seront présentés dans les chapitres ultérieurs. Nous ajoutons auparavant la Section ii.1 qui regroupe les définitions et notations utilisées pour une plus grande clarté de la présentation. Les Chapitres iv, v, vi et vii sont constitués de nos publications sur le problème des guides d'ondes bidimensionnels, tandis que le Chapitre viii est consacré aux résultats qui n'ont pas encore été publiés.

ii.1 Définitions et préliminaires

Il s'agit ici de définir à la fois le domaine $\Omega \subset \mathbb{R}^3$ qui va jouer le rôle de l'espace des configurations et l'opérateur $-\Delta_D^\Omega$ qui décrit la particule quantique dans cette région.

On utilise la notation en composante standard de l'analyse tensorielle [70]. Par convention, les indices de covariance sont placés en bas d'un tenseur et les indices de contravariance en haut. La valeur des indices sera $1, 2$ pour les lettres grecques et $1, 2, 3$ pour latines. Ces indices sont associés aux coordonnées (q, u) introduites ci-dessous par l'identification $(1, 2, 3) \leftrightarrow (q^1, q^2, u)$. Dans toute la suite, on adopte la convention d'Einstein qui stipule qu'un même indice placé en haut et en bas d'une même expression donne lieu à une sommation. La montée ou la descente d'un indice se fait alors par un tenseur métrique où ses composantes contravariantes sont définies comme les composantes de la matrice inverse du tenseur métrique covariant. Les dérivées partielles seront marquées par les *virgules*, par exemple $p_{,\mu} = \partial p / \partial q^\mu$, *etc.* Nous nous référons en particulier à l'ouvrage [60] pour les divers concepts de géométrie différentielle utilisés dans cette thèse.

ii.1.1 La surface de référence

Soit Σ une surface de classe C^2, complète, non-compacte, simplement connexe et plongée dans $\mathbb{R}^3$. C'est un résultat purement topologique qu'une telle variété est alors difféomorphe à $\mathbb{R}^2$. On peut la définir globalement par une représentation paramétrique régulière

$$p : \Sigma_0 \to \mathbb{R}^3 : \left\{q \equiv (q^1, q^2) \mapsto p(q)\right\}, \qquad p(\Sigma_0) = \Sigma, \tag{ii.1}$$

où Σ_0 est un ensemble ouvert dans $\mathbb{R}^2$. Avec le produit vectoriel des vecteurs tangents $p_{,\mu}$ on définit la normale unité n qui nous donne une orientation de Σ.

On introduit le tenseur métrique $g_{\mu\nu} := p_{,\mu} \cdot p_{,\nu}$ et la deuxième forme fondamentale $h_{\mu\nu} := -n_{,\mu} \cdot p_{,\nu}$ de Σ où le *point* désigne le produit scalaire usuel dans $\mathbb{R}^3$. Remarquons que $h_{\mu\nu}$ n'est pas un tenseur dans le sens strict, car elle dépend aussi de l'orientation de Σ, c'est-à-dire de la façon dont la surface est plongée dans $\mathbb{R}^3$ – *cf.* [11]. Cette remarque est également valable pour le tenseur de Weingarten $h_\mu{}^\nu = h_{\mu\rho} g^{\rho\nu}$ qui joue un rôle principal dans cette thèse, puisqu'il détermine les invariants fondamentaux de la surface, c'est-à-dire la courbure de Gauss $K := \det(h_\mu{}^\nu)$ et la moyenne $M := \frac{1}{2}\operatorname{tr}(h_\mu{}^\nu)$. On dit que la surface Σ est *asymptotiquement plate* si ces invariants "s'annulent à l'infini", ce que l'on désigne par

$$\boxed{\langle \Sigma 0 \rangle \quad K, M \xrightarrow{\infty} 0}$$

Nous préciserons cette limite plus tard dans les cas particuliers mais une définition générale peut être donnée par

$$K \xrightarrow{\infty} 0 :\Longleftrightarrow \lim_{t\to\infty} \sup_{\Sigma_t} \left|K \circ p^{-1}\right| = 0, \qquad \text{où} \quad \Sigma_t := \{x \in \Sigma \,|\, d(x, o) \geq t\},$$

o est un point fixé de Σ et $d(\cdot,\cdot)$ désigne la fonction distance Riemannienne sur la surface [53, Déf. 2.15].

En utilisant l'élément d'aire $d\Sigma = g^{\frac{1}{2}} d^2q$, où $g := \det(g_{\mu\nu})$, on peut introduire quelques quantités géométriques globales de la surface, notamment la *courbure de Gauss totale* $\mathcal{K}$ et la *courbure moyenne totale* $\mathcal{M}$ qui sont définies respectivement par les intégrales

$$\mathcal{K} := \int_\Sigma K d\Sigma \qquad \text{et} \qquad \mathcal{M}^2 := \int_\Sigma M^2 d\Sigma. \tag{ii.2}$$

La deuxième courbure intégrale existe toujours (elle peut être infinie positive), tandis que $\mathcal{K}$ est bien définie si l'on suppose

$$\boxed{\langle \Sigma 1 \rangle \quad K \in L^1(\Sigma_0, d\Sigma)}$$

ii.1.2 L'espace des configurations

Soient $a > 0$, $I := (-a, a)$ et $\Omega_0 := \Sigma_0 \times I$. On introduit alors l'application [83, Prob. 12 du Chap. 3]

$$\mathcal{L} : \Omega_0 \to \mathbb{R}^3 : \{(q, u) \mapsto p(q) + un(q)\}\,, \qquad \mathcal{L}(\Omega_0) =: \Omega, \tag{ii.3}$$

qui définit un guide d'ondes bidimensionnel Ω d'épaisseur $d := |I| = 2a$ comme l'espace entre deux surfaces parallèles $\Sigma_\pm := (p \pm an)(\Sigma_0)$ représentant les deux frontières du guide. Dans le langage général de [50] ou de [6, Sec. 2.7], le guide d'ondes Ω est le tube de rayon a autour de la surface Σ plongée dans $\mathbb{R}^3$ ou encore le a-voisinage tubulaire de Σ.

Pour que Ω soit une sous-variété de $\mathbb{R}^3$, nous demandons que l'application $\mathcal{L} : \Omega_0 \to \Omega$ soit un difféomorphisme. Si Σ était une surface compacte, on pourrait toujours assurer cette propriété en prenant a suffisamment petit, d'après [6, Thm. 2.7.12]. Dans notre cas où la surface de référence est non-compacte, nous faisons l'hypothèse directe que

$\boxed{\langle \Omega 0 \rangle \quad \Omega \text{ ne se recoupe pas}}$ *c.à.d.*, $\mathcal{L}$ est injective.

Mais il faut encore assurer que $\mathcal{L} : \Omega_0 \to \Omega$ soit une immersion, c'est-à-dire énoncer une condition qui assure l'absence de points critiques pour cette application. Pour cela, on calcule le tenseur métrique $G_{ij} := \mathcal{L}_{,i} \cdot \mathcal{L}_{,j}$ de Ω et on arrive ainsi à une forme par blocs suivante

$$(G_{ij}) = \begin{pmatrix} (G_{\mu\nu}) & 0 \\ 0 & 1 \end{pmatrix}, \qquad G_{\nu\mu} = (\delta^\sigma_\nu - uh_\nu{}^\sigma)(\delta^\rho_\sigma - uh_\sigma{}^\rho)g_{\rho\mu}\,, \tag{ii.4}$$

où on a utilisé l'identité $n_{,\mu} \cdot n_{,\nu} = h_{\mu\rho}\, g^{\rho\sigma} h_{\sigma\nu}$ qui est établie notamment dans la Proposition iv.1. Comme les valeurs propres du tenseur de Weingarten sont les courbures principales k_+, k_- de Σ, on trouve immédiatement que

$$G := \det(G_{ij}) = g\,[(1 - uk_+)(1 - uk_-)]^2 = g(1 - 2Mu + Ku^2)^2, \tag{ii.5}$$

car $K = k_+k_-$ et $M = \frac{1}{2}(k_+ + k_-)$. Cette expression définit incidemment l'élément de volume $d\Omega = G^{\frac{1}{2}} d^2q\, du$ de l'espace des configurations. Supposons

$\boxed{\langle \Omega 1 \rangle \quad a < \rho_m := (\max\{\|k_+\|_\infty, \|k_-\|_\infty\})^{-1}}$

où ρ_m peut être interprété comme le *rayon de courbure minimal* de Σ. Sous cette condition et puisque $g > 0$ sur Σ_0, on obtient $G > 0$ pour tous les points de Ω_0. En conséquence du théorème d'inversion locale [82, Thm. 2-11], l'application $\mathcal{L} : \Omega_0 \to \Omega$ est donc un difféomorphisme et la matrice inverse G^{ij} existe. Remarquons que les normes dans la définition de ρ_m sont nécessairement finies puisqu'on a supposé que l'épaisseur d du guide d'ondes est non nulle.

ii.1.3 L'hamiltonien

Dans la Section i.1, on a déjà choisi l'opérateur (i.1) comme hamiltonien quantique non-relativiste d'une particule confinée dans Ω. Il s'agit du laplacien dont la forme quadratique associée Q_D^Ω est définie comme suit

$$Q_D^\Omega(\psi,\phi) := \int_\Omega \sum_{j=1}^3 \frac{\partial\psi}{\partial x^j}\frac{\partial\phi}{\partial x^j}\, d^3x\,, \qquad \mathrm{Dom}\, Q_D^\Omega := W_0^{1,2}(\Omega),$$

où $x \equiv (x^1,x^2,x^3)$ sont des coordonnées cartésiennes dans l'espace ambiant $\mathbb{R}^3$. D'après [17, Chap. 6], cette forme est fermée sur son domaine et l'hamiltonien $-\Delta_D^\Omega$ correspondant est un opérateur non-négatif autoadjoint. Son action est simple :

$$-\Delta_D^\Omega\psi = -\sum_{j=1}^3 \frac{\partial^2\psi}{(\partial x^j)^2}\,,$$

mais il faut s'assurer que ψ soit égale à zéro sur les frontières $\partial\Omega$, ce qui est compliqué en général dans les coordonnées ambiantes.

La stratégie est d'exprimer ce laplacien dans nos coordonnés (q,u) à l'aide de l'implémentation unitaire U de $\mathcal{L}$ entre $L^2(\Omega)$ et $L^2(\Omega_0,d\Omega)$ définie par $\psi \mapsto \psi\circ\mathcal{L}$, ce qui conduit à un opérateur de la forme de Laplace-Beltrami

$$H := U(-\Delta_D^\Omega)U^{-1} = -G^{-\frac12}\partial_i G^{\frac12} G^{ij}\partial_j \qquad \text{sur} \qquad L^2(\Omega_0,d\Omega) \tag{ii.6}$$

avec la forme quadratique associée

$$Q(\psi,\phi) = \int_{\Omega_0} \psi_{,i}\, G^{ij}\, \phi_{,j}\; G^{\frac12} d^2q\, du\,, \qquad \mathrm{Dom}\, Q = W_0^{1,2}(\Omega_0,d\Omega). \tag{ii.7}$$

La norme et le produit scalaire correspondant à l'espace de Hilbert de (ii.6) seront indiqués par l'indice "G", tandis que "g" est réservé à l'espace de surface $L^2(\Sigma_0,d\Sigma)$. La structure différentielle de l'opérateur H est maintenant plus compliquée mais l'espace des configurations Ω_0 ainsi rectifié est simple pour contrôler les conditions aux bords de Dirichlet. Tout ce qui concerne les propriétés spectrales du guide d'ondes bidimensionnel est caché dans la forme (ii.7) qui est en fait l'héroïne de notre histoire.

Ultérieurement, nous utiliserons la famille des fonctions propres $\{\chi_n\}_{n=1}^\infty$ du laplacien Dirichlet $-\Delta_D^I$ sur $L^2(I)$. Elle est donnée par

$$\chi_n(u) := \begin{cases} \sqrt{\frac{2}{d}}\cos\kappa_n u & \text{si } n \text{ est impair,} \\ \sqrt{\frac{2}{d}}\sin\kappa_n u & \text{si } n \text{ est pair,} \end{cases} \tag{ii.8}$$

où $\kappa_n^2 := (\kappa_1 n)^2$ avec $\kappa_1 := \pi/d$ sont les valeurs propres correspondantes.

ii.1.4 La motivation

Nous sommes avant tout intéressés à l'*existence* d'états liés dans les guides d'ondes bidimensionnels. Si Ω est borné, le spectre de $-\Delta_D^\Omega$ est purement discret car sa résolvante est compacte [17, Thm. 6.2.3]. Pour que le phénomène de l'existence ne soit pas trivial, on suppose que Σ n'est pas bornée. Trouver des conditions suffisantes pour qu'une surface dans $\mathbb{R}^3$ soit non bornée est une question intéressante indépendamment du sujet de cette thèse [8, Sec. 6.4]. Par exemple, sous les hypothèses sur Σ déjà imposées, il suffit de supposer en plus que l'aire $|\Sigma|$ ne soit pas finie pour garantir cette propriété dans notre cas. Expliquons maintenant pourquoi l'on attend que le spectre discret de $-\Delta_D^\Omega$ soit non-vide même si l'espace des configurations Ω est non borné.

Supposons que Σ est de classe C^4. On introduit la transformation unitaire $\hat{U} : L^2(\Omega_0, d\Omega) \to L^2(\Omega_0, d\Sigma\, du) : \{\psi \mapsto (1 - 2Mu + Ku^2)^{\frac{1}{2}}\psi\}$ qui conduit à l'opérateur $\hat{H} := \hat{U}H\hat{U}^{-1}$ contenant un potentiel

$$\hat{H} = -g^{-\frac{1}{2}}\partial_i g^{\frac{1}{2}} G^{ij}\partial_j + V, \qquad V = g^{-\frac{1}{2}}(g^{\frac{1}{2}}G^{ij}J_{,j})_{,i} + J_{,i}G^{ij}J_{,j}\,, \tag{ii.9}$$

où $J := \ln(1 - 2Mu + Ku^2)^{\frac{1}{2}}$. Etudions cet hamiltonien dans la situation où le guide d'ondes bidimensionnel est *fin*, c'est-à-dire l'épaisseur est petite, $a \ll \rho_m$. Pour cela, on effectue la limite formelle $u \to 0$ dans l'expression de $\hat{H}$ en utilisant les formules (ii.4) et (ii.5). On arrive à l'opérateur $\hat{H}_q + \hat{H}_u$ sur $L^2(\Sigma) \otimes L^2(I)$ qui est découplé en deux parties

$$\hat{H}_q := -\Delta_g + K - M^2 \qquad \text{et} \qquad \hat{H}_u := -\partial_3^2 \tag{ii.10}$$

où les variables q et u sont séparés. L'hamiltonien $\hat{H}_q$ est la somme de l'opérateur de Laplace-Beltrami $-\Delta_g$ de la surface Σ exprimé dans les coordonnées q, et d'un potentiel additionnel attractif puisque d'une part $K - M^2 = -\frac{1}{4}(k_+ - k_-)^2$ est négatif et que d'autre part $K - M^2$ tend vers zéro à l'infini d'après $\langle\Sigma 0\rangle$. Remarquons que ce potentiel est identiquement égal à zéro seulement si la surface Σ est un plan ($k_+ = k_- = 0$) ou une sphère ($k_+ = k_- = cte$), ce qui est exclu aussitôt que l'on considère les surfaces non-compactes et courbées d'une manière non-triviale. En conséquence, un argument variationnel simple montre que ce potentiel crée au moins un état lié au-dessous du spectre essentiel de l'hamiltonien limite $\hat{H}_q$. On espère que cet état survivra dans les guides d'ondes de taille non nulle.

Cette observation est à la base des travaux [61, 56, 14, 15, 84] nommés au début de la Section i.3.1 ou de [71] où l'espace ambiant est une variété générale. Rappelons que ce processus limite n'est que formel puisque le spectre de l'opérateur transverse $\hat{H}_u$ diverge lorsque $d \to 0$. Néanmoins, l'intérêt à ce problème a été renouvelé récemment quand l'évolution temporelle d'une particule dans un voisinage d'une variété compacte de dimension n plongée dans $\mathbb{R}^{n+m}$ a été traitée d'une manière rigoureuse dans [47]

où le piégeage sur la variété a été réalisé par un potentiel harmonique. Remarquons aussi que le potentiel effectif serait proportionnel à $\hbar^2$ si l'on ne posait pas $\hbar$ égale à 1. Ce fait indique que l'effet de localisation dû à la courbure est un phénomène d'origine purement quantique.

ii.2 ad Chapitre iv : La courbure locale

Ce travail a fait l'objet d'une publication dans *Ukrainian Journal of Physics* sous le titre : "Locally curved quantum layers" (2000) en collaboration avec P. Duclos et P. Exner.

Dans cette partie, on suppose que Σ est une surface de classe C^∞ qui est un plan en dehors d'une partie $\mathcal{A}$ compacte courbée. Une telle surface est non bornée, asymptotiquement plate $\langle\Sigma 0\rangle$, vérifie $\langle\Sigma 1\rangle$, et la courbure de Gauss totale $\mathcal{K}$ est égale à zéro, ce que l'on peut vérifier à l'aide du théorème de Gauss-Bonnet [60, Sec. 6.3]. Les épaisseurs d des guides d'ondes bidimensionnels construits autour de Σ qui conviennent du point de vue des hypothèses $\langle\Omega 0\rangle$ et $\langle\Omega 1\rangle$ sont caractérisées uniquement par la géométrie de la partie déformée $\mathcal{A}$.

Dans la Section iv.2, nous définissons le guide d'ondes quantique bidimensionnel d'une manière générale et détaillée sans faire d'hypothèses sur la géométrie particulière de la surface de référence. La formulation correspond à celle qui a été effectuée dans la Section ii.1 précédente mais, à la place de l'opérateur unitaire (ii.9), on introduit un autre hamiltonien (iv.16), défini sur l'espace de Hilbert $L^2(\Omega_0)$.

Dans la Section iv.3, nous utilisons le fait que Σ peut être paramétrée par les coordonnées polaires usuelles $q \equiv (r, \vartheta) \in (r_0, \infty) \times S^1$ à l'extérieur d'un disque $\mathcal{B}_{r_0} \subset \Sigma$ de rayon $r_0 > 0$ qui contient $\mathcal{A}$. Pour localiser le spectre essentiel, on construit dans la Proposition iv.2 deux opérateurs de comparaison H^N et H^D en ajoutant respectivement une condition de Neumann ou Dirichlet sur la bande cylindrique $\partial\mathcal{B}_{r_0} \times I$. On trouve facilement que l'infimum du spectre essentiel est égal à κ_1^2 pour les deux hamiltoniens et comme $H^N \leq H \leq H^D$, on obtient aussi le même résultat pour H en vertu du principe du mini-max.

Le résultat essentiel concernant l'existence d'au moins un état lié, et obtenu par une méthode variationnelle, est énoncé dans le Théorème iv.3. La stratégie est de trouver une fonction d'essai $\psi \in \mathrm{Dom}\, Q$ telle que

$$\tilde{Q}[\psi] := Q[\psi] - \kappa_1^2 \|\psi\|_G^2 < 0. \tag{ii.11}$$

Grâce au principe de Rayleigh-Ritz [17, Sec. 4.5], il existe alors au moins une valeur propre de H située entre 0 et $Q[\psi]/\|\psi\|_G^2$. On commence en cherchant une suite de fonctions qui annule le fonctionnel (ii.11) dans sa limite. Il est facile de vérifier formellement que $\tilde{Q}[\chi_1] = \mathcal{K} = 0$. La raison pour laquelle on utilise cette fonction est que χ_1 est un vecteur propre généralisé d'énergie κ_1^2

du laplacien Dirichlet dans le guide d'ondes bidimensionnel droit. Comme χ_1 n'appartient pas au $\mathrm{Dom}\, Q$, on la multiplie par une fonction appropriée de variable radiale r qui est égale à 1 sur $\mathcal{B}_{r_0}$ et décroît suffisamment vite à l'infini en dehors de ce disque de telle façon que $\varphi\chi_1 \in \mathrm{Dom}\, Q$. Pour que la contribution à $\tilde{Q}[\varphi\chi_1]$ de cette régularisation soit éliminée, on considère en même temps une dilatation $r \mapsto \sigma r$ qui définit alors une famille de fonctions $\{\varphi_\sigma\}$ vérifiant $\varphi_\sigma \to 1$ ponctuellement lorsque $\sigma \to 0$. En plus, on montre que $\tilde{Q}[\varphi_\sigma\chi_1] \to 0$ lorsque $\sigma \to 0$ et $\psi_\sigma := \varphi_\sigma\chi_1$ est donc la suite désirée. Pour obtenir une valeur négative, on ajoute à ψ_σ une perturbation $\varepsilon\Theta$, où $\varepsilon \in \mathbb{R}$ et $\Theta := j^2(H - \kappa_1^2)\psi_\sigma$ avec une fonction j supportée sur une certaine partie courbée de $\mathcal{B}_{r_0} \times I$. Comme

$$\tilde{Q}[\psi_\sigma + \varepsilon\Theta] = \tilde{Q}[\psi_\sigma] + 2\varepsilon\tilde{Q}(\Theta, \psi_\sigma) + \varepsilon^2\tilde{Q}[\Theta] \tag{ii.12}$$

avec $\tilde{Q}(\Theta, \psi_\sigma) = \|j(H - \kappa_1^2)\psi_\sigma\|_G^2 > 0$ et que le deuxième et troisième morceaux de (ii.12) ne dépendent pas en fait de σ, on choisit ε assez petit et de signe négatif pour que la somme de ces deux morceaux soit négative. Il reste à choisir σ assez petit pour que la somme des trois termes soit négative. C'est un résumé de la preuve appuyée sur l'idée de [49] et [22, Thm. 2.1]. Le résultat récapitulé du Chapitre iv est alors compris dans le Corollaire iv.4.

Remarques.

a) On n'est pas obligé de supposer que la surface de référence est de classe C^∞. Il est suffisant de la prendre de classe C^2 pour obtenir tous les résultats.

b) Le résultat $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = \kappa_1^2$ est suffisant pour démontrer l'existence d'états liés au-dessous du spectre essentiel. Mais comme $\Omega \setminus \Omega_0$ est un ensemble relativement compact et $\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [\kappa_1^2, \infty)$, on voit immédiatement que tout l'intervalle $[\kappa_1^2, \infty)$ appartient aussi à ce type du spectre de l'opérateur $-\Delta_D^\Omega$.

ii.3 ad Chapitre v : La courbure globale

Ce travail a fait l'objet d'une publication qui va paraître aux *Communications in Mathematical Physics* sous le titre : "Bound States in Curved Quantum Layers" (2001) en collaboration avec P. Duclos et P. Exner.

Il s'agit essentiellement de donner ici une liste de conditions suffisantes pour que le spectre discret ne soit pas vide dans les guides d'ondes bidimensionnels plus généraux où les courbures K et M de la surface de référence ne sont pas obligées de s'annuler en dehors d'un compact. Les hypothèses $\langle\Sigma 0\rangle$ et $\langle\Sigma 1\rangle$ ne sont pas trivialement vérifiée dans ce cas-là et la courbure de Gauss totale $\mathcal{K}$ peut admettre des valeurs différentes déterminées par le comportement de la géométrie de Σ à l'infini. Dans toute la suite de cette partie, on fait l'hypothèse non-triviale que la surface admet au moins un

pôle, c'est-à-dire un point à partir duquel elle peut être paramétrée globalement par les coordonnées géodésiques polaires $q \equiv (s, \vartheta) \in (0, \infty) \times S^1$ qui sont définies à l'aide de l'application exponentielle [60, Sec. 5.3].

Dans la Section v.3 préliminaire, on introduit le guide d'ondes bidimensionnel comme dans la Section ii.1 et on discute en particulier la géométrie de Σ exprimée dans le système des coordonnées spéciales considérées.

Dans la Section v.4, la condition $\langle \Sigma 0 \rangle$ signifie que les courbures K et M tendent vers zéro uniformément par rapport à ϑ lorsque $s \to \infty$. Sous cette hypothèse, il est encore possible de localiser le spectre essentiel. On considère dans le Théorème v.2 un opérateur auxiliaire H^N obtenu à partir de H en ajoutant une condition de Neumann sur la bande $\mathcal{L}(\{s_0\} \times S^1 \times I)$. Comme $s_0 > 0$ peut être choisi arbitrairement grand et que la surface est asymptotiquement plate on obtient facilement que $\inf \sigma_{\mathrm{ess}}(H^N) \geq \kappa_1^2$. D'après le principe de minimax, cela doit être aussi vrai pour H car $H \geq H^N$.

La Section v.5 est consacrée à une recherche de la fonction d'essai appropriée pour laquelle on obtient une valeur négative de la fonctionnelle (ii.11). Rappelons que ce fait montre l'existence d'au moins un état lié de l'opérateur $-\Delta_D^\Omega$. Dans le Théorème v.3, on commence avec la fonction d'essai ψ_σ qui a été utilisée dans la section précédente où les variables s et s_0 jouent le rôle de r et r_0. Comme $\tilde{Q}[\psi_\sigma] \to \mathcal{K}$ lorsque $\sigma \to 0$, on obtient immédiatement l'existence d'états liés si la courbure de Gauss totale est négative. Si $\mathcal{K} = 0$, on pourrait ajouter la perturbation $\varepsilon\Theta$ avec la fonction Θ proposée dans la section précédente, mais on lui préfère $\Theta := ju\psi_\sigma$ où $q \mapsto j(q)$ est une fonction supportée dans une certaine partie de Σ_0 sur laquelle $\varphi_\sigma = 1$, M ne change pas le signe et cette courbure n'est pas identiquement égale à zéro. Comme $\tilde{Q}(\Theta, \psi_\sigma) = -(j, M)_g \neq 0$, on choisit ε, σ assez petits et ε d'un signe convenable pour que (ii.12) soit négative.

Si la courbure de Gauss totale est positive, on n'obtient aucun résultat avec cette fonction d'essai qui peut être écrite comme $(1 + \varepsilon ju)\psi_\sigma$. Néanmoins, le Théorème v.4 considère une autre fonction d'essai de la forme similaire $(1 + Mu)\psi_\sigma$ qui démontre l'existence d'états liés dans le cas où soit (a) l'épaisseur du guide d'ondes bidimensionnel d est suffisamment petite, soit (b) la courbure moyenne totale $\mathcal{M}$ est infinie. Dans la preuve, il faut supposer que la surface de référence soit de classe C^3 et que l'hypothèse $\langle \Sigma 2 \rangle$ $\nabla_g M \in L^2(\Sigma_0, d\Sigma)$ soit vérifiée, où ∇_g désigne la dérivée covariante sur Σ. En fait, à l'aide d'une fonction d'essai plus adaptée, il est même possible de retirer la condition $\langle \Sigma 2 \rangle$ dans le cas (a).

Même si on peut démontrer l'existence d'états liés dans une grande variété de guides d'ondes quantiques bidimensionnels grâce à ces deux fonctions d'essai introduites, la liste des conditions suffisantes obtenues ne couvrent pas tous les cas possibles où l'on attend ce phénomène. Cela reste une question ouverte sauf dans le cas où la surface de référence possède la symétrie cylindrique, cas qui est étudié dans la Section v.6.

Dans ce cas particulier, nous profitons de la connaissance d'une paramétrisation explicite de Σ via les coordonnées géodésiques polaires pour établir le comportement de la courbure moyenne M à l'infini. Notamment, comme corollaire du Lemme v.5, on obtient que si $\mathcal{K} > 0$ la courbure totale $\mathcal{M}$ est infinie, c'est-à-dire M n'est pas négligeable à l'infini dans le sens intégral. D'autre part, grâce à $\langle\Sigma 1\rangle$, on peut éliminer une telle contribution de la courbure de Gauss K en construisant une suite de fonctions d'essai localisée à l'infini. C'est l'idée essentielle de notre stratégie.

Nous supposons que $\mathcal{K} \in (0, 2\pi]$ car si $\mathcal{K} = 0$ nous avons déjà obtenu le résultat sur le spectre discret par le Théorème v.3 et les cas $\mathcal{K} < 0$ ne sont pas permis dès que Σ est une surface de révolution difféomorphe au plan. Si on prend la suite $\psi_n(s,u) := \varphi_n(s)\chi_1(u)$, où φ_n sont des fonctions appropriées de supports compacts grossissants et localisés à l'infini lorsque $n \to \infty$, la valeur de $\tilde{Q}$ en ψ_n converge vers zéro lorsque $n \to \infty$, puisqu'on suppose $\langle\Sigma 1\rangle$. On dispose donc d'une suite de fonctions qui annule $\tilde{Q}$ dans la limite. On la perturbe en ajoutant $\varepsilon_n\Theta_n$, où $\Theta_n := ju\psi_n$ avec $j(s) := s^{-1}$ et où $\{\varepsilon_n\}$ est une suite numérique. Comme $\tilde{Q}(\Theta_n, \psi_n) \sim -(\varphi_n, jM\varphi_n)_g$ pour n large et comme on sait grâce au Lemme v.5 que M n'est pas intégrable et ne change pas de signe à l'infini, on vérifie qu'un choix convenable pour ε_n est $(\varphi_n, jM\varphi_n)_g^{-1}$, parce qu'alors la somme du premier et du troisième terme de l'expression analogue à (ii.12) converge vers zéro lorsque $n \to \infty$, tandis que la limite du deuxième terme reste finie et négative. Par conséquent, on peut trouver n assez grand pour que la forme (ii.11) avec $\psi_n + \varepsilon_n\Theta_n$ soit négative.

En mettant tous les résultats ensemble, on arrive aux quatre conditions suffisantes indépendantes qui impliquent l'existence d'états liés dans les guides d'ondes quantiques bidimensionnels – *cf.* Théorème v.1 Ces conditions sont alors illustrées par des exemples.

Un cas de guide d'ondes bidimensionnel qui ne possède pas d'états liés est étudié dans la Section v.7. Il s'agit du cas où la surface de référence est un cylindre fermé par un hémisphère. Comme ce n'est pas une surface asymptotiquement plate, le spectre essentiel descend au-dessous de κ_1^2 et on montre à l'aide d'un opérateur de comparaison que, pour cette géométrie particulière, il n'y a pas d'états liés au-dessous du seuil de $-\Delta_D^\Omega$.

Remarques.

a) Parmi les surfaces possédante des pôles, citons les quadriques, les surfaces de Hadamard-Cartan et les surfaces de révolution. Néanmoins, il existe des surfaces sans pôle [52].

b) Le résultat $\inf\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \geq \kappa_1^2$ est suffisant pour démontrer l'existence d'états liés au-dessous du spectre essentiel. Certaines conditions suffisantes pour que tout l'intervalle $[\kappa_1^2, \infty)$ appartienne à ce type du spectre seront introduites dans la Section viii.1.

ii.4 ad Chapitre vi : La courbure faible

Ce travail a fait l'objet d'une publication dans *Journal of Physics A : Mathematical and General* sous le titre : "Bound States in Mildly Curved Layers" (2001) en collaboration avec P. Exner.

On a vu dans les deux sections précédentes que les guides d'ondes quantiques bidimensionnels peuvent posséder des états liés au-dessous de son spectre essentiel. Après avoir démontré leur existence, on est naturellement intéressé aux propriétés de ces états, en particulier à la taille de l'écart entre la valeur propre correspondante et le seuil du spectre essentiel. Il s'agit ici d'étudier cette question dans le cas où cet écart est petit, ce que l'on appelle la "liaison faible". Puisque les états liés dans les guides d'ondes quantiques proviennent uniquement de la courbure, on s'attend à ce que cette liaison faible se produise dans les guides d'ondes Ω faiblement courbés. Nous les modélisons en prenant une famille Σ_ε de surfaces de référence qui sont définies par l'équation $x^3 = \varepsilon f(x^1, x^2)$, où (x^1, x^2, x^3) sont des coordonnées cartésiennes dans l'espace ambiant $\mathbb{R}^3$, f est une fonction de classe C^4, et $\varepsilon > 0$ petit est alors le paramètre du couplage faible. Le guide d'ondes bidimensionnel est introduit dans la Section vi.2, où l'on présente aussi une liste des hypothèses faites sur la fonction f et le résultat principal inclus dans le Théorème vi.1. Remarquons seulement que Σ_ε sera asymptotiquement plate $\langle\Sigma 0\rangle$ si l'on fait les hypothèses que les premières dérivées de f sont bornées et que les secondes s'annulent uniformément à l'infini. Les conditions $\langle\Omega 0\rangle$ et $\langle\Omega 1\rangle$ sont vérifiées pour ε suffisamment petit.

La stratégie adaptée de [22, Sec. 4] est d'estimer l'hamiltonien (ii.9) par un opérateur de Schrödinger de la forme $-\Delta_D^{\Omega_0} + \varepsilon V(\varepsilon)$ auquel on applique la technique usuelle de Birman-Schwinger et l'on trouve ainsi le comportement asymptotique par rapport à ε de l'unique valeur propre. La marche à suivre est la suivante : dans la Section vi.3, on développe la méthode de Birman-Schwinger dans une situation générale, où Ω_0 est un voisinage tubulaire arbitraire du plan. Nous trouvons ainsi une condition nécessaire et suffisante pour que l'opérateur de Schrödinger correspondant possède un état lié unique dans le régime du couplage faible et nous déterminons un développement asymptotique de la valeur propre. Cette partie revêt un intérêt propre indépendamment de son application aux guides d'ondes quantiques. L'application à notre situation présente est alors effectuée dans la Section vi.4. Entrons maintenant dans les détails.

Dans la Section vi.3, on s'intéresse donc au spectre discret de l'opérateur

$$H_\lambda := -\Delta - \Delta_D^M + \lambda V \qquad \text{sur} \qquad L^2(\mathbb{R}^2 \times M) \tag{ii.13}$$

pour $\lambda > 0$ petit, où $-\Delta$ désigne le laplacien dans $\mathbb{R}^2$, M est un ensemble ouvert pré-compact dans $\mathbb{R}^m$ et V est une fonction réelle sur $\mathbb{R}^2 \times M$ telle que $\inf \sigma_{\mathrm{ess}}(H_\lambda) \geq \inf \sigma(-\Delta_D^M) =: \kappa_1^2$. Les autres hypothèses sur ce potentiel sont regroupées au début de cette Section vi.3. D'après le principe

de Birman-Schwinger [81], $\alpha^2 \in [0, \kappa_1^2)$ est une valeur propre de H_λ si et seulement si le nombre -1 est une valeur propre de l'opérateur intégral

$$K(\alpha) := \lambda |V|^{\frac{1}{2}} \left(-\Delta - \Delta_D^M - \alpha^2\right)^{-1} V^{\frac{1}{2}}, \tag{ii.14}$$

où $V^{\frac{1}{2}} := |V|^{\frac{1}{2}} \operatorname{sgn} V$. On écrit $K(\alpha) = L_\alpha + M_\alpha$, où L_α est un opérateur de rang un contenant la partie singulière de (ii.14) pour $\alpha = \kappa_1$. On montre à l'aide de cette décomposition que la condition $\lambda K(\alpha)\psi = -\psi$ conduit à une équation algébrique (vi.9)

$$w = \frac{\lambda}{2\pi} \left(V^{\frac{1}{2}} \chi_1, (I + \lambda M_{\alpha(w)})^{-1} |V|^{\frac{1}{2}} \chi_1 \right) \tag{ii.15}$$

où $w^{-1} := \ln(\kappa_1^2 - \alpha^2)^{\frac{1}{2}}$, et χ_1 désigne le vecteur propre de $-\Delta_D^M$ correspondant à κ_1^2. En résolvant (ii.15) pour λ petit, on arrive au développement asymptotique de w par rapport à λ et à la condition $(\chi_1, V\chi_1) \leq 0$ sous laquelle $\alpha(\lambda)^2 = \kappa_1^2 - \exp 2w(\lambda)^{-1}$ est la valeur propre associée à l'état lié. Les résultats obtenus sont énoncés dans le Théorème vi.5, tandis que le Lemme vi.4 contient les propriétés de l'opérateur M_α.

Dans la Section vi.4.1, on introduit les quantités géométriques de Σ_ε et du guide d'ondes bidimensionnel Ω_ε correspondant. En particulier, on obtient que les métriques $g_{\mu\nu}$ et G_{ij} sont uniformément elliptiques. Cela nous permet ensuite dans la Section vi.4.2 d'encadrer l'hamiltonien (ii.9) entre deux opérateurs du type (ii.13). Le potentiel est exprimé par des dérivées covariantes des courbures K et M, donc lui-même dépend maintenant du paramètre ε, mais c'est la seule différence par rapport à (ii.13). Dans la Section vi.4.3, on vérifie à l'aide du Théorème vi.5 que les deux opérateurs possèdent précisément une valeur propre et ses développements asymptotiques coïncident pour ε suffisamment petit. En conséquence du principe du minimax, on obtient ainsi le même développement asymptotique pour la valeur propre unique dans le guide d'ondes bidimensionnel qui est faiblement courbé. Dans la Section vi.4.4, on discute ce résultat dans la situation où le guide d'ondes est fin, c'est-à-dire l'épaisseur d est petite. En particulier, on obtient alors que le terme principal du développement asymptotique s'exprime à l'aide du potentiel $K - M^2$, ce qui est attendu grâce aux arguments développés dans la Section ii.1.4.

ii.5 ad Chapitre vii : Les bosses et les creux

Ce travail a fait l'objet d'une publication aux *Annales Henri Poincaré* sous le titre : "Bound States in Weakly Deformed Strips and Layers" (2001) en collaboration avec D. Borisov, P. Exner et R. Gadyl'shin.

On considère ici une autre déformation du guide d'ondes bidimensionnel droit $\Omega_0 := \mathbb{R}^2 \times (0, d)$ qui induit l'apparition d'états liés. L'espace des

configurations est défini comme Ω_0 dont on perturbe la frontière localement. Comme on s'intéresse au cas particulier où la déformation est faible, on prend une famille Ω_λ avec $\lambda > 0$ définie par

$$\phi : \Omega_0 \to \mathbb{R}^3 : \left\{(x,u) \mapsto \left(x^1, x^2, (1+\lambda v(x))\, u\right)\right\}, \qquad \phi(\Omega_0) =: \Omega_\lambda, \quad \text{(ii.16)}$$

où les coordonnées cartésiennes $x \equiv (x^1, x^2)$ paramètrent $\mathbb{R}^2$ et la fonction arbitraire $v \in C_0^\infty(\mathbb{R}^2)$ définit la bosselure.

En supprimant une composante de x dans l'application ϕ, on obtient le guide d'ondes unidimensionnel plan qui a été étudié par W. Bulla *et al.* dans [7]. Les auteurs ont démontré par la technique de Birman-Schwinger que $-\Delta_D^{\Omega_\lambda}$ possède précisément un état lié pour λ suffisamment petit si $\langle v\rangle := \int_{\mathbb{R}} v(x)\,dx > 0$. Cette condition dit que l'aire des bosses déformant Ω_0 doit être plus grande que l'aire des creux ou, en d'autres termes, que le changement de l'aire de la perturbation $\Omega_\lambda \setminus \Omega_0$ est positive. Dans ce cas-là, on montre que la valeur propre est analytique en λ et on trouve le premier terme de son développement limité. D'autre part, le spectre discret est vide si $\langle v\rangle < 0$. Pour étudier le cas limite $\langle v\rangle = 0$ dans le cadre de [7], on devrait calculer le terme suivant dans le développement limité mais cela serait très compliqué. Cependant, P. Exner et S. A. Vugalter [46] ont utilisé une méthode variationnelle pour trouver à la fois une condition sous laquelle les états liés existent aussi dans ce cas limite et une condition sous laquelle le spectre discret est vide. Néanmoins, ces conditions ne sont pas optimales, c'est-à-dire qu'elles ne couvrent pas toutes les déformations v possibles avec $\langle v\rangle = 0$.

Le but de la partie présente est double. Dans la Section vii.2, on utilise la technique de Birman-Schwinger pour généraliser le résultat de [7] aux guides d'ondes quantiques bidimensionnels définis par (ii.16). En particulier, on montre l'existence d'un état lié unique sous la condition $\langle v\rangle := \int_{\mathbb{R}^2} v(x)\,dx > 0$ et que la valeur propre correspondante peut être exprimée comme $\kappa_1^2 - \exp 2w^{-1}$, où $\lambda \mapsto w(\lambda)$ est une fonction analytique dont le développement limité à l'ordre un est calculé. Le spectre discret est vide si $\langle v\rangle < 0$ et de nouveau on n'obtient aucun résultat dans la situation limite $\langle v\rangle = 0$. C'est pourquoi on développe dans la Section vii.3 une méthode alternative qui permet de calculer facilement le terme suivant dans le développement limité. Cette approche est appliquée en même temps au cas des bandes [7] et les conditions non optimales de [46] peuvent ainsi être vérifiées. En plus, nous avons maintenant un critère général d'existence d'états liés pour une fonction v arbitraire donnée. Entrons maintenant dans les détails.

La stratégie de la Section vii.2 est de transformer l'espace des configurations compliqué Ω_λ en l'espace Ω_0 rectifié. On le réalise à l'aide de la transformation unitaire U entre $L^2(\Omega_\lambda)$ et $L^2(\Omega_0)$ définie par $\psi \mapsto G^{\frac{1}{4}}\psi \circ \phi$

qui transforme l'hamiltonien $-\Delta_D^{\Omega_\lambda}$ en l'opérateur

$$H_\lambda := U(-\Delta_D^{\Omega_\lambda})U^{-1} = -G^{-\frac{1}{4}}\partial_i G^{\frac{1}{2}} G^{ij}\partial_j G^{-\frac{1}{4}} \qquad \text{sur} \qquad L^2(\Omega_0),$$

où $G_{ij} := \phi_{,i} \,.\, \phi_{,j}$ est le tenseur métrique de Ω_λ exprimé dans les coordonnées (x, u). Remarquons qu'une technique semblable a été utilisée dans le travail récent [2]. La structure différentielle de cet opérateur est compliquée mais, en utilisant l'expression explicite pour la métrique (vii.7), on vérifie qu'on peut écrire

$$H_\lambda = -\Delta_D^{\Omega_0} + \lambda C_\lambda^* D, \tag{ii.17}$$

où C_λ et D sont des opérateurs différentiels d'ordre un et de support compact entre $L^2(\Omega_0)$ et $L^2(\Omega_0) \otimes \mathbb{C}^7$. On obtient ainsi un hamiltonien de la forme (ii.13) à la différence près que le potentiel n'est pas une fonction scalaire. Remarquons que comme Ω_0 est déformé seulement localement, on a $\sigma_{\text{ess}}(H_\lambda) = [\kappa_1^2, \infty)$. On s'intéresse à la valeur propre $\alpha^2 \in [0, \kappa_1^2)$ de H_λ qui existe d'après le principe de Birman-Schwinger – *cf.* Proposition vii.1 – si et seulement si l'opérateur

$$K_\lambda^\alpha := \lambda D\big(- \Delta_D^{\Omega_0} - \alpha^2\big)^{-1} C_\lambda^* \tag{ii.18}$$

possède le nombre -1 comme valeur propre. On écrit $K_\lambda^\alpha = \hat{L}_\lambda + \hat{M}_\lambda$, où $\hat{L}_\lambda$ contient la singularité de (ii.18) pour $\alpha = \kappa_1$, tandis que la partie régulière $\hat{M}_\lambda$ est un opérateur borné et analytique par rapport à la variable auxiliaire $w := 2[\ln(\kappa_1^2 - \alpha^2)]^{-1}$ près de zéro. On démontre cette propriété dans le Lemme vii.3 en utilisant essentiellement la borne de Schur-Holmgren – *cf.* Lemme vii.2 – et la projection de $\hat{M}_\lambda$ sur les fonctions propres χ_j de $-\Delta_D^{(0,d)}$. Après cela, on montre que la condition $\lambda K_\lambda^\alpha \psi = -\psi$ conduit à une équation algébrique de la forme (ii.15), où il faut seulement mettre respectivement $C_\lambda, \hat{M}_\lambda$ et D à la place de $V^{\frac{1}{2}}, \lambda M_\alpha$ et $|V|^{\frac{1}{2}}$. D'après le théorème des fonctions implicites, on obtient que la fonction $\lambda \mapsto w(\lambda)$ est analytique et on calcule facilement le premier terme de son développement limité qui est proportionnel à la valeur $-\langle v \rangle$. Si $\langle v \rangle > 0$, ce terme est donc négatif et en conséquence la fonction $\alpha(\lambda)^2 = \kappa_1^2 - \exp 2w(\lambda)^{-1}$ représente une valeur propre de H_λ puisqu'elle tend vers κ_1^2 par valeurs inférieures lorsque $\lambda \to 0$. Ces résultats obtenus sont énoncés dans le Théorème vii.4.

Pour étudier le spectre discret dans le cas limite $\langle v \rangle = 0$, il faut calculer le terme suivant dans le développement limité de $w(\lambda)$ et déterminer son signe. Mais ceci serait très laborieux dans le cadre de la technique de Birman-Schwinger puisque les opérateurs C_λ et $\hat{M}_\lambda$ dépendent de λ d'une manière non-triviale. Nous cherchons donc dans la Section vii.3 le développement limité par une autre méthode qui nous permet de dériver facilement les termes d'ordres supérieurs. Nous y effectuons en même temps le traitement pour différentes dimensions en complétant aussi les résultats connus sur les

bandes [7, 46] mais, pour simplifier l'exposition, nous ne décrivons dans ce résumé que le cas des guides d'ondes quantiques bidimensionnels (ii.16). D'après le résultat précédent, la fonction $\lambda \mapsto w(\lambda)$ est analytique et on peut donc écrire (vii.17)

$$w(\lambda) = -\sum_{i=1}^{\infty} \lambda^i m_i,$$

où $-m_i$ désignent alors les coefficients du développement limité cherché. Soit $f \in C_0^\infty(\mathbb{R}^2)$ telle que $\operatorname{supp} f \cap \operatorname{supp} v = \emptyset$ et $\langle f \rangle \neq 0$. La stratégie est de construire une solution $\psi_\lambda(x, u; m)$ du problème de Dirichlet (vii.18)

$$\begin{aligned} \left(\Delta + \kappa_1^2\right) \psi_\lambda = m^2 \psi_\lambda + \left[(\ln m)^{-1} - w(\lambda)\right] f\chi_1 \qquad & \text{dans} \quad \Omega_\lambda \\ \psi_\lambda = 0 \qquad & \text{sur} \quad \partial\Omega_\lambda, \end{aligned} \tag{ii.19}$$

où $-\Delta$ désigne le laplacien standard dans $\mathbb{R}^3$ et $m > 0$ car si une telle solution est bornée et ne s'annule pas pour m petit, alors $\psi_\lambda(x, u; \exp w^{-1})$ est la fonction propre de $-\Delta_D^{\Omega_\lambda}$. En écrivant (vii.19)

$$\psi_\lambda(x, u; m) = \sum_{i=0}^{\infty} \lambda^i \psi_i(x, u; m)\,,$$

on obtient un système d'équations aux dérivées partielles (vii.20)–(vii.21) pour les fonctions ψ_i dans la région droite Ω_0 mais avec des conditions aux bords $\partial\Omega_0$ plus compliquées. Chacune de ces équations peut être résolue par la méthode de Fourier standard en utilisant le Lemme vii.5 dans lequel un problème plus général est traité. On arrive ainsi aux développements limités des ψ_i par rapport à $(\ln m)^{-1}$ et à la condition (vii.25)

$$m_i = -\sqrt{\frac{2}{d}}\,\frac{\kappa_1}{\langle f \rangle} \sum_{j=1}^{i} \left\langle \frac{d^j (-v)^j}{j!} \frac{\partial^j \psi_{i-j}}{\partial u^j}(\cdot, 0; 0) \right\rangle, \tag{ii.20}$$

qui assure que les solutions sont continues par rapport à m dans le voisinage de $m = 0$ et décroissantes lorsque $|x| \to \infty$ pour $m > 0$. Comme $\psi_0(\cdot; 0) = -\langle f \rangle \chi_1/(2\pi)$, on obtient immédiatement que le premier terme du développement limité de $w(\lambda)$ coïncide avec celui qui a été trouvé par la méthode de Birman-Schwinger dans la section précédente. Dans la Section vii.3.2, on calcule le développement limité de ψ_1 qui, joint à celui de ψ_0, suffit – *cf.* (vii.27) – pour établir l'expression (vii.32) pour m_2. Comme nous l'avons souligné plusieurs fois, ce résultat est nécessaire seulement pour l'étude du cas critique $\langle v \rangle = 0$, quand le premier coefficient m_1 égale zéro car m_2 détermine alors l'ordre principal du développement limité de $w(\lambda)$. Dans cette situation, on établit dans la Section vii.3.3 le Théorème vii.7 qui confirme en outre les résultats spectraux de [46].

ii.6 ad Chapitre viii : Sur le spectre des variétés non-compactes

Dans cette section sont présentés des résultats non encore publiés qui ont été élaborés lors de l'étude du sujet de cette thèse.

L'objet de cette partie est une petite contribution à la vaste question : "Quel est le spectre d'une variété non-compacte ?" Notre guide d'ondes bidimensionnel Ω est une telle variété qui est de plus non-complète. Nous avons vu que $-\Delta_D^\Omega$ peut posséder des états liés au-dessous du spectre essentiel si la surface de référence Σ est asymptotiquement plate $\langle\Sigma 0\rangle$. Sous cette hypothèse, nous avons trouvé une borne inférieure κ_1^2 du spectre essentiel. Dans la Section viii.1, nous cherchons des conditions suffisantes pour que tout l'intervalle $[\kappa_1^2, \infty)$ soit un spectre de ce type. Les résultats analogues concernant l'analyse spectrale d'un guide d'ondes unidimensionnel sont récapitulés dans la Section viii.2. Dans la Section viii.3, nous étudions le spectre du laplacien sur les variétés non-compactes qui sont complètes et possèdent au moins un pôle. Puis nous nous concentrons sur les variété à symétrie radiale et les surfaces. Dans ces cas particuliers, nous établissons que le spectre est l'intervalle $[0, \infty)$ en posant certaines conditions supplémentaires sur la décroissance des courbures à l'infini. Entrons maintenant dans le résumé détaillé.

Soit Σ une surface de classe C^3 qui possède au moins un pôle, est asymptotiquement plate $\langle\Sigma 0\rangle$, et vérifie l'hypothèse $\langle\Sigma 1\rangle$. La Section viii.1.1 est consacrée à l'étude de la géométrie d'une telle variété paramétrée par les coordonnées géodésiques polaires. Considérons autour de Σ un guide d'ondes bidimensionnel Ω qui vérifie $\langle\Omega 0\rangle$ et $\langle\Omega 1\rangle$. Dans le Théorème v.2, nous avons établi que le seuil du spectre essentiel de $-\Delta_D^\Omega$ est minoré par la valeur κ_1^2 mais la question est de savoir si tout l'intervalle $[\kappa_1^2, \infty)$ appartient au spectre essentiel. Dans le Théorème viii.5 de la Section viii.1.2, nous montrons que c'est le cas si on suppose en plus que les deux conditions suivantes sont vérifiées

$$\langle\sigma 1\rangle \quad h_{\mu\,;\rho}^{\ \ \nu} \xrightarrow{\infty} 0, \qquad \langle\sigma 2\rangle \quad k_g \xrightarrow{\infty} 0.$$

Ici, nous notons par le *point-virgule* la dérivée covariante et k_g désigne la courbure géodésique des cercles géodésiques sur Σ. La stratégie est de construire une suite de Weyl pour l'opérateur H et pour toutes les valeurs de l'intervalle $[\kappa_1^2, \infty)$. On définit

$$\hat{\psi}_n(s,u) := \Big(\langle r\rangle^{-\frac{1}{2}} \jmath_n\Big)(s)\, \chi_1(u)\, e^{i\lambda s} \tag{ii.21}$$

où $\lambda \in \mathbb{R}^+$, $\langle r\rangle$ désigne le périmètre des cercles géodésiques, et $\jmath_n$ est une suite de fonctions à supports compacts grossissants et localisés à l'infini lorsque $n \to \infty$. En utilisant $\langle\Sigma 0\rangle$, $\langle\sigma 1\text{–}2\rangle$ et $\langle\Sigma 1\rangle$, on montre que la famille des fonctions $\{\hat{\psi}_n / \|\hat{\psi}_n\|_G\}_{n=1}^\infty$ constitue la suite de Weyl désirée. Remarquons que $\langle\sigma 1\rangle$ est une hypothèse covariante tandis que $\langle\sigma 2\rangle$ doit être

vérifiée dans les coordonnées géodésiques polaires. Dans la Section viii.1.3, nous montrons que $\langle \sigma 2 \rangle$ peut être éliminée si Σ est une surface de révolution.

La Section viii.1.4 est constituée des *addenda* concernant ce cas particulier où l'on peut décomposer l'hamiltonien $-\Delta_D^\Omega$ par rapport aux sous-espaces des moments angulaires. Nous introduisons deux approches alternatives pour établir cette décomposition. La première utilise le fait que Ω peut être reconstruit en connaissant seulement la courbure de la courbe du profil tandis que dans la deuxième, on transforme l'opérateur H par une implémentation unitaire d'un changement de métrique. Les deux approches conduisent à une somme directe d'opérateurs de la forme d'un hamiltonien d'une bande dans le plan avec un terme centrifuge additionnel.

Dans la Section viii.2, nous utilisons l'analyse spectrale développée dans le Chapitre v et dans la Section viii.1 pour récapituler et préciser les résultats connus dans le cas des guides d'ondes quantiques unidimensionnels [22]. La région Ω est maintenant une bande infinie dans le plan dont l'épaisseur est constante. En particulier, nous obtenons qu'il suffit de supposer que la courbure de la courbe de référence s'annule à l'infini pour démontrer l'existence d'états liés. En d'autres termes, on n'est pas obligé de faire une hypothèse quelconque sur la dérivée de la courbure pour obtenir ce résultat. Par contre, la condition que cette dérivée s'annule à l'infini garantit que le spectre essentiel de $-\Delta_D^\Omega$ coïncide avec l'intervalle $[\kappa_1^2, \infty)$, c'est-à-dire qu'il n'y a pas de lacunes.

La Section viii.3 est consacrée à l'analyse spectrale du laplacien sur une variété de dimension n non-compacte et complète. Nous rappelons au début certains résultats connus qui garantissent que le spectre est l'intervalle $[0, \infty)$. Comme l'opérateur considéré est positif, le spectre est donc purement essentiel. Nous établissons ensuite d'autres conditions suffisantes garantissant cette propriété. Le laplacien est introduit dans la Section viii.3.1 où l'on fait aussi l'hypothèse sur l'existence d'au moins un pôle sur la variété et où l'on exprime la métrique dans les cordonnées géodésiques polaires.

Dans la Section viii.3.2, nous étudions la situation où la variété de classe C^3 a une symétrie radiale. En conséquence, le laplacien admet une décomposition par rapport aux sous-espaces des moments angulaires et il est unitairement équivalent à une somme directe d'opérateurs $\hat{H}_\ell$ unidimensionnels. Chacun des $\hat{H}_\ell$ est un opérateur sur $L^2(\mathbb{R}^+)$ qui est constitué de la somme du laplacien unidimensionnel avec le potentiel centrifuge standard et le potentiel (viii.23)

$$V := -\frac{n-1}{2}\, K(s) + \frac{(n-1)(n-3)}{4} \left[\frac{\dot{r}(s)}{r(s)}\right]^2 . \tag{ii.22}$$

Ici K désigne la courbure sectionnelle radiale (la courbure de Gauss dans le cas des surfaces) et r est la solution de l'équation de Jacobi (viii.1)

$$\ddot{r} + K\, r = 0 \qquad \text{avec} \qquad r(0,\vartheta) = 0,\ \dot{r}(0,\vartheta) = 1. \tag{ii.23}$$

La partie centrifuge ne contribue pas au mode $\ell = 0$ et comme le spectre d'une somme directe d'opérateurs est égal à la réunion des spectres individuels, il suffit de démontrer que $[0, \infty)$ appartient au spectre de $\hat{H}_0$.

D'après le critère de Weyl, cela sera vrai si l'on trouve une suite d'intervalles sur $\mathbb{R}^+$ qui vérifie les conditions suivantes : 1) la taille des intervalles grossit pour qu'on puisse éliminer la contribution de l'énergie cinétique de $\hat{H}_0$ en choisissant des fonctions d'essai appropriées localisées sur ces intervalles ; 2) la restriction du potentiel V sur ces intervalles tend vers zéro. Comme nous supposons que la courbure K s'annule à l'infini on est conduit à imposer que ces intervalles tendent vers l'infini. Bien que ne sachant pas si le deuxième terme du potentiel (ii.22) tend aussi vers zéro à l'infini, nous avons réussi à démontrer que c'était le cas au moins sur une suite d'intervalles bien choisie tendant vers l'infini et sous l'hypothèse supplémentaire que la courbure totale correspondant à K existe. La stratégie est d'étudier séparément tous les comportements possibles de $\dot{r}r^{-1}$ et d'utiliser ensuite l'équation de Jacobi (ii.23). La démonstration détaillée est effectuée dans la preuve du Théorème viii.12 qui dit que le spectre d'une variété à symétrie radiale, complète, simplement connexe et non-compacte est égale à $[0, \infty)$ sous la condition que K s'annule à l'infini et que la courbure totale existe.

Dans la Section viii.3.3, nous considérons une variété de dimension $n = 2$ qui possède au moins un pôle mais n'a pas nécessairement une symétrie radiale. En construisant une suite de Weyl d'une façon similaire à celle dans le Théorème viii.5, nous montrons que $[0, \infty)$ constitue le spectre d'une telle surface sous la condition que $K \to 0$ lorsque $s \to \infty$ et sous les hypothèses additionnelles $\langle \Sigma 1 \rangle$ et $\langle \sigma 2 \rangle$.

Chapitre iii

Conclusion

Dans ce travail, nous avons étudié les propriétés spectrales du laplacien Dirichlet $-\Delta_D^\Omega$ sur une variété Ω de dimension trois plongée dans l'espace euclidien $\mathbb{R}^3$. Il s'agit du voisinage tubulaire d'épaisseur d constante qui est construit autour d'une surface Σ complète et difféomorphe au plan. Nous avons appelé ce système *guide d'ondes quantique bidimensionnel* puisque $-\Delta_D^\Omega$ réalise un modèle raisonnable pour l'hamiltonien quantique d'une particule vivant dans un film conducteur déposé sur une surface isolante. L'adjectif "bidimensionnel" provient du fait que l'épaisseur de ces films est d'ordre bien inférieur à celui de la taille longitudinale donc le transport éventuel se passe le long de la surface de référence.

La géométrie différentielle des courbes dans le plan est relativement plus facile à étudier que celle des surfaces dans l'espace. C'est sans aucun doute pourquoi les premiers résultats spectraux du laplacien Dirichlet sur les domaines tubulaires ont été obtenus dans les guides d'ondes unidimensionnels, c'est-à-dire dans les cas où Ω est une bande d'épaisseur constante dans le plan. Il est maintenant bien connu [22] que l'opérateur $-\Delta_D^\Omega$ correspondant possède toujours des états liés au-dessous du spectre essentiel, dès que la bande est courbée et asymptotiquement droite. Des résultats analogues ont été obtenus aussi pour les tubes dans $\mathbb{R}^3$ mais la généralisation au cas des guides modelés sur une surface n'avaient pas encore été traitée.

C'est l'objet principal de cette thèse de montrer que l'*effet de localisation dû à la courbure* se réalise aussi dans les guides d'ondes quantique bidimensionnels. La différence essentielle à retenir est que la surface de référence Σ possède deux invariants fondamentaux, la courbure moyenne et la courbure de Gauss. Alors que la première courbure peut être considérée comme l'analogue de la courbure ordinaire d'une courbe dans le plan, la courbure de Gauss est une caractéristique nouvelle n'ayant aucune contrepartie dans les guides d'ondes unidimensionnels. En conséquence, la méthode standard pour démontrer l'existence d'états liés adaptée du cas unidimensionnel ne marche que pour certaines classes de guides d'ondes bidimensionnels –

cf. Théorème v.3. En particulier, on obtient sans difficulté le résultat pour les guides d'ondes construits autour des surfaces à la *courbure de Gauss totale* non-positive, c'est-à-dire les surfaces qui sont "suffisamment ouvertes" à l'infini. Un contre-exemple où cette courbure totale est strictement positive est fourni par le paraboloïde de révolution.

Pour inclure des cas de guides d'ondes autour des surfaces à courbure de Gauss totale positive, il a donc fallu développer de nouvelles méthodes. Notamment au Chapitre v, nous introduisons deux fonctions d'essai originales qui conduisent aussi, à l'aide d'une preuve variationnelle, à l'existence d'états liés dans les guides d'ondes bidimensionnels ayant la symétrie cylindrique, ou ayant l'épaisseur d suffisamment petite, ou qui sont construits autour d'une surface à la courbure moyenne totale infinie avec le gradient de la courbure moyenne est L^2-intégrable. Néanmoins, nos conditions suffisantes ne couvrent pas tous les cas possibles des guides d'ondes bidimensionnels où l'on attend des états liés. Il reste, par exemple, à démontrer que le guide d'ondes correspondant à la surface sans la symétrie cylindrique ou l'épaisseur suffisamment petite possède des états liés même si la courbure moyenne n'est pas L^2-intégrable – *cf.* Exemple 6 du Chapitre v.

Un autre problème que nous avons rencontré lors des tentatives de généralisation des guides d'ondes unidimensionnels a concerné la question de savoir comment on pourrait paramétrer effectivement la surface de référence Σ. Nous rappelons qu'on peut toujours paramétrer globalement une courbe par sa longueur d'arc. Dans le cas des surfaces, la paramétrisation analogue est fournie par les *coordonnées géodésiques polaires* mais toutes les surfaces ne peuvent pas être paramétrées globalement de cette façon. Même si nous avons supposé l'existence de telles coordonnées globale sur Σ pendant tout le Chapitre v, nous ne l'avons fait qu'à cause de raisons techniques pour disposer d'une paramétrisation simple de la surface de référence. Néanmoins, il serait suffisant de considérer cette sorte de paramétrisation seulement à l'extérieur d'une partie compacte de Σ mais cette question n'est pas encore complètement résolue. L'idée est similaire à celle du Chapitre iv où nous avons étudié les guides d'ondes bidimensionnels construits atour d'un plan déformé localement. Ici, la courbure de Gauss totale est égale à zéro et l'existence d'états liés découle donc du Chapitre v sous la condition que le plan déformé peut être paramétré par les coordonnées géodésiques polaires. Cependant, la stratégie du Chapitre iv montre qu'on peut se passer de cette hypothèse additionnelle puisqu'on dispose des coordonnées polaires usuelles dans le plan à l'extérieur de la partie courbée, et ce fait est suffisant pour obtenir tous les résultats spectraux.

Pendant toute l'étude, nous avons supposé que la surface de référence est difféomorphe à $\mathbb{R}^2$. En conséquence, une telle surface est nécessairement simplement connexe et elle peut être paramétrée par une seule carte. Les cas où Σ n'est pas simplement connexe pourraient être englobés en considérant plusieurs cartes. Cette généralisation concerne, par exemple, les surfaces avec

poignées variées et constitue une direction de la recherche future, excepté les surfaces possédant la symétrie cylindrique en dehors d'une partie courbée où c'est trivial. Une autre question ouverte est d'englober les surfaces qui ne sont pas de classe C^2.

Les états liés, dont l'existence avait été établie dans les Chapitres iv et v, ont été étudiés plus profondément dans le Chapitre vi. Nous nous sommes concentrés sur les guides d'ondes bidimensionnels qui sont *faiblement courbés*. Pour trouver le développement asymptotique de la valeur propre par rapport au paramètre décrivant ce couplage faible, nous avons généralisé la méthode utilisée pour la situation analogue dans les guides d'ondes unidimensionnels [22, Sec. 4]. Comme l'appareil principal que nous avons employé a été basé sur la technique de Birman-Schwinger d'un opérateur de Schrödinger dans un voisinage tubulaire de dimension quelconque du plan, nous croyons qu'on pourrait de la même façon traiter les guides d'ondes bidimensionnels construits dans les espaces euclidiens de dimensions plus grandes que trois.

Plus généralement, un domaine de recherche future pourrait être l'extension du concept des guides d'ondes bidimensionnels dans la direction suivante : alors que nous avons supposé que Ω est un voisinage tubulaire d'une surface Σ dans $\mathbb{R}^3$ on pourrait aussi étudier les situations où la surface est plongée dans $\mathbb{R}^n$ avec $n \geq 3$ ou encore dans une variété Riemannienne générale de dimension n.

Dans le Chapitre vii, nous étudions le guide d'ondes bidimensionnel droit mais avec une frontière déformée localement par des *bosses* et des *creux*. Nous généralisons la méthode de Birman-Schwinger utilisée dans le cas unidimensionnel correspondant [7] et trouvons ainsi le premier terme du développement limité de la valeur propre unique par rapport au volume de déformation. Nous estimons ici que notre formulation du problème et la "rectification" successive du guide d'ondes déformé est plus accessible dans notre approche géométrique qui utilise le formalisme tensoriel. En plus, pour établir aussi le deuxième terme du développement limité qui joue un rôle principal dans le cas critique où le volume de déformation égale zéro, nous développons une nouvelle méthode qui est en même temps applicable aux guides d'ondes unidimensionnels. On pense que les résultats obtenus par la technique de Birman-Schwinger dans la première partie peuvent être généralisés facilement au cas où l'on considère à la place de l'ensemble transversal $(0, d)$ une région arbitraire de $\mathbb{R}^m$ avec $m \geq 1$ qui est bornée, connexe et ouverte.

Le *spectre essentiel* des guides d'ondes bidimensionnels a été étudié dans la première partie du Chapitre viii. En utilisant le critère de Weyl, nous avons trouvé certaines conditions suffisantes pour que ce spectre soit égal au spectre du guide d'ondes droit. Comme cette analyse est nouvelle même pour les guides d'ondes unidimensionnels, nous avons précisé dans la Section viii.2 les résultats spectraux connus dans ce cas-là.

Dans la Section viii.3, nous avons abordé le problème du *spectre d'une variété complète et non-compacte* de dimension $n \geq 1$ qui est paramétrée par les coordonnées géodésiques polaires. Sous certaines hypothèses appropriées sur la décroissance des courbures, nous avons montré que le spectre était constitué de tout l'intervalle $[0, \infty)$ dans les cas à symétrie radiale ou le cas $n = 2$. Une question ouverte est d'englober aussi les variétés générales qui ne peuvent pas être paramétrée par les coordonnées géodésiques polaires.

Parmi les recherches en perspective dans le domaine des guides d'ondes bidimensionnels, en plus de toutes les améliorations et généralisations ayant déjà été nommées dans cette conclusion, il y a aussi les problèmes de diffusion et de résonance. Par ailleurs, il serait particulièrement intéressant d'étudier plus précisément les propriétés des états liés par des méthodes numériques.

Deuxième partie

Chapitre iv

La courbure locale

Résumé

Nous considérons une particule quantique dans un voisinage tubulaire d'épaisseur constante construit dans $\mathbb{R}^3$ autour d'une surface infinie de classe C^∞. Nous supposons que la surface est un plan déformé localement et que les frontières de l'espace tubulaire sont impénétrables. Sous ces hypothèses, nous démontrons que l'hamiltonien de la particule possède des états liés dûs à la géométrie.

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Notation

Afin d'éviter les malentendus, nous fournissons ici un tableau qui compare la notation de ce chapitre à celle présentée initialement dans le Chapitre ii.

notation de ce Chapitre iv	notation du Chapitre ii
ϕ	$\mathcal{L}$
$\mathsf{Tot}(\Sigma)$	$\mathcal{K}$
$\hat{H}$	H
$\hat{U}$	U
H	$G^{\frac{1}{4}} H G^{-\frac{1}{4}}$
U	$G^{\frac{1}{4}} U$
$q[\cdot]$	$Q[\cdot]$
$t[\cdot]$	$\tilde{Q}[\cdot]$

Locally curved quantum layers

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We consider a quantum particle constrained to a curved layer of a constant width built over an infinite smooth surface. We suppose that the latter is a locally deformed plane and that the layer has the hard-wall boundary. Under this assumptions we prove that the particle Hamiltonian possesses geometrically induced bound states.

iv.1 Introduction

Relations between geometry and spectral properties are one of the trademark topic of mathematical physics, in fact, an abstraction of various acoustic problems can be found in the roots of this discipline. For a long time, however, it seemed that such questions were restricted to the area of classical physics. This was mostly because geometrical properties of quantum systems were supposed to result from their dynamics, and as such they were not accessible to experimenters choice and manipulation. Interesting results dependent on geometry existed, of course, such as chaotic behaviour of certain quantum billiards observed first in [BGS] and studied in numerous subsequent papers, but they remained to be mostly academic exercises.

The situation has changed dramatically with the advent of mesoscopic techniques which allow us to produce tiny structures of various shapes devised and reproducible in the laboratory and yet small enough to exhibit quantum effects. Moreover, the physical nature of these objects makes it possible to describe them by a simple model in which a free particle (with an effective mass) is confined to the spatial region of the structure – see [DE] and references therein – borrowing the terminology one can speak about quantum waveguides, resonators, *etc.*

Theoretical studies of such systems have brought interesting results, some of them being purely quantum, without a classical counterpart. Among the most beautiful is the binding effect of curvature due to which infinitely extended regions with hard walls and a constant width can exhibit localized states. The effect was in fact observed a long time ago – see, *e.g.*, [dC1, dC2, Tol] and references therein – in formal attempts to justify quantization on nontrivial manifolds, but only in [EŠ] it was placed into a proper quantum-waveguide context and the existence of geometrically induced discrete spectrum for a curved planar strip was rigorously proven. This was followed by numerous other studies in which the results were improved and properties of the bound states were investigated – see, *e.g.*, [DE, GJ, RB].

Much less is known about analogous system in higher dimensions starting from the physically interesting case of a curved layer. This may seem strange at a glance, since the leading term of the effective potential for a general n-dimensional manifold in $\mathbb{R}^{m+n}$ was computed more than two decades ago [Tol]. However, going beyond the formal limit of infinitely thin layer one has to be able to estimate the next terms which is not an easy task. The aim of the present paper is to stimulate an investigation of the "two-in-three" case; we will concentrate at the simplest case where the deformation of a planar layer is infinitely smooth and compactly supported.

Let us describe the contents of the paper. In the next section we will formulate the problem and introduce a technique to handle it based on a suitable change of coordinates. The main results are given in Section iv.3. We will show first that under our assumption the essential spectrum starts at the first transverse eigenvalue. Then we will present a variational argument showing that a local deformation of the layer pushes the bottom of the spectrum below this value inducing thus a nonempty discrete spectrum. Properties of these bound states will be discussed elsewhere.

iv.2 Formulation of the problem

Let Σ_0 be an open set in $\mathbb{R}^2$; its points will be denoted by $q = (q^1, q^2) \in \mathbb{R}^2$. Let a regular and simple *surface* Σ of class $\boldsymbol{C}^\infty$ in the space $\mathbb{R}^3$ be given by a mapping

$$p : \Sigma_0 \to \mathbb{R}^3 : \{q \mapsto p(q) \in \Sigma\} \tag{iv.1}$$

such that the vectors $p_{,\mu} \equiv \partial_\mu p := \partial p/\partial q^\mu$, $\mu = 1, 2$, are linearly independent. We have in mind in this paper surfaces diffeomorphic to the plane, but since we will use different parametrizations, it is reasonable to consider Σ_0 generally as a subset of $\mathbb{R}^2$. Under the linear independence condition a unit normal of the surface

$$n : \Sigma_0 \to \mathbb{R}^3 : \left\{ q \mapsto n(q) := \frac{p_{,1} \times p_{,2}}{|p_{,1} \times p_{,2}|} \in \mathbb{R}^3 \right\} \tag{iv.2}$$

is a well-defined smooth function, which defines an orientation of Σ. Together they determine a *layer* Ω of a width $d = 2a > 0$ over the surface Σ by virtue of the mapping

$$\phi : \Omega_0 \to \mathbb{R}^3 : \{(q, u) \mapsto \phi(q, u) := p(q) + un(q) \in \Omega\}, \tag{iv.3}$$

where $\Omega_0 := \Sigma_0 \times (-a, a)$.

iv.2.1 Properties of the reference surface

Recall first basic facts about the three fundamental forms of Σ. The coefficients of the first fundamental form $\mathbf{I}$ of the surface can be identified with the covariant components of its *metric tensor*

$$g_{\mu\nu} := p_{,\mu} \cdot p_{,\nu} \qquad g := \det(g_{\mu\nu}) \tag{iv.4}$$

while for the second one, $\mathbf{II}$, we use the common notation

$$h_{\mu\nu} := -n_{,\mu} \cdot p_{,\nu} \qquad h := \det(h_{\mu\nu}). \tag{iv.5}$$

The Weingarten map h^ν_μ (*cf.* [Kli, Def. 3.3.4 & Prop. 3.5.5]) determines the *Gauss curvature* of Σ, $K := \det(h^\nu_\mu) = \frac{h}{g}$, and its *mean curvature*, $M := \frac{1}{2}\operatorname{Tr}(h^\nu_\mu) = \frac{1}{2}g^{\mu\nu}h_{\mu\nu}$. The third fundamental form $\mathbf{III} := (n_{,\mu}\,.\,n_{,\nu})$ may be expressed by means of the first and second fundamental forms as follows :

Proposition iv.1. $n_{,\mu}\,.\,n_{,\nu} = -Kg_{\mu\nu} + 2Mh_{\mu\nu} = h_{\mu\rho}\,g^{\rho\sigma}\,h_{\sigma\nu}$

Proof : The first relation is equivalent to the identity $\mathbf{III} - 2M\mathbf{II} + K\mathbf{I} = 0$ – *cf.* [Kli, Prop. 3.5.6] or [LR, Problem 7.53] for a general dimension. To prove the second one, we use the fact that K, M are determined by the characteristic equation

$$k_\pm^2 - 2Mk_\pm + K = 0, \tag{iv.6}$$

where k_+, k_- are the *principal curvatures*, *i.e.* the eigenvalues of h^σ_μ. Let $T^\pm_\sigma$ be the principal direction, *i.e.* the eigenvector of h^σ_μ, corresponding to $k_\pm$. Multiplying (iv.6) by this vector we get $h^\rho_\mu h^\sigma_\rho T^\pm_\sigma - 2Mh^\sigma_\mu T^\pm_\sigma + K\delta^\sigma_\mu T^\pm_\sigma = 0$. Since the principal directions forms locally an orthogonal basis in $\mathbb{R}^2$, the same must hold in the matrix sense, $h^\rho_\mu h^\sigma_\rho - 2Mh^\sigma_\mu + K\delta^\sigma_\mu = 0$. The desired equality is then obtained by multiplication with $g_{\sigma\nu}$. ∎

Remark. We use the standard *summation convention* about repeated indices; the Greek and Latin ones run through $1, 2$ and $1, 2, 3$, respectively. The indices are associated with the above coordinates by $(1, 2, 3) \leftrightarrow (q^1, q^2, u)$. Furthermore, upper and lower indeces denote components of contravariant and covariant tensors, respectively. Indices are raised and lowered by the corresponding metric tensor. For instance, the matrix of the Weingerten map is given by $h^\nu_\mu = h_{\mu\rho}\,g^{\rho\nu}$. The same applies to the metric tensor G_{ij} in the layer Ω which we shall introduce below.

Next we use the Jacobian $g^{\frac{1}{2}}$ to write down the invariant surface element

$$d\Sigma := g^{\frac{1}{2}}d^2q \equiv g^{\frac{1}{2}}dq^1dq^2.$$

It makes it possible to define a global quantity characterizing Σ, namely the *total curvature* of our surface as

$$\mathsf{Tot}(\Sigma) := \int_\Sigma K d\Sigma.$$

Suppose that $\mathcal{G} \subset \Sigma$ is a region encircled by a simple closed curve $\mathcal{C}$ of class $\boldsymbol{C}^2$, then the Gauss-Bonnet theorem [LR, 7.6.45] claims that

$$\mathsf{Tot}(\mathcal{G}) + \oint_{\mathcal{C}} k_g d\ell = 2\pi, \tag{iv.7}$$

where k_g is the geodesic curvature of $\mathcal{C}$ (traversed in the positive sense) and ℓ denotes its arc length. For the purpose of this paper it is important that the geodesic curvature of a circle in the plane is equal to its reciprocal radius. Consequently, an infinite surface obtained by a compactly supported deformation of a plane has $\mathsf{Tot}(\Sigma) = 0$.

iv.2.2 Metric properties of the layer

It is clear from the definition (iv.3) that the metric tensor of the layer as a manifold in $\mathbb{R}^3$ is of the following form

$$G_{ij} := \phi_{,i}\,.\,\phi_{,j} \qquad (G_{ij}) = \begin{pmatrix} G_{11} & G_{12} & 0 \\ G_{12} & G_{22} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{iv.8}$$

where $G_{\mu\nu} = g_{\mu\nu} - 2\,u\,h_{\mu\nu} + u^2\,n_{,\mu}\,.\,n_{,\nu}$. In view of Proposition iv.1 we can rewrite the last expression as

$$G_{\mu\nu} = g_{\mu\rho}(\delta^\rho_\sigma - uh^\rho_\sigma)(\delta^\sigma_\nu - uh^\sigma_\nu), \tag{iv.9}$$

which makes it easy to compute the determinant because the matrix of the Weingarten map h^ν_μ has the principal curvatures k_+, k_- as eigenvalues. Hence

$$G := \det(G_{\mu\nu}) = g\,[(1-uk_+)(1-uk_-)]^2 = g(1-2Mu+Ku^2)^2, \tag{iv.10}$$

where in the second step we employed the relations $K = k_+k_-$ and $M = \frac{1}{2}(k_+ + k_-)$. As above,

$$d\Omega := G^{\frac{1}{2}}d\Omega_0 \equiv G^{\frac{1}{2}}d^2q\,du$$

defines the volume element of the layer.

The "straightening" transformation employed below requires that the mapping ϕ defining the layer is a diffeomorphism. In view of the regularity assumptions imposed on Σ and the inverse function theorem it is sufficient that $G_{\mu\nu}$ has an inverse bounded uniformly in Ω. This imposes a restriction of the layer thickness d. Define $\rho_m := (\max\{\|k_\nu(q)\|_\infty : \nu = \pm,\, q \in \Sigma_0\})^{-1}$. It follows from (iv.9) that $G_{\mu\nu}$ can be estimated by the surface metric,

$$C_- g_{\mu\nu} \le G_{\mu\nu} \le C_+ g_{\mu\nu}, \tag{iv.11}$$

where the constants $C_\pm := \left(1 \pm a\rho_m^{-1}\right)^2$ are well defined since $\rho_m > 0$ by definition. Hence for a smooth surface Σ the bijectivity of ϕ is ensured as long as $a < \rho_m$.

iv.2.3 Various expressions of the Hamiltonian

After these preliminaries let us define the Hamiltonian $\tilde{H}$ of our model. As we have said, the particle is supposed to be free within Ω and the boundary of the layer is a hard wall, *i.e.*, the wavefunctions should satisfy the Dirichlet boundary condition there. For the sake of simplicity we set the Planck's constant $\hbar = 1$ and the effective mass of the electron $m_* = 1/2$; then $\tilde{H}$ can be identified with the Dirichlet Laplacian

$$\tilde{H} := -\Delta_D^\Omega \quad \text{on} \quad \boldsymbol{L}^2(\Omega), \tag{iv.12}$$

which is defined for an open set $\Omega \subset \mathbb{R}^3$ as the Friedrichs extension of the operator $-\Delta$ with the domain $\boldsymbol{C}_0^\infty(\Omega)$ – *cf.* [RS, Sec. XIII.15].

A natural way to investigate the operator (iv.12) is to pass to the intrinsic coordinates (q, u) in which it acquires the Laplace-Beltrami form,

$$\hat{H} := -G^{-\frac{1}{2}}\partial_i G^{\frac{1}{2}} G^{ij}\partial_j \quad \text{on} \quad \boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}}d^2q\,du). \tag{iv.13}$$

To find its action explicitly, we employ (iv.8) together with the expression of the determinant (iv.10). Then $\hat{H}$ splits into a sum of two parts,

$$\hat{H} = \hat{H}_1 + \hat{H}_2,$$

given by

$$\hat{H}_1 = -G^{-\frac{1}{2}}\partial_\mu G^{\frac{1}{2}} G^{\mu\nu}\partial_\nu = -\partial_\mu G^{\mu\nu}\partial_\nu - \frac{1}{2}G^{-1}G_{,\mu}\,G^{\mu\nu}\partial_\nu \tag{iv.14}$$

$$\hat{H}_2 = -G^{-\frac{1}{2}}\partial_3 G^{\frac{1}{2}}\partial_3 = -\partial_3^2 - 2\,\frac{Ku - M}{1 - 2Mu + Ku^2}\,\partial_3\,. \tag{iv.15}$$

The above coordinate change is nothing else than the unitary transformation

$$\hat{U} : \boldsymbol{L}^2(\Omega) \to \boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du) : \{\psi \mapsto \hat{U}\psi := \psi \circ \phi\}$$

which relates the two operators by $\hat{H} = \hat{U}\tilde{H}\hat{U}^{-1}$.

At the same time, it is useful to have an alternative form of the Hamiltonian which is symmetric w.r.t. G and has the Jacobian removed from the inner product. It is obtained by another unitary transformation,

$$U : \boldsymbol{L}^2(\Omega) \to \boldsymbol{L}^2(\Omega_0) : \{\psi \mapsto U\psi := G^{\frac{1}{4}} \psi \circ \phi\},$$

which leads to the unitarily equivalent operator

$$H := U\tilde{H}U^{-1} = -G^{-\frac{1}{4}} \partial_\mu G^{\frac{1}{2}} G^{\mu\nu} \partial_\nu G^{-\frac{1}{4}} - G^{-\frac{1}{4}} \partial_3 G^{\frac{1}{2}} \partial_3 G^{-\frac{1}{4}} \tag{iv.16}$$

with the domain

$$D(H) := \{\psi \in \boldsymbol{W}_2^2(\Omega_0) |\ \forall q \in \Sigma_0 : \psi(q, -a) = \psi(q, a) = 0\},, \tag{iv.17}$$

where $\boldsymbol{W}_2^2(\Omega_0)$ is the appropriate local Sobolev space in the sense of [RS, Sec. XIII.14]. Commuting $G^{-\frac{1}{4}}$ with the gradient components we cast the operator (iv.16) into a form which has a simpler kinetic part but contains an effective potential,

$$H = -\partial_\mu G^{\mu\nu} \partial_\nu - \partial_3^2 + V, \tag{iv.18}$$

with

$$V = F^i_{,i} + F_i F^i, \quad F_i := (\ln G^{\frac{1}{4}})_{,i}.$$

This expression of the potential is valid for any smooth metric G_{ij}. If we employ the particular form (iv.8) of the metric tensor, we can write again (iv.18) as a sum of two parts, $H \equiv H_1 + H_2$ with $V = V_1 + V_2$, where

$$\begin{aligned}
H_1 &= -\partial_\mu G^{\mu\nu} \partial_\nu + V_1 && \text{(iv.19)}\\
V_1 &:= \frac{1}{4} \partial_\mu G^{-1} G^{\mu\nu} G_{,\nu} + \frac{1}{16} G^{-2} G_{,\mu} G^{\mu\nu} G_{,\nu} \\
&= -\frac{3}{16} G^{-2} G_{,\mu} G^{\mu\nu} G_{,\nu} + \frac{1}{4} G^{-1} G^{\mu\nu} G_{,\mu\nu} + \frac{1}{4} G^{-1} G_{,\mu} G^{\mu\nu}{}_{,\nu} && \text{(iv.20)}\\
H_2 &= -\partial_3^2 + V_2 && \text{(iv.21)}\\
V_2 &:= \frac{K - M^2}{(1 - 2Mu + Ku^2)^2} && \text{(iv.22)}
\end{aligned}$$

iv.2.4 Coordinate decoupling

While the operator $H_1 + V_2$ depends on all the three coordinates, in thin layers its "leading term" depend on the longitudinal coordinates q only. The transverse coordinate $u = q^3$ is isolated in $H_2 - V_2 = -\partial_3^2$, so up to higher-order terms in a the Hamiltonian decouples into a sum of the operators

$$\begin{aligned}
H_q &= -g^{-\frac{1}{4}} \partial_\mu g^{\frac{1}{2}} g^{\mu\nu} \partial_\nu g^{-\frac{1}{4}} + K - M^2, && \text{(iv.23)}\\
H_u &= -\partial_3^2. && \text{(iv.24)}
\end{aligned}$$

This observation is behind the formal limit $a \to 0+$ mentioned in the introduction [dC1, dC2, Tol] in which the transverse part is thrown away and the thin-layer Hamiltonian is replaced by the surface operator H_q, with the energy appropriately renormalized. This procedure can be given meaning in the perturbation-theory framework, in analogy with [DE], as we shall discuss elsewhere.

Here we use it for motivation purposes. The effective "surface potential" $K - M^2$ can be rewritten by means of the principal curvatures of Σ as follows

$$K - M^2 = -\frac{1}{4}(k_+ - k_-)^2. \tag{iv.25}$$

If the curvature vanishes at large distances, we get a potential well which could imply existence of bound states that would persist in layers of a finite thickness. In distinction to the "one-in-two" case of a curved planar strip the effective potential may vanish if the surface is locally spherical, $k_+ = k_-$, however, this cannot happen everywhere at a locally deformed plane. Let us also remark that similar Laplace-Beltrami operators penalized by a quadratic function of the curvature lead on compact surfaces to interesting isoperimetric problems [Ha, HL, EHL].

In the next section we shall also need the eigenfunctions $\{\chi_n\}_{n=1}^{\infty}$ of the transverse operator H_u. They are given by

$$\chi_n(u) = \begin{cases} \sqrt{\frac{2}{d}} \cos \kappa_n u & \text{if} \quad n \text{ is } \textit{odd} \\ \\ \sqrt{\frac{2}{d}} \sin \kappa_n u & \text{if} \quad n \text{ is } \textit{even} \end{cases} \tag{iv.26}$$

and the corresponding eigenvalues are $\kappa_n^2 = (\kappa_1 n)^2$ with $\kappa_1 = \frac{\pi}{d}$.

iv.3 Spectrum of locally deformed planar layers

In what follows we shall consider a class of layers over surfaces which are smooth local deformations of a plane. More specifically, suppose that the deformed part of the surface is $\mathcal{A} \subset \Sigma$ and denote $\operatorname{supp} K \cup \operatorname{supp} M = p^{-1}(\mathcal{A}) =: \mathcal{A}_0$; it is clear that $\Sigma \setminus \mathcal{A}$ is a plane with a "hole", not necessarily a simply connected one.

Let $(X, \delta_{\mu\nu})$ be a natural representation of $\Sigma \setminus \mathcal{A}$ in Cartesian coordinates $(x^1, x^2) \in X \subset \mathbb{R}^2$ given by an isometry

$$\mathcal{C} : \Sigma_0 \setminus \mathcal{A}_0 \to X : \{q \mapsto (x^1, x^2) =: \mathcal{C}(q)\}.$$

In view of the compact-support assumption we can choose $r_0 > 0$ in such a way that $\mathcal{B}_{r_0} := \{w \in \Sigma : |\mathcal{C} \circ p^{-1}(w)| \le r_0\}$ contains $\mathcal{A}$ and thus $\Sigma_{r_0} := \Sigma \setminus \mathcal{B}_{r_0}$ is the undeformed plane with the disc of radius r_0 removed. It is useful to introduce a polar-coordinate parametrization of Σ_{r_0} given by the isometry

$$\mathcal{P} : (r_0, \infty) \times S^1 \to X : \{(r, \vartheta) \mapsto (x^1, x^2) =: (r\cos\vartheta, r\sin\vartheta)\}; \tag{iv.27}$$

the corresponding metric tensor acquires then the form $\operatorname{diag}(1, r^2)$.

iv.3.1 The essential spectrum

In a planar layer the essential spectrum starts from the lowest transverse eigenvalue. We will use the standard bracketing argument [RS, Sec. XIII.15] in combination

with the minimax principle to prove that the same remains true after a compactly supported deformation.

Proposition iv.2. $\inf \sigma_{\rm ess}(\tilde{H}) = \kappa_1^2$.

PROOF : We cut the layer Ω perpendicularly at the boundary of $\mathcal{B}_{r_0}$ and impose there the Neumann or Dirichlet condition respectively; this enables us to squeeze H between a pair of operators

$$H_{int}^N \oplus H_{ext}^N \le H \le H_{int}^D \oplus H_{ext}^D, \tag{iv.28}$$

which have both the form of an orthogonal sum. The spectrum of the interior parts is purely discrete, so the essential components are determined by the exterior part only, $\sigma_{\rm ess}(H_{int}^\beta \oplus H_{ext}^\beta) = \sigma_{\rm ess}(H_{ext}^\beta) = \sigma(H_{ext}^\beta)$, $\beta = N, D$. The latter can be simply localized employing the polar-coordinate parametrization (iv.27) of Σ_{r_0}. In particular, let

$$U_{\mathcal{P}} : \ \boldsymbol{L}^2\left(\Omega_0 \setminus p^{-1}(\Sigma_{r_0}) \times (-a,a)\right) \to \boldsymbol{L}^2\left((r_0,\infty) \times S^1 \times (-a,a)\right)$$

be the substitution-type unitary operator $(U_{\mathcal{P}}\psi)(r,\vartheta,u) := \psi(\mathcal{P}^{-1} \circ \mathcal{C}(q), u)$. It is clear that the spectrum of the corresponding exterior Hamiltonians

$$U_{\mathcal{P}} H_{\rm ext}^\beta U_{\mathcal{P}}^{-1} = -\partial_r^2 - \frac{1}{r^2}\partial_\vartheta^2 - \partial_u^2 - \frac{1}{4r^2}$$

contains all points $\kappa_1^2 + \epsilon_\beta$, where ϵ_β belongs to the spectrum of the s-wave radial part, $h^\beta := -\partial_r^2 - (4r^2)^{-1}$ in $\boldsymbol{L}^2(r_0,\infty)$ with the appropriate b.c. at $r = r_0$. We have

$$-(\partial_r^2)_N - \frac{1}{4r_0^2} \le h^N \quad \text{and} \quad h^D \le -(\partial_r^2)_D$$

in the sense of quadratic forms and $\inf \sigma_{\rm ess}(-(\partial_r^2)_\beta) = 0$. Since r_0 can be chosen arbitrary large, the claim follows from (iv.28) by the minimax principle. ∎

iv.3.2 Existence of Bound States

Now comes the main result of this paper. We are going to show that the conjecture about existence of a discrete spectrum in locally curved layers formulated in Sec. iv.2.4 is true, even for layers which may not be thin. The variational proof of the following results is based on the idea adapted from [GJ], see also [DE, Thm. 2.1].

Theorem iv.3. *Suppose that the layer is not planar and the deformation satisfies the smoothness and compact support assumptions. Then* $\inf \sigma(\tilde{H}) < \kappa_1^2$.

PROOF : Denote the norm in $\boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du)$ as $\|\cdot\|_G$; then it follows from (iv.13) that the quadratic form associated with our Hamiltonian $\hat{H}$ is given by

$$q[\psi] := \|\hat{H}^{\frac{1}{2}}\psi\|_G^2 = q_1[\psi] + q_2[\psi]$$

where

$$q_1[\psi] := \|\hat{H}_1^{\frac{1}{2}}\psi\|_G^2 \quad = \quad (\psi_{,\mu}, G^{\frac{1}{2}} G^{\mu\nu}\psi_{,\nu}) \tag{iv.29}$$

$$q_2[\psi] := \|\hat{H}_2^{\frac{1}{2}}\psi\|_G^2 \quad = \quad \|G^{\frac{1}{4}}\psi_{,3}\|^2. \tag{iv.30}$$

It acts on $Q(\hat{H})$, the quadratic form domain of $\hat{H}$. In order to prove the claim it is sufficient to find a trial function $\psi \in Q(\hat{H})$ such that

$$t[\psi] := q[\psi] - \kappa_1^2 \|\psi\|_G^2 < 0.$$

(a) We begin the construction of a trial function with $\psi(q,u) := \varphi(q)\chi_1(u)$, where χ_1 is the lowest transverse-mode function (iv.26) and φ is a function from the Schwartz space $\mathcal{S}(\mathbb{R}^2)$, arbitrary for a moment. It yields

$$q_1[\psi] = \left(\varphi_{,\mu}, \langle G^{\frac{1}{2}} G^{\mu\nu} |\chi_1|^2\rangle_u \, \varphi_{,\nu}\right)_q \tag{iv.31}$$

$$q_2[\psi] = \left(\varphi, \langle G^{\frac{1}{2}} |\chi_1'|^2\rangle_u \, \varphi\right)_q \tag{iv.32}$$

$$\|\psi\|_G^2 = \left(\varphi, \langle G^{\frac{1}{2}} |\chi_1|^2\rangle_u \, \varphi\right)_q \tag{iv.33}$$

where $\langle\cdot\rangle_u$ means a "transverse" expectation and the subscripts q, u mark the fact that we integrate w.r.t. the corresponding coordinate only.

Taking into account the explicit expression (iv.10) for G and using the trivial fact that $|\chi_1|$, $|\chi_1'|$ are *even* functions and that we integrate over a symmetric interval $(-a,a)$, and consequently, that we can consider just the *even* powers of u in $\langle\cdot\rangle$, we get

$$\langle G^{\frac{1}{2}} |\chi_1'|^2\rangle_u - \kappa_1^2 \langle G^{\frac{1}{2}} |\chi_1|^2\rangle_u = K g^{\frac{1}{2}};$$

we have employed at that the identity $\langle u^2(|\chi_1'|^2 - \kappa_1^2|\chi_1|^2)\rangle_u = 1$. By virtue of (iv.11), we can estimate the remaining term as

$$q_1[\psi] \leq C^+ \left(\varphi_{,\mu}, g^{\frac{1}{2}} g^{\mu\nu} \varphi_{,\nu}\right)_q . \tag{iv.34}$$

Suppose now that $\varphi(q) = 1$ on $p^{-1}(\mathcal{B}_{r_0})$ and that the function is radially symmetric in the sense $\tilde{\varphi}(r,\vartheta) = \tilde{\varphi}(r)$, where $\tilde{\varphi} := \varphi \circ \mathcal{C}^{-1} \circ \mathcal{P}$. Passing then to the polar coordinates ($g^{\frac{1}{2}} d^2q = r\,dr\,d\vartheta$) in (iv.34) we arrive at

$$q_1[\psi] \leq C^+ \int_{\mathbb{R}^+ \times S^1} |\dot{\tilde{\varphi}}|^2 r \, dr d\vartheta =: C^+ \, \|\dot{\tilde{\varphi}}\|_{\mathcal{P}},$$

where the dot denotes the derivative w.r.t. r. The *r.h.s.* of this inequality depends on the surface geometry through the constant C^+ only. Summing up the results we have

$$t[\psi] \leq C^+ \, \|\dot{\tilde{\varphi}}\|_{\mathcal{P}}^2 + (\varphi, K g^{\frac{1}{2}} \varphi)_q \, . \tag{iv.35}$$

(b) In the next step we shall specify further the function $\tilde{\varphi}$ in a way which allows us to make the *r.h.s.* of (iv.35) arbitrary small. Let us define the family $\{\tilde{\varphi}_\sigma : \sigma \in (0,1]\}$ by an external scaling (in the region $r > r_0$) of a suitable function. The idea is analogous to [GJ] or [DE, Thm. 2.1], however, since we deal with a two-dimensional integral we have to be more careful about the decay properties. We can adopt for this purpose the mollifier employed in [EV, BCEZ], which is expressed in terms of Macdonald functions (or modified Bessel functions in the terminology of [AS]) as

$$\tilde{\varphi}_\sigma(r) := \min\left\{1, \frac{K_0(\sigma r)}{K_0(\sigma r_0)}\right\}$$

Since K_0 is strictly decreasing, the corresponding $\psi_\sigma := \varphi_\sigma \chi_1$ will not be smooth at $r = r_0$ but it remains continuous, hence it is an admissible trial function as an element of $Q(\hat{H})$.

To estimate the first term at the *r.h.s.* of (iv.35), let us compute the norm of the scaled function using [AS, Sec. 9.6] and [GR, 5.54] :

$$\begin{aligned}
\|\dot{\tilde{\varphi}}_\sigma\|^2_{\mathcal{P}} &= \frac{2\pi}{K_0(\sigma r_0)^2}\int_{r_0}^{\infty} \dot{K}_0(\sigma r)^2\, r\, dr = \frac{2\pi}{K_0(\sigma r_0)^2}\int_{\sigma r_0}^{\infty} K_1(t)^2\, t\, dt \\
&= \frac{\pi\,(\sigma r_0)^2}{K_0(\sigma r_0)^2}\,\left[K_0(\sigma r_0)K_2(\sigma r_0) - K_1(\sigma r_0)^2\right] \\
&= \frac{\pi\,(\sigma r_0)^2}{K_0(\sigma r_0)^2}\,\left[K_0(\sigma r_0)^2 + \frac{2}{\sigma r_0}K_0(\sigma r_0)K_1(\sigma r_0) - K_1(\sigma r_0)^2\right] \\
&= -\frac{\pi}{\ln \sigma r_0}\Bigg[-(\sigma r_0)^2 \ln \sigma r_0 - 2\sigma r_0 \ln \sigma r_0\, \frac{K_1(\sigma r_0)}{K_0(\sigma r_0)} \\
&\qquad\qquad + (\sigma r_0)^2 \ln \sigma r_0 \left(\frac{K_1(\sigma r_0)}{K_0(\sigma r_0)}\right)^2\Bigg]
\end{aligned}$$

Next we use the small-argument asymptotic expressions [AS, Sec. 9.6]

$$\begin{aligned}
K_0(x) &= -\ln x + \mathcal{O}(1) \\
K_1(x) &= \frac{1}{x} + \mathcal{O}(\ln x)
\end{aligned}$$

which imply that $x \ln x \frac{K_1(x)}{K_0(x)}$ remains bounded as $x \to 0+$, hence

$$\|\dot{\tilde{\varphi}}_\sigma\|^2_{\mathcal{P}} < \frac{b}{|\ln \sigma r_0|} \tag{iv.36}$$

holds for a positive constant b and σr_0 small enough.

(c) To handle the second term at the *r.h.s.* of (iv.35) for $\varphi = \varphi_\sigma$ we employ the dominated convergence theorem : since $|\varphi_\sigma| \leq 1$ and $\varphi_\sigma \to 1$ pointwise as $\sigma \to 0+$, we have

$$(\varphi_\sigma, Kg^{\frac{1}{2}}\,\varphi_\sigma)_q \to (1, Kg^{\frac{1}{2}})_q \equiv \mathsf{Tot}(\Sigma)$$

by definition. Notice that the total curvature integral is well defined because the Gauss curvature K of a surface obtained by a smooth compactly supported deformation of a plane belongs to $\boldsymbol{L}^1(\Sigma_0, g^{\frac{1}{2}}d^2q)$. In view of (iv.35), (iv.36) and the last formula we have therefore

$$t[\psi_\sigma] \to \mathsf{Tot}(\Sigma) \tag{iv.37}$$

as $\sigma \to 0+$. Recall that in Sec. iv.2.1 we have used the Gauss-Bonnet theorem (iv.7) to show that $\mathsf{Tot}(\Sigma) = 0$ holds for surfaces obtained by a smooth local deformation of a plane. Thus $t[\psi_\sigma]$ can be made arbitrarily small by choosing σ small enough. Since we want to make the form negative, we have to modify the trial function ψ_σ further in analogy with [GJ].

(d) To this aim we pick $j \in \boldsymbol{C}_0^\infty(\mathcal{A}_0 \times (-a, a))$ and set $\Theta := j^2(\hat{H} - \kappa_1^2)\psi_\sigma$. From (iv.14)–(iv.15) and the fact that the scaling acts out of the support of the

localization function j, we immediately get the following explicit expression

$$\begin{aligned}\Theta(q,u) &= j(q,u)^2\,\pi\left(\frac{2}{d}\right)^{\frac{3}{2}}\frac{Ku-M}{Ku^2-2Mu+1}\,\sin\kappa_1 u\\ &= j(q,u)^2\,\pi\left(\frac{2}{d}\right)^{\frac{3}{2}}(\ln G^{\frac{1}{4}})_{,3}\,\sin\kappa_1 u\,.\end{aligned}$$

Notice that by construction the function Θ does not depend on σ. It is non-zero as an element of $\boldsymbol{L}^2(\Omega_0, G^{\frac{1}{2}}d^2q\,du)$ for a non-zero j unless G is independent of u. In view of (iv.10), however, the last named situation occurs only if K, M are zero identically on the whole surface which is impossible because Σ is not a plane by assumption.

Since both ψ_σ and Θ belong to $Q(\hat{H})$, we have

$$t[\psi_\sigma+\varepsilon\,\Theta] = t[\psi_\sigma] + 2\,\varepsilon\,\|j(\hat{H}-\kappa_1^2)\psi_\sigma\|_G^2 + \varepsilon^2\,t[\Theta]\,.$$

For all sufficiently small *negative* ε the sum of the last two terms is negative, and the above arguments show that we can choose σ so that $t[\psi_\sigma+\varepsilon\,\Theta]<0$; recall that the second term on the right side is independent of σ. ∎

Remark. Notice that the choice of the Macdonald function $K_0(r)$ for the mollifier $\tilde{\varphi}$ in the part **(b)** is not indispensable. One can modify this part of the proof, *e.g.*, by using $e^{-r}\ln r$. However, the choice we made is the most natural in a sense, because it employs the Green's function kernel at zero energy.

The obtained conclusion about the bottom of the spectrum can be combined with Proposition iv.2 to get the result announced at the beginning of Sec. iv.3.2.

Corollary iv.4. *Let Ω be a curved layer built over Σ which is a nontrivial, local, and smooth deformation of a plane, with the half-thickness strictly smaller than the minimum curvature radius of Σ* – cf. (iv.11). *Then $\tilde{H}$ has at least one bound state with energy below κ_1^2.*

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Chapitre v

La courbure globale

Résumé

Nous considérons une particule quantique non-relativiste dans un voisinage tubulaire d'épaisseur constante construit autour d'une surface non-compacte plongée dans $\mathbb{R}^3$. Nous supposons que la surface est paramétrée par les coordonnées géodésiques polaires et que les frontières de l'espace tubulaire sont impénétrables. Sous l'hypothèse que les courbures de la surface s'annulent à l'infini, nous trouvons des conditions suffisantes garantissant l'existence des états liés dûs à la géométrie.

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Bound States in Curved Quantum Layers

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Abstract

We consider a nonrelativistic quantum particle constrained to a curved layer of constant width built over a non-compact surface embedded in $\mathbb{R}^3$. We suppose that the latter is endowed with the geodesic polar coordinates and that the layer has the hard-wall boundary. Under the assumption that the surface curvatures vanish at infinity we find sufficient conditions which guarantee the existence of geometrically induced bound states.

Key-Words : waveguides, layers, constrained systems, Dirichlet Laplacian, bound states, surface geometry, curvature, integral curvatures, geodesic polar coordinates

v.1 Introduction

Relations between the geometry of a region Ω in $\mathbb{R}^n$, boundary conditions at $\partial\Omega$, and spectral properties of the corresponding Laplacian are one of the vintage problems of mathematical physics. Recent years brought new motivations and focused attention to aspects of the problem which attracted little attention earlier.

A strong impetus comes from mesoscopic physics, where new experimental techniques make it possible to fabricate semiconductor systems which can be regarded with a reasonable degree of accuracy as waveguides, resonators, etc., for effectively free quantum particles. Often potential barriers at their boundaries can be modeled as a hard wall, in which case it is natural to identify the system Hamiltonian – up to a constant which is usually unimportant – with the Dirichlet Laplacian, $-\Delta_D^\Omega$, defined as the Friedrichs extension – *cf.* Section v.3.3. Moreover, the mentioned solid-state physics advances inspired new insights into classical physics, because analogous problems involving the Dirichlet Laplacian arise also in flat electromagnetic waveguides. For more information about the physical background see [DE, LCM] and references therein.

On the mathematical side a new interesting effect is the binding due to the curvature, supposed to be nonzero and asymptotically vanishing, of an infinitely stretched tubular region in $\mathbb{R}^n$, $n = 2, 3$. Such "trapped modes" may be generated by other local perturbations of a straight tube as well – see, *e.g.*, [BGRS] – but in the bent-tube case they are of a purely quantum origin because there are no

classical closed trajectories, apart from a zero measure set of initial conditions in the phase space.

More generally, quantum motion in the vicinity of a manifold with a potential constraint or Dirichlet condition was studied a long time ago [JK, dC1, dC2, T] in formal attempts to justify quantization on submanifolds. For a thin neighbourhood one excludes the transverse part of the Hamiltonian which gives rise to normal oscillations and the Hamiltonian is replaced by a tangential operator on the submanifold with the energy appropriately renormalized. Interest in this problem has been renewed recently when time evolution around a compact n-dimensional manifold in $\mathbb{R}^{n+m}$ was treated in a rigorous way and compared with the corresponding classical dynamics [FH]. The confinement was realized by a harmonic potential transverse to the manifold and the thin-neighborhood limit was performed by means of a dilation procedure followed by averaging in the normal direction. If the normal bundle is trivial, which is the case, *e.g.*, for manifolds of codimension one, the resulting tangential Hamiltonian contains two terms; the first is proportional to the Laplace-Beltrami operator on the constraint manifold and the second is an effective potential which depends not only on the intrinsic quantities, but also on the external curvature of the constraint manifold. Notice also that if $\mathbb{R}^{n+m}$ is replaced by a manifold of the same dimension, the effective potential depends also on the curvature of this ambient space [M].

The said potential is important also in the situation when the width of the "fat manifold" is finite and fixed. This was first noticed for bent planar Dirichlet strips in the paper [EŠ] which was followed by numerous studies on which the existence conditions and properties of the geometrically induced discrete spectrum were further investigated – see, in particular, [GJ, DE, RB], the first two papers also for a generalization to curved tubes in $\mathbb{R}^3$. On the other hand, much less is known about other possible generalizations of this problem to higher dimensions starting from the physically interesting case of curved layers in $\mathbb{R}^3$.

This is the question we address in the present paper. While the strategy will be the same as in the work mentioned above, using suitable curvilinear coordinates to transform the Laplacian, the two-dimensional character of the underlying manifold bring new features. To characterize them briefly, recall that in the simplest $(1+1)$-case the effective potential is $-\frac{1}{4}\kappa^2$, where κ is the curvature, which is negative whenever the curvature is nonzero. In case of a layer, $n=2$ and $m=1$, which we consider here, the (leading term of the) effective potential is given by $-\frac{1}{4}(k_1-k_2)^2$ – see the derivation of (v.12) – where k_1, k_2 are the principal curvatures of the surface. This expression may vanish also if the surface is locally spherical, $k_1 = k_2$, but the last relation cannot be valid everywhere at a non-compact surface unless the latter is a plane, $k_1 = k_2 = 0$. Thus the effective potential has again an attractive component, which now combines with a more complicated tangential operator – the surface Laplace-Beltrami – since in distinction to a curve the surface cannot be fully rectified. This makes the layer case richer and more interesting.

v.2 Survey of the Paper

The ultimate objective of this work is to set a list of sufficient conditions to guarantee the existence of curvature-induced bound states. We restrict ourselves naturally to non-compact layers only, since the spectrum of the Dirichlet Laplacian in a bounded region of $\mathbb{R}^n$ is always discrete [Dav, Chap. 6].

The layer configuration space Ω itself is properly defined in Section v.3 as a tubular neighbourhood of width d built over a surface Σ embedded in $\mathbb{R}^3$ which is diffeomorphic to $\mathbb{R}^2$. To make it more visual, we can understand Ω as a part of $\mathbb{R}^3$ between a pair of parallel surfaces. For technical reasons we suppose from the beginning that the surface admits at least one *pole* from which we can parametrize the surface globally by geodesic polar coordinates. We stress already here that the existence of a pole in Σ is a strong geometric assumption and that there may be no poles in general [GM]. We introduce first quantities describing the layer geometry and formulate some basic assumptions. In the subsequent part, the Dirichlet Laplacian, $-\Delta_D^\Omega$, is expressed in terms of the couple $q = (q^1, q^2)$ of the surface (called also longitudinal) coordinates together with the normal (transverse) coordinate u.

In Section v.4, we estimate the threshold of the essential spectrum of the Hamiltonian under the assumption $\langle\Sigma 0\rangle$ that the reference surface is *asymptotically planar* in the sense that its Gauss and mean curvatures vanish at large distances. We find that this part of spectrum is bounded from below by $\kappa_1^2 := \left(\frac{\pi}{d}\right)^2$, which is the lowest transverse-mode energy.

Section v.5 is dedicated to the analysis of the discrete part of the spectrum. We find here three sufficient conditions and illustrate them on examples. Since these results leave open the existence question for thick layers of positive total Gauss curvature, we present in Section v.6 an alternative method, which covers the case of asymptotically planar layers that are cylindrically symmetric. Finally, we conclude in Section v.7 with an example of a layer which has no bound states; the reference surface here is not asymptotically planar.

To state here the main results of the paper we need to mention some assumptions which will be discussed in more detail below : $\langle\Sigma 1\rangle$ and $\langle\Sigma 2\rangle$ means respectively the integrability of the Gauss curvature K and the square of $\nabla_g M$, where M is the mean curvature, and $\langle\Omega 1\rangle$ requires the layer half-width to be less than the minimum normal curvature radius of Σ. The integral (total) curvatures corresponding to K and M are defined in (v.3).

Theorem v.1. *Let Σ be a C^2-smooth complete simply connected non-compact surface with a pole embedded in $\mathbb{R}^3$. Let the layer Ω built over the surface be not self-intersecting. If the surface is not a plane but it is asymptotically planar, then any of the conditions*

- $\langle\Sigma 1\rangle$ *and the* total Gauss curvature is non-positive
- Σ *is C^3-smooth and the layer is* sufficiently thin
- Σ *is C^3-smooth,* $\langle\Sigma 1\rangle$, $\langle\Sigma 2\rangle$, *and the* total mean curvature is infinite
- $\langle\Sigma 1\rangle$ *and Σ is* cylindrically symmetric

is sufficient for the Laplace operator $-\Delta_D^\Omega$ to have at least one isolated eigenvalue of finite multiplicity below $\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega)$ *for all the layer half-widths satisfying* $\langle\Omega 1\rangle$.

While this theorem covers various wide classes of layers, the list is not exhaustive. For instance, it remains to be clarified whether one can include also thick layers without cylindrical symmetry built over surfaces with strictly positive total Gauss curvature which, however, do not satisfy the assumption $\langle\Sigma 2\rangle$. Another open question is whether one can replace $\langle\Sigma 1\rangle$ by an assumption including the existence of the total Gauss curvature only, defined in the principal value sense. Finally, it is desirable to find existence results also for layers over more general surfaces which do not possess poles or are not diffeomorphic to $\mathbb{R}^2$.

Properties of the obtained curvature-induced bound states will be discussed elsewhere. Let us just mention that in analogy to bent strips [DE] one can perform

the Birman-Schwinger analysis for slightly curved planar layers (weak-coupling regime) which yields the first term in the asymptotic expansion for the gap between the eigenvalue and the threshold of the essential spectrum. We also remark that the weak coupling analysis of bent "fat" manifolds is similar to that of a local one-sided deformation of a straight strip [BGRS] or planar layer [BEGK].

We use the standard component notation of the tensor analysis, the range of indices being $1,2$ for Greek and $1,2,3$ for Latin. The indices are associated with the above mentioned coordinates by $(1,2,3) \leftrightarrow (q^1, q^2, u) \equiv (s, \vartheta, u)$. The partial derivatives are denoted by *commas*, however, we use also the *dot* notation for the derivatives w.r.t. s.

v.3 Preliminaries

Let Σ be a C^2-smooth surface in $\mathbb{R}^3$ which has at least one *pole*, *i.e.*, a point $o \in \Sigma$ such that the exponential mapping, $\exp_o : \mathrm{T}_o\Sigma \to \Sigma$, is a diffeomorphism. The existence of a pole in Σ is a nontrivial assumption which has important topological consequences. In particular, Σ is necessarily diffeomorphic to $\mathbb{R}^2$ and as such it is simply connected and non-compact. Using the *geodesic polar coordinates* we can parametrize the surface (with the exception of the pole o) by a unique patch $p : \Sigma_0 \to \mathbb{R}^3$, where $\Sigma_0 := (0,\infty) \times S^1$. The tangent vectors $p_{,\mu} := \partial p/\partial q^\mu$ are linearly independent and their cross-product defines a unit normal field n on Σ.

Put $\Omega_0 := \Sigma_0 \times (-a, a)$. We define a *layer* $\Omega := \mathcal{L}(\Omega_0)$ of width $d = 2a > 0$ over the surface Σ by virtue of the mapping $\mathcal{L} : \Omega_0 \to \mathbb{R}^3$ which acts as (*cf.* [Sp3, Prob. 12 of Chap. 3])

$$\mathcal{L}(q,u) := p(q) + un(q). \tag{v.1}$$

v.3.1 The Surface Geometry

The induced surface metric in the geodesic polar coordinates has the diagonal form, $(g_{\mu\nu}) = \mathrm{diag}(1, r^2)$, where $r^2 \equiv g := \det(g_{\mu\nu})$ is the square of the Jacobian of the exponential mapping which satisfies the classical Jacobi equation

$$\ddot{r}(s,\vartheta) + K(s,\vartheta)\, r(s,\vartheta) = 0 \qquad \text{with} \qquad r(0,\vartheta) = 0,\ \dot{r}(0,\vartheta) = 1. \tag{v.2}$$

The *Gauss curvature* K, together with the *mean curvature* M, can be determined via the Weingarten tensor $h_\mu{}^\nu$ – *cf.* [Kli, Prop. 3.5.5].

By means of the invariant surface element, $d\Sigma := g^{\frac{1}{2}} d^2q$, we may introduce some global quantities characterizing Σ, namely the *total Gauss curvature* $\mathcal{K}$ and the *total mean curvature* $\mathcal{M}$ which are defined, respectively, by the integrals

$$\mathcal{K} := \int_\Sigma K d\Sigma \qquad \text{and} \qquad \mathcal{M}^2 := \int_\Sigma M^2 d\Sigma. \tag{v.3}$$

The latter always exists (it may be $+\infty$), while the former is well defined provided

$\boxed{\langle \Sigma 1 \rangle \quad K \in L^1(\Sigma_0, d\Sigma)}$

If this condition is not satisfied, one can understand the above integral as the principal-value defined through the area restricted by the geodesic circle $p(s,\cdot)$ of

radius $s \to \infty$. Assuming $\mathcal{K}$ to be finite, an integration of (v.2) yields the following useful estimate :

$$\exists C > 0 \; \forall s \in (0, \infty) : \quad \int_0^{2\pi} r(s, \vartheta)\, d\vartheta \leq Cs. \tag{v.4}$$

The norm and the inner product in the Hilbert space $L^2(\Sigma_0, d\Sigma)$ will be indicated by the subscript "g".

v.3.2 The Layer Geometry

It is clear from the definition (v.1) that the metric tensor of the layer as a manifold in $\mathbb{R}^3$ has the block form

$$(G_{ij}) = \begin{pmatrix} (G_{\mu\nu}) & 0 \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad G_{\nu\mu} = (\delta_\nu^\sigma - u h_\nu{}^\sigma)(\delta_\sigma^\rho - u h_\sigma{}^\rho) g_{\rho\mu}. \tag{v.5}$$

This formula is well suited for calculation of the determinant, $G := \det(G_{ij})$, because the eigenvalues of the matrix of the Weingarten map are the *principal curvatures* k_1, k_2, and $K = k_1 k_2$, $M = \frac{1}{2}(k_1 + k_2)$. Hence

$$G = g\,[(1 - uk_1)(1 - uk_2)]^2 = g(1 - 2Mu + Ku^2)^2. \tag{v.6}$$

In particular, this expression defines through $d\Omega := G^{\frac{1}{2}} d^2q\, du$ the volume element of Ω.

Henceforth, we shall assume

$\boxed{\langle \Omega 0 \rangle \quad \Omega \text{ is not self-intersecting}}$ *i.e.*, $\mathcal{L}$ is injective.

We have to require also that $\mathcal{L}$ is a diffeomorphism. In view of the regularity assumptions imposed on Σ and the inverse function theorem, it is equivalent to assuming that $1 - 2Mu + Ku^2$ does not vanish on Ω_0, which can be guaranteed by imposing a restriction on the layer thickness :

$$\boxed{\langle \Omega 1 \rangle \quad a < \rho_m := (\max\{\|k_1\|_\infty, \|k_2\|_\infty\})^{-1}}$$

The number ρ_m is naturally interpreted as the *minimal normal curvature radius* of Σ (for planar surfaces one can put $\rho_m := \infty$). It follows from (v.5) that $C_- \leq 1 - 2Mu + Ku^2 \leq C_+$ holds with $C_\pm := \left(1 \pm a\rho_m^{-1}\right)^2$. The lower bound explains why we assume $\langle \Omega 1 \rangle$ (together with $\langle \Omega 0 \rangle$) to get the global diffeomorphism. On the other hand, the supremum norms in the definition of ρ_m are necessarily finite since a meaningful layer must have a non-zero width. Another consequence of the considerations is that under the assumption $\langle \Omega 1 \rangle$, $G_{\mu\nu}$ can be immediately estimated by the surface metric,

$$C_- g_{\mu\nu} \leq G_{\mu\nu} \leq C_+ g_{\mu\nu} \qquad \text{with} \qquad 0 < C_- \leq 1 \leq C_+ < 4. \tag{v.7}$$

Remark. We stress the following which will be supposed through all the paper but will not be always referred to hereafter :

- We consider surfaces which can be parametrized by means of the geodesic polar coordinates. This requires the existence of at least one pole.
- Since Σ is assumed to be of class C^2, the surface curvatures K, M are C^0 and as such bounded locally.
- Moreover, since we assume layers with non-zero widths, the principal curvatures have to be bounded uniformly on all Σ_0 due to $\langle \Omega 1 \rangle$. By virtue of the relation between k_1, k_2 and K, M, the same is true for the latter.

v.3.3 The Hamiltonian

After these geometric preliminaries let us define the Hamiltonian of our model. We consider a nonrelativistic spinless particle confined to Ω which is free within it and suppose that the boundary of the layer is a hard wall, *i.e.*, the wavefunctions satisfy the Dirichlet boundary condition there. For the sake of simplicity we set Planck's constant $\hbar = 1$ and the mass of the particle $m = \frac{1}{2}$. Then the Hamiltonian can be identified with the Dirichlet Laplacian $-\Delta_D^\Omega$ on $L^2(\Omega)$, which is defined for an open set $\Omega \subset \mathbb{R}^3$ as the Friedrichs extension of the free Laplacian with the domain defined initially on $C_0^\infty(\Omega)$ – *cf.* [RS4, Sec. XIII.15] or [Dav, Chap. 6]. The domain of the closure of the corresponding quadratic form is the Sobolev space $W_0^{1,2}(\Omega)$.

A natural way to investigate this operator is to pass to the coordinates (q, u) in which it acquires the Laplace-Beltrami form ($G_{ij}G^{jk} := \delta_i^k$)

$$H := -G^{-\frac{1}{2}}\partial_i G^{\frac{1}{2}} G^{ij}\partial_j \qquad \text{on} \qquad L^2(\Omega_0, G^{\frac{1}{2}} d^2q\, du). \tag{v.8}$$

This coordinate change is nothing else than the unitary transformation

$$U : L^2(\Omega) \to L^2(\Omega_0, d\Omega) : \{\psi \mapsto U\psi := \psi \circ \mathcal{L}\}$$

which relates the two operators by $H = U(-\Delta_D^\Omega)U^{-1}$. If Σ is not C^3-smooth, the operator H has to be understood in the form sense

$$Q[\psi] := \|H^{\frac{1}{2}}\psi\|_G^2 = (\psi_{,i}, G^{ij}\psi_{,j})_G, \quad \mathrm{Dom}\, Q = W_0^{1,2}(\Omega_0, d\Omega). \tag{v.9}$$

Here the subscript "G" indicates the norm and the inner product in the Hilbert space of (v.8). Employing the block form (v.5) of G_{ij}, we can split H into a sum of two parts, $H = H_1 + H_2$, given by

$$H_1 := -G^{-\frac{1}{2}}\partial_\mu G^{\frac{1}{2}} G^{\mu\nu}\partial_\nu = -\partial_\mu G^{\mu\nu}\partial_\nu - 2F_{,\mu}G^{\mu\nu}\partial_\nu\,, \tag{v.10}$$

$$H_2 := -G^{-\frac{1}{2}}\partial_3 G^{\frac{1}{2}}\partial_3 = -\partial_3^2 - 2\,\frac{Ku - M}{1 - 2Mu + Ku^2}\,\partial_3\,, \tag{v.11}$$

where we have introduced $F := \ln G^{\frac{1}{4}}$ and expressed $F_{,3}$ explicitly for H_2.

At the same time, it is useful to have an alternative form of the Hamiltonian which has the factor $1 - 2Mu + Ku^2$ removed from the weight $G^{\frac{1}{2}}$ of the inner product. It is obtained by another unitary transformation,

$$\hat{U} : L^2(\Omega_0, d\Omega) \to L^2(\Omega_0, d\Sigma\, du) : \{\psi \mapsto \hat{U}\psi := (1 - 2Mu + Ku^2)^{\frac{1}{2}}\psi\},$$

which leads to the unitarily equivalent operator $\hat{H} := \hat{U}H\hat{U}^{-1}$. This operator makes sense if we impose a stronger regularity assumption on Σ, namely that the latter is piecewise C^4-smooth (or C^3 if $\hat{H}$ is considered in the form sense). The operator $\hat{H}$ can be rewritten by means of an effective potential V using $J := \frac{1}{2}\ln(1-2Mu+Ku^2)$ as follows :

$$\hat{H} = -g^{-\frac{1}{2}}\partial_i g^{\frac{1}{2}} G^{ij}\partial_j + V, \qquad V = g^{-\frac{1}{2}}(g^{\frac{1}{2}}G^{ij}J_{,j})_{,i} + J_{,i}G^{ij}J_{,j}$$

and again, employing the particular form of G_{ij}, the operator $\hat{H}$ can be split into a sum, $\hat{H}_1 + \hat{H}_2$. The first operator is defined by the part of $\hat{H}$ where one sums over the Greek indices and

$$\hat{H}_2 = -\partial_3^2 + V_2, \qquad V_2 = \frac{K - M^2}{(1 - 2Mu + Ku^2)^2}.$$

To motivate the considerations of the following sections let us look at this transformed operator from a heuristic point of view. While the operator $\hat{H}_1 + V_2$ depends on all three coordinates, in thin layers ($a \ll \rho_m$) its leading term depends up to an error $\mathcal{O}(a\rho_m^{-1})$ on the longitudinal coordinates q only. One can estimate the former in the form sense by means of (v.7) and use the fact that $C_\pm = 1 + \mathcal{O}(a\rho_m^{-1})$. The transverse coordinate u is isolated in $\hat{H}_2 - V_2 = -\partial_3^2$, so up to higher-order terms in a the Hamiltonian decouples into a sum of the operators

$$H_q := -g^{-\frac{1}{2}}\partial_\mu g^{\frac{1}{2}} g^{\mu\nu}\partial_\nu + K - M^2 \qquad \text{and} \qquad H_u := -\partial_3^2\,, \tag{v.12}$$

the first one being the Laplace-Beltrami operator of Σ, except for the additional potential $K - M^2$ which can be rewritten by means of the principal curvatures as $-\frac{1}{4}(k_1 - k_2)^2$. This is the attractive interaction mentioned in the introduction. Let us remark that similar Laplace-Beltrami operators penalized by a quadratic function of the curvature lead on compact surfaces to interesting isoperimetric problems [H, HL, EHL, F].

In what follows we shall use the family of eigenfunctions $\{\chi_n\}_{n=1}^\infty$ of the transverse operator $(-\partial_3^2)_D$ which is given by

$$\chi_n := \begin{cases} \sqrt{\frac{2}{d}}\cos\kappa_n u & \text{if } n \text{ is odd,} \\ \sqrt{\frac{2}{d}}\sin\kappa_n u & \text{if } n \text{ is even.} \end{cases}$$

Here $\kappa_n^2 := (\kappa_1 n)^2$ with $\kappa_1 := \pi/d$ are the corresponding eigenvalues.

v.4 Essential Spectrum

The essential spectrum of a planar layer ($K, M \equiv 0$) is clearly $[\kappa_1^2, \infty)$. By a bracketing argument [DEK, Sec. 3.1] and using an appropriate Weyl sequence, it is easy to see that the same remains true if Ω is obtained by a compactly supported deformation of a planar layer. In this section we will prove the inclusion $\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \subseteq [\kappa_1^2, \infty)$ under the assumption that the surface Σ is *asymptotically planar* in the sense

$$\boxed{\langle\Sigma 0\rangle \quad K, M \to 0 \qquad \text{as} \quad s \to \infty}$$

Theorem v.2. *Suppose* $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ *and assume that the surface is asymptotically planar* $\langle\Sigma 0\rangle$. *Then*

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^\Omega) \geq \kappa_1^2.$$

Proof: We divide the layer Ω into an exterior and interior part by putting $\Omega_{\mathrm{ext}} := \mathcal{L}(\Omega_{0,s_0})$ and $\Omega_{\mathrm{int}} := \Omega \setminus \overline{\Omega}_{\mathrm{ext}}$, respectively, where $\Omega_{0,s_0} := \Sigma_{0,s_0} \times (-a, a)$, $\Sigma_{0,s_0} := (s_0, \infty) \times S^1$ for some $s_0 > 0$. Imposing the Neumann boundary condition at the common boundary of the two parts, $s = s_0$, we arrive at the decoupled Hamiltonian $H^N = H^N_{\mathrm{int}} \oplus H^N_{\mathrm{ext}}$. More precisely, it is obtained as the operator associated with the quadratic form Q^N acting as (v.9), however with the domain $\mathrm{Dom}\, Q^N := \mathrm{Dom}\, Q^N_{\mathrm{int}} \oplus \mathrm{Dom}\, Q^N_{\mathrm{ext}}$, where

$$\mathrm{Dom}\, Q^N_\omega := \{\psi \in W^{1,2}(\Omega_\omega, d\Omega) \mid \psi(\cdot, \pm a) = 0\}, \qquad \omega \in \{\mathrm{int}, \mathrm{ext}\}.$$

Since $H \geq H^N$ and the spectrum of H^N_{int} is purely discrete [Dav, Chap. 7], the minimax principle gives the estimate $\inf \sigma_{\mathrm{ess}}(H) \geq \inf \sigma_{\mathrm{ess}}(H^N_{\mathrm{ext}}) \geq \inf \sigma(H^N_{\mathrm{ext}})$.

Hence it is sufficient to find a lower bound on $H^N_{\rm ext}$. However, by virtue of (v.9) and (v.5), we have for all $\psi \in \mathrm{Dom}\, Q^N_{\rm ext}$:

$$\begin{aligned} Q^N_{\rm ext}[\psi] &\geq \|\psi_{,3}\|^2_{G,\rm ext} \geq \inf_{\Omega_{0,s_0}} \{1 - 2Mu + Ku^2\} \|\psi_{,3}\|^2_{L^2(\Omega_0, d\Sigma du),\rm ext} \\ &\geq \left(1 - \sup_{\Sigma_{0,s_0}} \{2a|M| + a^2|K|\}\right) \kappa_1^2 \|\psi\|^2_{L^2(\Omega_0, d\Sigma du),\rm ext} \\ &\geq \frac{1 - \sup_{\Sigma_{0,s_0}} \{2a|M| + a^2|K|\}}{1 + \sup_{\Sigma_{0,s_0}} \{2a|M| + a^2|K|\}} \kappa_1^2 \|\psi\|^2_{G,\rm ext} \\ &=: (1 + \epsilon(s_0))\ \kappa_1^2 \|\psi\|^2_{G,\rm ext}, \end{aligned}$$

where ϵ denotes a function which goes to zero as $s_0 \to \infty$ due to $\langle \Sigma 0 \rangle$. The subscript "ext" indicates the restriction of the norm to the exterior part. In the second line we have used $(-\partial_3^2)_D \geq \kappa_1^2$. The claim then easily follows by the fact that s_0 can be chosen arbitrarily large. □

Remark. This threshold estimate is sufficient for the subsequent investigation of the discrete spectrum which is our goal in this paper. In order to show that all energies above κ_1^2 belong to the spectrum, one has to construct an appropriate Weyl sequence to check the opposite conclusion $\sigma_{\rm ess}(-\Delta^\Omega_D) \supseteq [\kappa_1^2, \infty)$. This can be done under an assumption stronger than $\langle \Sigma 0 \rangle$ which involves derivatives of the Weingarten tensor as well.

v.5 Discrete Spectrum

The aim of this section is to prove three different conditions sufficient for the Hamiltonian to have a non-empty spectrum below κ_1^2. Since we have shown that the essential spectrum does not start below this value for the layers built over asymptotically planar surfaces, the conditions yields immediately the existence of curvature-induced bound states. All the proofs here are based on the variational idea of finding a trial function Ψ from the form domain of H such that

$$\tilde{Q}[\Psi] := Q[\Psi] - \kappa_1^2 \|\Psi\|^2_G < 0.$$

It is convenient to split Q into two parts, $Q = Q_1 + Q_2$, which are associated with H_1 and H_2 of (v.10) and (v.11), respectively.

A powerful method in this situation is to construct a trial function by deforming the transverse-threshold resonance wavefunction separately in the central and tail regions. The idea goes back to Goldstone and Jaffe [GJ], see also [DE, Thm. 2.1], [RB] and [DEK, Sec. 3.2].

Theorem v.3. *Assume* $\langle \Omega 0 \rangle$, $\langle \Omega 1 \rangle$, $\langle \Sigma 1 \rangle$, *and suppose that* Σ *is not planar. If the surface has a non-positive total Gauss curvature,* i.e., $\mathcal{K} \leq 0$, *then*

$$\inf \sigma(-\Delta^\Omega_D) < \kappa_1^2.$$

PROOF: We begin the construction of Ψ by considering a radially symmetric function $\psi(s, \vartheta, u) := \varphi(s)\chi_1(u)$, where φ is arbitrary for a moment. Employing the explicit form (v.11) of H_2 we get immediately

$$Q_2[\psi] - \kappa_1^2 \|\psi\|^2_G = (\varphi, K\varphi)_g, \tag{v.13}$$

while the "longitudinal kinetic part" $Q_1(\psi)$ can be estimated by virtue of (v.7) and (v.4) as

$$Q_1[\psi] \leq C_1 \int_0^\infty |\dot{\varphi}(s)|^2 s \, ds. \tag{v.14}$$

The r.h.s. of this inequality depends on the surface geometry through the constant $C_1 := (C_+/C_-)^2 C$ only. To make this integral arbitrarily small we replace φ by the family $\{\varphi_\sigma : \sigma \in (0,1]\}$ of elements which are equal to 1 on a compact set, $s \leq s_0$, for some $s_0 > 0$, and outside they are given by scaled Macdonald functions [AS, Sec. 9.6] :

$$\varphi_\sigma(s) := \min\left\{1, \frac{K_0(\sigma s)}{K_0(\sigma s_0)}\right\}.$$

Since K_0 is strictly decreasing, the corresponding $\psi_\sigma := \varphi_\sigma \chi_1$ will not be smooth at $s = s_0$ but it remains continuous, hence it is an admissible trial function as an element of $\mathrm{Dom}\, Q$. Using the properties of the Macdonald function [AS, Sec. 9.6] and [GR, 5.54], it is now easy to verify that for σs_0 small enough

$$\exists C_2 > 0 : \qquad \int_0^\infty |\dot{\varphi}_\sigma(s)|^2 s \, ds < \frac{C_2}{|\ln \sigma s_0|} \tag{v.15}$$

and therefore $Q_1[\psi_\sigma] \to 0+$ as $\sigma \to 0+$. On the other hand, since we assume $\langle \Sigma 1 \rangle$ and $|\varphi_\sigma| \leq 1$ together with $\varphi_\sigma \to 1-$ pointwise as $\sigma \to 0+$, we get by the dominated convergence theorem that (v.13) (after the replacement $\psi \mapsto \psi_\sigma$) converges to $\mathcal{K}$. Thus, by choosing σ small enough, $\tilde{Q}[\psi_\sigma]$ can be made strictly negative if the total Gauss curvature is strictly negative too.

In order to deal with the case $\mathcal{K} = 0$, in analogy to [GJ] we construct the trial function by a small deformation of ψ_σ in the central region. We set $\Psi_{\sigma,\varepsilon} := \psi_\sigma + \varepsilon\Theta$, where $\Theta(q,u) := j(q)u\chi_1(u)$ with $j \in C_0^\infty((0,s_0) \times S^1)$. Since Θ is evidently a function from $\mathrm{Dom}\, Q$ as well, we can write

$$\tilde{Q}[\Psi_{\sigma,\varepsilon}] = \tilde{Q}[\psi_\sigma] + 2\varepsilon \tilde{Q}(\Theta, \psi_\sigma) + \varepsilon^2 \tilde{Q}[\Theta]. \tag{v.16}$$

An explicit calculation where one employs the fact that the scaling acts out of the support of the localization function j yields : $\tilde{Q}(\Theta, \psi_\sigma) = -(j, M)_g$, which can be made non-zero by choosing j supported on a compact where M does not change sign. Let us stress that it is independent of σ, because $\varphi_\sigma = 1$ on $\mathrm{supp}\, j$; the same is true for $\tilde{Q}[\Theta]$. Now such a compact surely exists because it is supposed that Σ is not a plane and we can take the parameter s_0 arbitrarily large. If we choose now the sign of ε in such a way that the second term on the r.h.s. of (v.16) is negative, then also the sum with the last term will be negative for sufficiently small ε, and we can choose σ so small that $\tilde{Q}(\Psi_{\sigma,\varepsilon}) < 0$ because $\tilde{Q}(\psi_\sigma) \to \mathcal{K} = 0$ as $\sigma \to 0+$ here. □

Remarks. (a) The special choice of the Macdonald function K_0 for the mollifier φ is not indispensable. In analogy to [GJ] or [DE, Thm. 2.1] we need a family of suitable functions scaled exterior to $(0, s_0)$ in such a way that the integral (v.14) tends to zero as $\sigma \to 0+$. However, since this integral contains the extra factor s (the relic of integration in a higher dimension) we have to be more careful about the decay properties. We have adopted for this purpose the mollifier employed

in [EV, BCEZ], which is the most natural in a sense, because it employs the Green function kernel of the free 2-dimensional Laplacian at zero energy. Nevertheless, we would have succeeded equally if we had chosen for the scaled tail, *e.g.*, a compactly supported function similar to that of the proof of Theorem v.6.

(b) In the case $\mathcal{K} = 0$ we have not used the deformation proposed in [DE] : $\tilde{\Theta} := \tilde{\jmath}^2(H - \kappa_1^2)\psi_\sigma$ with $\tilde{\jmath} \in C_0^\infty((0, s_0) \times S^1 \times (-a, a))$, because it requires an extra condition on the surface regularity. The analogous condition in the strip case has been forgotten in [DE, Thm. 2.1]. Moreover, the localization function j used here is simpler since it is independent of u. We note that it corresponds in fact to the deformation part of the test function employed in [RB], however, we have found out about this just after the submission of the paper.

A class of layers to which the above theorem applies is represented by those built over *Cartan-Hadamard surfaces*, *i.e.*, geodesically complete simply connected non-compact surfaces with non-positive Gauss curvature. In view of the Cartan-Hadamard theorem [Kli, Thm. 6.6.4] each point is a pole and we can therefore construct infinitely many geodesic polar coordinate systems. Excluding the trivial planar case, the total Gauss curvature is always strictly negative and so all these layers possess at least one bound state provided they are asymptotically planar, $\mathcal{K}$ is finite, and the assumptions $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$ are satisfied.

EXAMPLE 1 (Hyperbolic Paraboloid). The simple quadric given in $\mathbb{R}^3$ by the equation $z = x^2 - y^2$ is an asymptotically planar surface with $\mathcal{K} = -2\pi$.

EXAMPLE 2 (Monkey Saddle). Take $z = x^3 - 3xy^2$. One can again check that $\langle\Sigma 0\rangle$ holds true and the total Gauss curvature now equals -4π.

A family of layers of the limit case $\mathcal{K} = 0$ was investigated in [DEK]. We consider there compactly supported deformations of a planar layer for which the zero value of $\mathcal{K}$ follows at once by the Gauss-Bonnet theorem. If such a deformed plane contains at least one pole, all the spectral results are trivial consequences of the present Theorems v.2 and v.3. On the other hand, the results of [DEK] are more general in the sense that due to the compact support assumption the technique works without the requirement on the existence of a pole.

EXAMPLE 3 (Compactly Perturbed Plane without Poles). Suppose that a plane with a circular hole is connected via a cylindrical tube perpendicular to it with a pierced sphere. Both interfaces can be made as smooth as needed. If the tube is sufficiently long there is only one pole o provided the surface has a cylindrical symmetry w.r.t. the axis of the tube ; it coincides with the intersection of the axis with the sphere. If we break now the symmetry by taking an ellipsoid instead of the sphere, we destroy the injectivity of the exponential mapping $\exp_o$ without creating new poles.

The Goldstone-Jaffe trick of choosing the ground state of the transverse operator as the generalized annulator of the shifted energy form $\tilde{Q}$ has proven its usefulness as a robust argument for demonstrating the existence of bound states. However, in the present context it reaches its limits because the above proof does not work for layers built over surfaces with positive total curvature, for instance :

EXAMPLE 4 (Elliptic Paraboloid). The surfaces $z = (x/x_0)^2 + (y/y_0)^2$ with $x_0, y_0 > 0$ are asymptotically planar but $\mathcal{K} = 2\pi > 0$. They always contain two poles given by its umbilics which coincide if it is a paraboloid of revolution.

On the other hand, due to the heuristic argument based on (v.12) one expects existence of bound states in any non-planar layer thin enough. This is indeed true.

This fact together with another sufficient condition are established in the next theorem.

Theorem v.4. *Assume* $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$, *and suppose that* Σ *is* C^3*-smooth, non-planar and obeys in addition*

$$\boxed{\langle\Sigma 2\rangle \quad \nabla_g M \in L^2(\Sigma_0, d\Sigma)}$$

Then $\inf\sigma(-\Delta_D^\Omega) < \kappa_1^2$ *if one of the following two conditions is satisfied :*

(a) *the layer is sufficiently thin,* i.e., *d is small enough,*

(b) $\langle\Sigma 1\rangle$ *and the total mean curvature is infinite,* i.e., $\mathcal{M} = \infty$.

For brevity we have introduced here the non-component notation ∇_g for the covariant derivative on Σ.

PROOF: We use $\Psi_\sigma(s,\vartheta,u) := (1 + M(s,\vartheta)u)\,\psi_\sigma(s,u)$, where $\psi_\sigma = \varphi_\sigma\chi_1$ is the trial function defined in the first part of the proof of Theorem v.3. Under the stated regularity assumption, Ψ_σ is an admissible trial function, *i.e.*, it belongs to $\mathrm{Dom}\,Q$. Using (v.7) together with Minkovski's inequality and (v.11), we get

$$Q_1[\Psi_\sigma] \le 2(C_+/C_-)^2 \left((1 + a\|M\|_\infty)^2 \|\dot\varphi_\sigma\|_g^2 + a^2 \|\varphi_\sigma \nabla_g M\|_g^2 \right)$$

$$Q_2[\Psi_\sigma] - \kappa_1^2 \|\Psi_\sigma\|_G^2 = \left(\varphi_\sigma, (K - M^2)\varphi_\sigma\right)_g + \frac{\pi^2 - 6}{12\kappa_1^2} \left(\varphi_\sigma, KM^2\varphi_\sigma\right)_g .$$

We start by checking the second sufficient condition. We recall that due to $\langle\Omega 1\rangle$, K and M are uniformly bounded. Thus, thanks to $\langle\Sigma 2\rangle$ and the hypotheses assumed in (b), it follows that $\tilde Q[\Psi_\sigma] \to -\infty$ as $\sigma \to 0+$.

We pass now to the first sufficient condition. Since $K - M^2$ is negative – *cf.* (v.12) – continuous and the surface is supposed to be non-planar, the first term at the r.h.s. of the second line is strictly negative, say $-c^2$, for a sufficiently large value of s_0 (the radius of the disc where $\psi_\sigma = \chi_1$). On the other hand, $\|\dot\varphi_\sigma\|_g$ is estimated by (v.15), so we can choose σ so small that it is less than $c^2/3$. Now we choose the layer half-width a so small that the sum of the remaining terms of the estimated $\tilde Q[\Psi_\sigma]$ is less than $c^2/3$ as well. For this we recall that κ_1^{-2} is proportional to a^2. Hence $\tilde Q[\Psi_\sigma] \le -c^2/3 < 0$ for σ, d small enough. □

Remark. In order to obtain the first sufficient condition, one can replace $\langle\Sigma 2\rangle$ by an assumption on the boundedness of $\nabla_g M$. Moreover, if we had used the compactly supported function φ_n from the proof of Theorem v.6 below instead of φ_σ, it would have been sufficient to assume that $\nabla_g M$ was bounded locally only, which is exactly the situation when Σ is of class C^3. This is why $\langle\Sigma 2\rangle$ is not included in the thin layer case of Theorem v.1.

We believe that the hypothesis $\langle\Sigma 2\rangle$ is technical – *cf.* Example 6. Even with it, however, the class of layers possessing bound states without any restriction on the layer thickness other than $\langle\Omega 1\rangle$ is extended significantly. For instance, it is an easy exercise to verify that all the conditions of Theorem v.4 (b) are fulfilled for the elliptic paraboloids and many other surfaces with a positive total Gauss curvature. Removing this technical condition is still an open question except for layers endowed with the cylindrical symmetry which we shall discuss below.

v.6 Cylindrically Symmetric Layers

Consider now layers which are invariant w.r.t. rotations around a fixed axis in $\mathbb{R}^3$. We may thus suppose that Σ is a surface of revolution parametrized by $p : \Sigma_0 \to \mathbb{R}^3$,

$$p(s,\vartheta) := (r(s)\cos\vartheta, r(s)\sin\vartheta, z(s)), \qquad \text{where} \quad r, z \in C^2((0,\infty)), \ r > 0.$$

It will be the geodesic polar coordinate chart if we impose the following condition on the *canonical* parametrization,

$$\dot{r}^2 + \dot{z}^2 = 1; \qquad \text{then also} \qquad \dot{r}\ddot{r} + \dot{z}\ddot{z} = 0. \tag{v.17}$$

An explicit calculation yields the diagonal form of the Weingarten tensor, $(h_\mu{}^\nu) = \mathrm{diag}(k_s, k_\vartheta)$, with the principal curvatures $k_s = \dot{r}\ddot{z} - \ddot{r}\dot{z}$ and $k_\vartheta = \dot{z}r^{-1}$. In fact, it is sufficient to know the function $s \mapsto k_s(s)$ only, since r, z can be constructed from the relations

$$\begin{aligned} r(s) &= \int_0^s \cos b(\xi)\, d\xi \\ z(s) &= \int_0^s \sin b(\xi)\, d\xi \end{aligned} \qquad \text{with} \qquad b(s) := \int_0^s k_s(\xi)\, d\xi. \tag{v.18}$$

Recall that by Theorem v.3 the spectrum bottom of any layer is strictly less than the first transverse eigenvalue provided $\mathcal{K} \leq 0$. However, only the case $\mathcal{K} = 0$ is relevant to the present situation of surfaces of revolution, because by the Gauss-Bonnet theorem (see also (v.2))

$$\mathcal{K} + 2\pi\dot{r}(\infty) = 2\pi, \qquad \text{where} \quad \dot{r}(\infty) := \lim_{s\to\infty} \dot{r}(s), \tag{v.19}$$

and $\dot{r}(\infty) > 1$ is not allowed because of (v.17). Notice, on the other hand, that $\dot{r}(\infty)$ always exists since the existence of the total Gauss curvature is supposed. Moreover, the positivity of r requires $\mathcal{K} \leq 2\pi$.

The goal of this section is to show that in the present special case of symmetric layers $\inf\sigma(-\Delta_D^\Omega) < \kappa_1^2$ holds true also for all admissible strictly positive values of $\mathcal{K}$, irrespective of the layer thickness. Our argument requires to exclude here the extreme case $\mathcal{K} = 0$ for which the result is already known, without any symmetry assumption. Hereafter we will therefore assume that $0 \leq \dot{r}(\infty) < 1$. It follows that there exist $0 < \delta' < \frac{1}{2}$ and $s_0 > 0$ such that for all $s \geq s_0$ one has $-\delta' \leq \dot{r}(s) \leq 1 - \delta'$. Using now the explicit dependence of k_ϑ on $r, \dot{z}$ and (v.17), we obtain the essential ingredients of our strategy :

Lemma v.5. *Assume $\mathcal{K} > 0$. There exist $\delta > 0$ and $s_0 > 0$ such that*

$$\forall s \geq s_0 : \quad \frac{\delta}{r(s)} \leq |k_\vartheta(s)| \leq \frac{1}{r(s)} \quad \text{and} \quad k_\vartheta(s) \text{ does not change sign.}$$

In particular, employing (v.4), it follows that k_ϑ is not integrable in $L^1(\mathbb{R}^+)$. On the other hand, the meridian curvature k_s is integrable under the assumption $\langle\Sigma 1\rangle$, which is seen by the regularity properties imposed on p and the following estimate :

$$\infty > \int_0^\infty |K(s)|\, r(s)\, ds \geq \int_{s_0}^\infty |k_s(s)k_\vartheta(s)|\, r(s)\, ds \geq \delta \int_{s_0}^\infty |k_s(s)|\, ds.$$

This is the essence of what we are going to use in our method. Even if M may decay at infinity it is not negligible in the integral sense there. However, K is supposed to be integrable and it will enable us to eliminate the unpleasant contribution of the corresponding total curvature – *cf.* (v.13) – by going to large distances by means of a family of trial functions supported there.

Theorem v.6. *Assume* $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$, $\langle\Sigma 1\rangle$, *and suppose that* Σ *is a surface of revolution. Then* $\inf\sigma(-\Delta_D^\Omega) < \kappa_1^2$.

PROOF: Since the result for $\mathcal{K} = 0$ is included in Theorem v.3, we suppose $\mathcal{K} > 0$ in the following. We use $\Psi_{n,\varepsilon}(s,u) := (\varphi_n(s) + \varepsilon\phi_n(s)u)\chi_1(u)$, where ε will be specified later and φ_n, ϕ_n are functions "localized at infinity" as $n \to \infty$. They are defined in the following way : Consider three sequences $b_1, b_2, b_3 : \mathbb{N} \to \mathbb{N}$ such that $0 < b_1 < b_2 < b_3$ and $b_1(n) \to \infty$ as $n \to \infty$. We set

$$\varphi_n(s) := \frac{\ln(s/b_i)}{\ln(b_j/b_i)}, \quad (i,j) \in \{(1,2),(3,2)\}, \qquad \text{and} \qquad \phi_n(s) := \frac{\varphi_n(s)}{s}$$

if $\min\{b_i, b_j\} < s \le \max\{b_i, b_j\}$, and assume that φ_n, ϕ_n are zero elsewhere. Defined in this way the functions are not smooth at the matching points, however, $\Psi_{n,\varepsilon}$ still belongs to $\mathrm{Dom}\, Q$ because they are continuous and of a compact support for each $n \in \mathbb{N}$. Next we note that they are positive and uniformly bounded (the maximum of ϕ_n is even decreasing as $n \to \infty$).

Using (v.7) and (v.4) we can estimate the longitudinal kinetic parts of $\tilde{Q}$ – *cf.* also (v.14) – by one-dimensional integrals

$$Q_1[\varphi_n\chi_1] \le C_1 \int_0^\infty \dot{\varphi}_n(s)^2 s\, ds, \qquad Q_1[\phi_n u\chi_1] \le \frac{d^2}{2} C_1 \int_0^\infty \dot{\phi}_n(s)^2 s\, ds,$$

and an explicit calculation yields that both converge to zero as $n \to \infty$ if we demand, in addition, that b_2/b_1 and b_3/b_2 tend to infinity as $n \to \infty$. The same is true for the mixed term $Q_1(\varphi_n\chi_1, \phi_n u\chi_1)$ by the Schwarz inequality. On the other hand, an explicit integration w.r.t. u for the rest of $\tilde{Q}$ yields

$$\begin{aligned} Q_2[\Psi_{n,\varepsilon}] - \kappa_1^2 \|\Psi_{n,\varepsilon}\|_G & \\ = (\varphi_n, K\varphi_n)_g - 2\varepsilon(\varphi_n, M\phi_n)_g + \varepsilon^2 & \left[\|\phi_n\|_g^2 + \frac{\pi^2 - 6}{3\kappa_1^2} (\phi_n, K\phi_n)_g \right]. \end{aligned}$$

For large n the contribution of the Gauss curvature will be negligible because of $\langle\Sigma 1\rangle$ and the facts that φ_n and ϕ_n are uniformly bounded and the infimum of their support tends to infinity as $n \to \infty$. Summing up the results, we arrive at

$$\lim_{n\to\infty} \tilde{Q}[\Psi_{n,\varepsilon}] = \lim_{n\to\infty} \left[\varepsilon^2 \|\phi_n\|_g^2 - 2\varepsilon(\varphi_n, M\phi_n)_g\right] \tag{v.20}$$

if the limit on the r.h.s. exists.

We put $\varepsilon \equiv \varepsilon_n := (\varphi_n, M\phi_n)_g^{-1}$ which will be seen in a moment as a reasonable choice because the integral tends to infinity as $n \to \infty$ for particular choices of b_j ; ε_n is thus well-defined for n large enough. Then the problem turns to comparing the number -2 to the limit

$$\lim_{n\to\infty} \frac{(\phi_n, \phi_n)_g}{(\varphi_n, M\phi_n)_g^2}.$$

In the special case of cylindrically symmetric surfaces when one has the information about the explicit behaviour of M at infinity, it is an easy matter. Indeed, since k_s is integrable in $L^1(\mathbb{R}^+)$ and ϕ_n is chosen in a way to eliminate the weight r with the help of (v.4), the meridian curvature does not contribute in the denominator, while in view of Lemma v.5, $k_\vartheta r$ can be replaced by a constant value near infinity. Using in addition (v.4) in the numerator, one is therefore seeking the zero limit of

$$\frac{\int_0^\infty \phi_n(s)^2 s\,ds}{\left(\int_0^\infty \varphi_n(s)\phi_n(s)ds\right)^2} = \frac{1}{\int_0^\infty \phi_n(s)^2 s\,ds} = \frac{3}{\ln(b_3/b_1)}.$$

One can choose, for instance, $\forall n \geq 2 : b_1(n) := n$, $b_2(n) := n^2$, $b_3(n) := n^3$, which fulfill also the other properties earlier required about these sequences. We conclude by $\tilde{Q}[\Psi_{n,\varepsilon}] \to -2$ as $n \to \infty$ so we can find a finite n_0 for which the form will be negative. □

Remark. Notice that (v.20) is a general result. We have not supposed anything of the surface symmetry when deriving this relation.

EXAMPLE 5 (Hyperboloid of Revolution). Consider one of the two sheets of the hyperboloid given by the equation $x^2 + y^2 - (z/z_0)^2 = -1$. It is an asymptotically planar surface of revolution and via the parameter $z_0 > 0$ we can get arbitrary value of the total Gauss curvature between 0 and 2π.

EXAMPLE 6 (Surface with Non Square Integrable $\nabla_g M$). Let us construct an asymptotically planar surface of revolution which satisfies $\langle\Sigma 1\rangle$ but contradicts $\langle\Sigma 2\rangle$. We define $k_s(s) := s^{-2}\sin s^2$ and use (v.18) to get the functions r, z and in this way the map p. One can easily check that there is a c such that $r(s) \geq cs$ for all $s \in \mathbb{R}^+$. Therefore $k_\vartheta = \dot{z}r^{-1} \to 0$ as $s \to \infty$ because $|\dot{z}| = |\sin b(s)| \leq 1$; the same limit holds, of course, for k_s. Since K, M are expressed by means of the principal curvatures, it follows that the surface is asymptotically planar $\langle\Sigma 0\rangle$. At the same time, $|K|r = |k_s\dot{z}| \leq |k_s|$ is integrable in $L^1(\mathbb{R}^+)$ which gives $\langle\Sigma 1\rangle$. On the other hand, while it is true that $\dot{k}_\vartheta = k_s r^{-1}\cos b - r^{-2}\sin b\cos b$ belongs to $L^2(\mathbb{R}^+, r(s)ds)$, the same does not hold for $\dot{k}_s$ by its definition. Hence, $\nabla_g M = (\dot{M}, 0)$ does not fulfil $\langle\Sigma 2\rangle$. We note that an explicit calculation together with (v.19) yields $\mathcal{K} = 2\pi\left(1 - \cos\sqrt{\frac{\pi}{2}}\right) \approx 1.38\,\pi$ in this example.

Remark. (*Partial Wave Decomposition*). An alternative approach is to decompose $-\Delta_D^\Omega$ with respect to angular momentum subspaces to investigate the spectral properties of layers endowed with the cylindrical symmetry. The obtained series of partial-wave Hamiltonians have a similar form as the pure strip Hamiltonian – *cf.* [EŠ, DE] – except for an additional centrifugal term and different operator domain for the lowest wave. This, however, makes the spectral analysis of layers more complicated than a direct use of the non-decomposed Hamiltonian H. At the same time, it gives an insight into the choice of the trial function in the proof of Theorem v.6 which has to be supported in the region where the influence of the centrifugal term is negligible.

v.7 A Layer without Bound States

Consider a semi-cylinder of radius R closed by a hemisphere; the total Gauss curvature is 2π. Since the mean curvature of the cylindrical part is constant, $M = (2R)^{-1} > 0$, such a surface is not asymptotically planar. We shall demonstrate that

the Hamiltonian $H := -\Delta_D^\Omega$ of the corresponding layer Ω built over this surface does not possess bound states for any $a < R$.

Imposing the Neumann or Dirichlet boundary condition on the segment of connection of the hemispherical and cylindrical layer, we get the bounds $H_{sph}^N \oplus H_{cyl}^N \le H \le H_{sph}^D \oplus H_{cyl}^D$. The spectrum of the hemispherical-segment Hamiltonians is purely discrete. By the minimax principle only the cylindrical part of the estimating operators contributes to the essential spectrum, while a possible eigenvalue of H below the essential spectrum is squeezed between the corresponding eigenvalues of H_{sph}^N and H_{sph}^D. In particular, for our purpose it is sufficient to show that $\inf\sigma(H_{sph}^N) > \inf\sigma_{\rm ess}(H_{cyl}^D)$. The spectral analysis of these operators becomes trivial if they are expressed in the spherical or cylindrical coordinates, respectively.

Due to mirror symmetry, the ground state energy of H_{sph}^N is the same as the lowest eigenvalue of the entire spherical layer which is κ_1^2. On the other hand, $\sigma(H_{cyl}^j) = \sigma_{\rm ess}(H_{cyl}^j) = [\epsilon_1, \infty)$ for both the conditions $j \in \{N, D\}$, where the threshold ϵ_1 is given by the first eigenvalue of the Dirichlet radial operator $-\partial_r^2 - (4r^2)^{-1}$ on $L^2((R-a, R+a))$. Since the latter is less than $-\partial_r^2 - (4(R+a)^2)^{-1}$, the Rayleigh principle yields $\epsilon_1 < \kappa_1^2$. It is now easy to conclude that the spectrum of the unified layer satisfies

$$\sigma(H) = \sigma_{\rm ess}(H) = [\epsilon_1, \infty). \tag{v.21}$$

Remark. The above example shows that without the condition $\langle\Sigma 0\rangle$, or at least without $M \to 0$ at infinity, one cannot guarantee the existence of bound states. Notice that the reference surface is not C^2-smooth in this counter-example and thus it does not belong to the class of manifolds considered from the beginning. Nevertheless, one can construct a sequence of domains which converges in an appropriate sense to the hemispherical layer and, at the same time, they can be connected to the cylindrical part in a sufficiently smooth way. It follows then from [RT, Thm. 1.5] that the spectral result (v.21) remains preserved for the domains sufficiently close to the limiting layer.

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Chapitre vi

La courbure faible

Résumé

On a montré récemment qu'une particule quantique non-relativiste dans un voisinage tubulaire d'épaisseur constante et avec des frontières impénétrables, construit autour d'une surface non-compacte, simplement connexe et géodésiquement complète peut avoir des états liés tant que la surface n'est pas un plan. Dans ce travail, nous étudions les développement asymptotiques de ces états liés dans le régime du couplage faible, c'est-à-dire la situation où la surface est un plan faiblement courbé. Sous des hypothèses appropriées sur la régularité et la décroissance des courbures de la surface, nous établissons l'ordre principal dans le développement asymptotique de la valeur propre par rapport au paramètre décrivant ce couplage faible. La preuve repose sur la méthode de Birman-Schwinger.

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Bound States in Mildly Curved Layers

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Abstract

It has been shown recently that a nonrelativistic quantum particle constrained to a hard-wall layer of constant width built over a geodesically complete simply connected noncompact curved surface can have bound states provided the surface is not a plane. In this paper we study the weak-coupling asymptotics of these bound states, *i.e.*, the situation when the surface is a mildly curved plane. Under suitable assumptions about regularity and decay of surface curvatures we derive the leading order in the ground-state eigenvalue expansion. The argument is based on Birman-Schwinger analysis of Schrödinger operators in a planar hard-wall layer.

vi.1 Introduction

The investigation of quantum particles constrained to a spatial region Ω of a prescribed shape, in particular, relations between its spectral properties and the geometry of Ω became an attractive problem when the technology progress made it possible to fabricate various mesoscopic systems for which this is a reasonable model – see, *e.g.*, [LCM]. Curvature induced bound states in hard-wall strips and tubes have been demonstrated more than a decade ago [EŠ] and studied subsequently in numerous papers – *cf.* [DE, LCM] and references therein.

Much less attention was paid to quantum mechanics in layers, apart of the trivial planar case. While for an experimenter it is easier to prepare a semiconductor film on a curved substrate than to fabricate a quantum wire, from the mathematical point of view the opposite is true, and solving the Schrödinger equation in a nontrivial layer is more complicated than the corresponding problem in a tube. It was noticed long time ago that in the formal limit of zero width the layer curvatures give rise to an effective attractive potential [KJ] but the first results for curved finite-width layers, with the particle Hamiltonian being a multiple of the Dirichlet Laplacian $-\Delta_D^\Omega$, appeared only recently.

We restrict ourselves to the case when Ω is non-compact and nontrivially curved. The first proof of existence of geometrically induced bound states was given in [DEK1] under the assumption that the planar layer is curved only locally. A more general case of curved layers which are *asymptotically* planar in the sense that the curvatures of the generating surface vanish at large distances has been discussed

in [DEK2]. We have derived there several sufficient conditions for the existence of bound states expressed in terms of geometric quantities characterizing the reference surface. While these conditions cover a wide class of layers, they do not represent an ultimate result : it is not clear, *e.g.*, whether bound states exist in layers built over surfaces of positive total Gauss curvature unless the latter are thin enough or endowed with a cylindrical symmetry.

After demonstrating their existence one is naturally interested in properties of the curvature-induced bound states. A particular question which we are going to address in the present paper concerns the weak-coupling regime. Since in our case the binding comes from the curvature alone, the described situation is expected to occur in *mildly curved* layers. We will show that the layer has then a unique eigenvalue and derive an asymptotic expansion for the gap between this eigenvalue and the threshold of the essential spectrum. The leading term in this formula will depend on the mean curvature of the reference surface.

Let us describe briefly the contents of the paper. In the next section we will give a precise formulation of the problem and describe the main result summarized in Theorem vi.1. The rest is devoted to the proof. The strategy is adopted from the "lower-dimensional" case of curved strips and tubes analyzed in [DE, Sec. 4]. First, in Section vi.3, we consider Schrödinger operators acting in a planar layer built over $\mathbb{R}^2$. We derive a necessary and sufficient condition under which such an operator has a bound state in the weak coupling limit and find the asymptotic expansion of the eigenvalue. The result contained in Theorem vi.5 is of an independent interest ; we prove it in a greater generality for a layer in $\mathbb{R}^{2+m}$, $m \geq 1$. Next, in Section vi.4, we apply it to the case of mildly curved quantum layers. We express the operator $-\Delta_D^\Omega$ in the coordinates (x, u), where $x \equiv (x^1, x^2) \in \mathbb{R}^2$ and $u \in I := (-a, a)$ with $a > 0$ parametrize the surface and its normal space, respectively, and pass to a unitarily equivalent operator with an effective potential, which can be consecutively estimated by operators to which Theorem vi.5 can be applied . We will also show how the leading term in the expansion looks like in the case of a thin layer.

vi.2 The results

To give a precise statement of the main result we need first to specify what we mean by mildly curved quantum layers. Let a family of surfaces $\Sigma_\varepsilon := p\,(\mathbb{R}^2)$ be given by a Monge patch

$$p : \mathbb{R}^2 \to \mathbb{R}^3, \qquad p\,(x^1, x^2; \varepsilon) := \big(x^1, x^2, \varepsilon f(x^1, x^2)\big)\,, \tag{vi.1}$$

where f is supposed to be a C^4-smooth function. Here $\varepsilon > 0$ is the parameter which controls the deformation ; it is supposed to be small so that Σ_ε is a mildly curved plane. The cross-product of the tangent vectors $p_{,\mu} := \partial p/\partial x^\mu$, $\mu = 1, 2$, defines a unit normal field n on Σ_ε. We put $\Omega_0 := \mathbb{R}^2 \times I$ and define a layer $\Omega_\varepsilon := \mathcal{L}(\Omega_0)$ of width $d = 2a$ over the surface Σ_ε by virtue of the mapping $\mathcal{L} : \Omega_0 \to \mathbb{R}^3$ which acts as

$$\mathcal{L}(x, u; \varepsilon) := p(x; \varepsilon) + u\, n(x; \varepsilon). \tag{vi.2}$$

The layer in question is thus the spatial region closed between two parallel surfaces – *cf.* [Sp3, Prob. 12 of Chap. 3] – represented by $p \pm an$. In this sense, we will hereafter

refer to the surface coordinates (x^1, x^2) as to longitudinal variables, while u will be the transverse variable.

We consider a nonrelativistic spinless particle confined to Ω_ε which is free within it, and suppose that the boundary of the layer is a hard wall, *i.e.*, the wavefunctions satisfy the Dirichlet boundary condition there. For the sake of simplicity we set Planck's constant $\hbar = 1$ and the mass of the particle $m = \frac{1}{2}$. Then the Hamiltonian of the system can be identified with the Dirichlet Laplacian $-\Delta_D^{\Omega_\varepsilon}$ on $L^2(\Omega_\varepsilon)$, which is defined for an open set $\Omega_\varepsilon \subset \mathbb{R}^3$ as the Friedrichs extension of the Laplacian acting on $C_0^\infty(\Omega_\varepsilon)$ – *cf.* [RS4, Sec. XIII.15] or [Dav, Chap. 6]. The domain of the closure of the corresponding quadratic form is the Sobolev space $W_0^{1,2}(\Omega_\varepsilon)$.

Next we must introduce some notation and formulate assumptions about the function f, in addition to the smoothness requirement mentioned above. We consider asymptotically planar surfaces – *cf.* [DEK2] – which means that the Gauss K and mean M curvatures of Σ_ε vanish at large distances from a fixed point. This will hold if we require

$\boxed{\langle \mathsf{d1} \rangle\ f_{,\mu} \in L^\infty(\mathbb{R}^2)}$ together with $\boxed{\langle \mathsf{d2} \rangle\ f_{,\mu\nu} \to 0 \ \text{ as } |x| \to \infty}$

for $\mu, \nu \in \{1, 2\}$. This allows us to localize the essential spectrum. Adapting from [DEK2, Thm. 4.1] a simple argument based on a Neumann bracketing one finds that $\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_\varepsilon}) \geq \kappa_1^2$. Here $\{\kappa_j^2 := (\kappa_1 j)^2\}_{j=1}^\infty$, with $\kappa_1 := \pi/d$, are the eigenvalues of $-\Delta_D^I$; the corresponding eigenfunctions will be denoted by χ_j. Assuming in addition

$\boxed{\langle \mathsf{d3} \rangle\ f_{,\mu\nu\rho} \to 0 \ \text{ as } |x| \to \infty}$ and $\boxed{\langle \mathsf{d4} \rangle\ f_{,\mu\nu\rho\sigma} \in L^\infty(\mathbb{R}^2)}$

for $\mu, \nu, \rho, \sigma \in \{1, 2\}$ we will be able to prove in Section vi.4.3 that the bound is sharp,

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_\varepsilon}) = \kappa_1^2. \tag{vi.3}$$

We have also to require that the derivatives of f satisfy the following integrability hypotheses :

$\boxed{\langle \mathsf{r1,2} \rangle\ f_{,\mu\nu}\,,\ f_{,\mu\nu\rho} \in L^2\left(\mathbb{R}^2, (1 + |x|^\delta)\, dx\right),\ \text{respectively}}$

and

$\boxed{\langle \mathsf{r3} \rangle\ f_{,\mu\nu\rho\sigma} \in L^1\left(\mathbb{R}^2, (1 + |x|^\delta)\, dx\right)}$ for some $\delta > 0$

and $\mu, \nu, \rho, \sigma \in \{1, 2\}$. The main result of the present work reads as follows :

Theorem vi.1. *Let Ω_ε be a family of layers generated by the surfaces Σ_ε given by* (vi.1). *Suppose that the function $f \in C^4(\mathbb{R}^2)$ satisfies the hypotheses* ⟨d1–4⟩ *and* ⟨r1–3⟩. *If Σ_1 is not planar, then for all ε small enough $-\Delta_D^{\Omega_\varepsilon}$ has exactly one isolated eigenvalue $E(\varepsilon)$ below the essential spectrum. Moreover, it can be expressed as*

$$E(\varepsilon) = \kappa_1^2 - e^{2w(\varepsilon)^{-1}},$$

where $w(\varepsilon)$ has the following asymptotic expansion

$$w(\varepsilon) = -\varepsilon^2 \sum_{j=2}^{\infty} (\chi_1, u\chi_j)_I^2 \left(\kappa_j^2 - \kappa_1^2\right)^2 \int_{\mathbb{R}^2} \frac{|\widehat{m_0}(\omega)|^2}{|\omega|^2 + \kappa_j^2 - \kappa_1^2}\, d\omega + \mathcal{O}(\varepsilon^{2+\gamma})$$

with $\gamma := \min\{1, \delta/2\}$. Here m_0 is the lowest-order term in the expansion of the mean curvature of Σ_ε w.r.t. ε – cf. (vi.16).

Remarks. (a) The subscript "I" indicates the norm and the inner product in the space $L^2(I)$. The sum runs in fact over even n only because one integrates over the interval $I = (-a, a)$ on which the function $u \mapsto \chi_1(u)u\chi_j(u)$ is odd for odd j.

(b) The expression for the leading-term coefficient w_1 in the expansion $w(\varepsilon) =: \varepsilon^2 w_1 + \mathcal{O}(\varepsilon^{2+\gamma})$ does not have a very transparent structure, however, for thin layers it can be rewritten as

$$w_1 = -\frac{1}{2\pi}\,\|m_0\|^2 + \frac{\pi^2 - 6}{24\pi^3}\,\|\nabla m_0\|^2 d^2 + \mathcal{O}(d^4). \tag{vi.4}$$

This formula is instructive because the first term comes from the surface attractive potential $K - M^2$ which dominates the picture in this case, while the $\mathcal{O}(d^4)$ error term expresses the contribution of higher transverse modes. We refer to Section vi.4.4 for more details.

vi.3 Weakly Coupled Schrödinger Operators in a Planar Layer

Let M be an open connected precompact set in $\mathbb{R}^m$, $m \geq 1$. The object of our interest in this section will be the operator

$$H_\lambda = -\Delta_D + \lambda V \qquad \text{with} \quad \lambda > 0 \qquad \text{on} \quad \mathcal{H} := L^2(\mathbb{R}^2) \otimes L^2(M), \tag{vi.5}$$

where $-\Delta_D$ is the Dirichlet Laplacian on $\mathbb{R}^2 \times M$ defined as the closure of $-\Delta \otimes I_m + I_2 \otimes -\Delta_D^M$. In the last expression the unindexed $-\Delta$ stays for the Laplace operator in $\mathbb{R}^2$. The potential V is supposed to be $H_0^{\frac{1}{2}}$-bounded, in other words

$$\boxed{\langle \mathsf{a1} \rangle \ \exists\, a, b \geq 0 \quad \forall \psi \in \operatorname{Dom} Q_0 : \quad \|V\psi\| \leq a\|\psi\| + b\left\|H_0^{\frac{1}{2}}\psi\right\|}$$

where $\operatorname{Dom} Q_0 = W_0^{1,2}(\mathbb{R}^2 \times M)$ is the form domain of H_λ.

The Dirichlet Laplacian $-\Delta_D^M$ on $L^2(M)$ has a purely discrete spectrum consisting of eigenvalues $\kappa_1^2 < \kappa_2^2 \leq \cdots \leq \kappa_j^2 < \ldots$; the corresponding normalized eigenfunctions will be denoted as χ_j, where $j = 1, 2, \ldots$. The lowest eigenvalue is, of course, simple and the eigenfunction χ_1 can be chosen positive – *cf.* [RS4, Sec. XIII. 12]. Important for our purpose are the transverse projections of the potential,

$$V_{jj'} := \int_M \bar{\chi}_j(y)\, V(\cdot, y)\, \chi_{j'}(y)\, dy$$

and the analogous quantities for other functions on $\mathbb{R}^2 \times M$, in particular for $|V|$. We shall adopt the assumptions

$$\boxed{\langle \mathsf{a2} \rangle \ |V|_{11} \in L^{1+\delta}\left(\mathbb{R}^2\right)} \quad \text{and} \quad \boxed{\langle \mathsf{a3} \rangle \ |V|_{11} \in L^1\left(\mathbb{R}^2, (1 + |x|^\delta)\, dx\right)}$$

for some $\delta > 0$. We also suppose that the essential spectrum of H_λ does not start below the lowest transverse-mode threshold, *i.e.*,

$$\boxed{\langle \mathsf{a0} \rangle \ \inf \sigma_{\mathrm{ess}}(H_\lambda) \geq \kappa_1^2}$$

This is true, in particular, if V vanishes at large distances from a fixed point.

The goal of this section is to show that for λ small enough the discrete spectrum of H_λ below κ_1^2 is not empty provided the projection of V onto χ_1 is not repulsive in the mean. This part of spectrum then contains only one eigenvalue $E(\lambda)$ for such

a small λ and it approaches κ_1^2 as λ tends to zero. The last claim follows from the following elementary fact.

Proposition vi.2. *Assume* $\langle$a1$\rangle$. *Then there are positive constants* λ_0 *and* c *such that for all* $\lambda \in (0, \lambda_0)$ *we have* $H_\lambda \geq \kappa_1^2 - c\lambda$.

PROOF: Using the Schwarz inequality and the assumption $\langle$a1$\rangle$ together with the inequality between the geometric and arithmetic means, we have for all $\psi \in \operatorname{Dom} Q_0$ the bound

$$\begin{aligned} Q_\lambda[\psi] := \left\| H_\lambda^{\frac{1}{2}} \psi \right\|^2 &\geq \left\| H_0^{\frac{1}{2}} \psi \right\|^2 - \lambda \|\psi\| \, \|V\psi\| \\ &\geq (1 - \lambda\, b/2) \left\| H_0^{\frac{1}{2}} \psi \right\|^2 - \lambda\, (a + b/2)\, \|\psi\|^2. \end{aligned}$$

Since $\left\| H_0^{\frac{1}{2}} \psi \right\| \geq \kappa_1 \|\psi\|$, we obtain the assertion by putting $\lambda_0 := 2/b$ and $c := a + (1 + \kappa_1^2)\, b/2$. □

vi.3.1 Birman-Schwinger Analysis

Using the orthonormal basis of $L^2(M)$ given by $\{\chi_j\}$, the free resolvent operator $R_0(\alpha) := (H_0 - \alpha^2)^{-1}$ is decoupled in the following way

$$R_0(\alpha) = \sum_{j=1}^{\infty} \chi_j \, \left(-\Delta + k_j(\alpha)^2 \right)^{-1} \bar{\chi}_j, \qquad k_j(\alpha) := \sqrt{\kappa_j^2 - \alpha^2}.$$

If we are interested in eigenvalues of H_λ below the lowest transverse mode, we have to consider $\alpha \in [0, \kappa_1)$ and the two-dimensional resolvent in the middle of the expansion is well defined for any $j = 1, 2, \ldots$. It can be expressed in terms of Hankel's function – *cf.* [AGHH, Chap. I.5]. Passing to Macdonald's functions K_0 by [AS, 9.6.4], we arrive at the following integral kernel formula

$$R_0(x, y, x', y'; \alpha) = \frac{1}{2\pi} \sum_{j=1}^{\infty} \chi_j(y)\, K_0\left(k_j(\alpha)|x - x'|\right)\, \bar{\chi}_j(y'). \tag{vi.6}$$

Define $K(\alpha) := |V|^{\frac{1}{2}} R_0(\alpha) V^{\frac{1}{2}}$, where we have employed the usual sign convention, $V^{\frac{1}{2}} := |V|^{\frac{1}{2}} \operatorname{sgn} V$. According to Birman-Schwinger principle – *cf.* [Sim] – the function $\alpha(\lambda)^2 \equiv E(\lambda)$ is an eigenvalue of H_λ if and only if the operator $\lambda K(\alpha)$ has the eigenvalue -1, *i.e.*,

$$\alpha^2 \in \sigma_{\mathrm{disc}}(H_\lambda) \iff -1 \in \sigma_{\mathrm{disc}}(\lambda K(\alpha)). \tag{vi.7}$$

The first term in the expansion (vi.6) referring to $j = 1$ has a singularity at $\alpha = \kappa_1$, and as usual in such problems we have to single it out. For this purpose we first introduce the following decomposition.

Lemma vi.3. *There are real-analytic functions* f *and* g *such that*

$$\forall u \in (0, \infty): \quad K_0(u) = f(u) \ln u + g(u)$$

and

(i) $f(u) = -1 + \mathcal{O}(u^2)$, $g(u) = (\ln 2 - \gamma_{\mathrm{E}}) + \mathcal{O}(u^2)$ *as* $u \to 0+$,

(ii) $\exists\, C_1 > 0\ \forall u \in (0, \infty):\ \max\{f(u), g(u)\} \leq C_1 e^{-u}$,

where $\gamma_{\rm E}$ denotes Euler's constant.

PROOF: Around the origin a good choice to approximate the Macdonald function K_0 would be $f := -I_0$, where I_0 is the other modified Bessel function [AS, 9.6] but it has a bad behaviour at large distances. Hence we use an interpolation, for instance,

$$\begin{aligned} f(u) &:= -e^{-u^2} I_0(u) - (1 - e^{-u^2})\, K_0(u) \\ g(u) &:= e^{-u^2} I_0(u)\, \ln u + \left[1 + (1 - e^{-u^2}) \ln u\right] K_0(u). \end{aligned}$$

Using the relation [AS, 9.6.13], we obtain the behaviour at the origin (i). On the other hand, it follows by [AS, 9.7.2] that f and g have a faster-than-exponential decay at infinity, which gives together with (i) that there is a positive C_1 such that (ii) holds. □

We will thus use the decomposition $K(\alpha) = L_\alpha + M_\alpha$, where

$$L_\alpha(x,y,x',y') := -\frac{1}{2\pi} |V(x,y)|^{\frac{1}{2}}\, \chi_1(y)\, \ln k_1(\alpha)\, \chi_1(y')\, V(x',y')^{\frac{1}{2}}$$

contains the singularity and the regular M_α splits into two parts again, $M_\alpha = A_\alpha + B_\alpha$. The operator B_α is given by the projection of the resolvent on higher transverse modes, *i.e.*, $B_\alpha := |V|^{\frac{1}{2}} R_0^\perp(\alpha) V^{\frac{1}{2}}$ with

$$R_0^\perp(\alpha) := \sum_{j=2}^{\infty} \chi_j \left(-\Delta + k_j(\alpha)^2\right)^{-1} \bar{\chi}_j, \tag{vi.8}$$

and the kernel of the remaining term is therefore

$$\begin{aligned} &A_\alpha(x,y,x',y') \\ &\quad := \frac{1}{2\pi} |V(x,y)|^{\frac{1}{2}}\, \chi_1(y) \left(K_0(k_1(\alpha)|x-x'|) + \ln k_1(\alpha)\right) \chi_1(y')\, V(x',y')^{\frac{1}{2}}. \end{aligned}$$

We note that M_α is by definition well defined for $\alpha = \kappa_1$. In particular,

$$A_{\kappa_1}(x,y,x',y') = -\frac{1}{2\pi} |V(x,y)|^{\frac{1}{2}}\, \chi_1(y) \left(\gamma_{\rm E} + \ln \frac{|x-x'|}{2}\right) \chi_1(y') V(x',y')^{\frac{1}{2}}.$$

Furthermore, we have the following lemma. Since its proof is purely technical, we postpone it to Section vi.3.2 below.

Lemma vi.4. *Assume* ⟨a1–3⟩. *Then there are positive C_2, C_3 and C_4 such that*

(i) $\forall \alpha \in [0, \kappa_1]: \quad \|M_\alpha\| < C_2$,

(ii) $\|M_\alpha - M_{\kappa_1}\| \le C_3 \lambda^\gamma$, *with* $\gamma := \min\{1, \delta/2\}$,

(iii) $\left\| \frac{dM_\alpha(w)}{dw} \right\| < C_4 |w|^{-1}$ *for λ sufficiently small, where* $w := (\ln k_1(\alpha))^{-1}$.

We recall that Proposition vi.2 yields $\alpha^2 \to \kappa_1^2-$ as $\lambda \to 0+$, and consequently, $k_1(\alpha) \to 0+$. Hence the auxiliary variable w is well defined and negative for λ small enough, and $w \to 0-$ as $\lambda \to 0+$.

By the Birman-Schwinger principle (vi.7) eigenvalues of H_λ correspond to singularities of the operator $(I + \lambda K(\alpha))^{-1}$ which we can equivalently express as

$$(I + \lambda K(\alpha))^{-1} = \left[I + \lambda (I + \lambda M_\alpha)^{-1} L_\alpha\right]^{-1} (I + \lambda M_\alpha)^{-1}.$$

Since M_α is bounded independently of α due to Lemma vi.4(i), we have $\|\lambda M_\alpha\| < 1$ for all sufficiently small λ, and therefore the second term on the right hand side of the last relation is a bounded operator. On the other hand, $\lambda(I+\lambda M_\alpha)^{-1}L_\alpha$ is a rank-one operator of the form $(\psi,\cdot)\varphi$, where

$$\begin{aligned}\psi(x,y) &:= -\frac{\lambda}{2\pi}\,\ln k_1(\alpha)\,V(x,y)^{\frac12}\,\chi_1(y),\\ \varphi(x,y) &:= [(I+\lambda M_\alpha)^{-1}|V|^{\frac12}\chi_1](x,y),\end{aligned}$$

so it has just one eigenvalue which is (ψ,φ). The requirement that the latter equals -1 yields the implicit equation

$$w = F(\lambda,w), \qquad F(\lambda,w) := \frac{\lambda}{2\pi}\left(V^{\frac12}\chi_1, \left(I+\lambda M_{\alpha(w)}\right)^{-1}|V|^{\frac12}\chi_1\right), \tag{vi.9}$$

where we use the auxiliary variable w defined in Lemma vi.4 which determines the energy via $\alpha^2 = \kappa_1^2 - e^{2w^{-1}}$. Solving (vi.9), we arrive at the main result of this section.

Theorem vi.5. *Assume* ⟨a0–3⟩ *and exclude the trivial case, $V\equiv 0$. Then H_λ has for sufficiently small $\lambda>0$ exactly one eigenvalue $E(\lambda)$ if and only if*

$$\int_{\mathbb{R}^2} V_{11}(x)\,dx \le 0, \tag{vi.10}$$

and in this case we can express it as $E(\lambda) = \kappa_1^2 - e^{2w(\lambda)^{-1}}$, where $w(\lambda)$ has the following asymptotic expansion :

$$\begin{aligned} w(\lambda) &= \frac{\lambda}{2\pi}\int_{\mathbb{R}^2} V_{11}(x)\,dx\\ &+ \left(\frac{\lambda}{2\pi}\right)^2\left\{\int_{\mathbb{R}^2\times\mathbb{R}^2} V_{11}(x)\left(\gamma_{\mathrm{E}}+\ln\frac{|x-x'|}{2}\right)V_{11}(x')\,dx\,dx'\right.\\ &\quad \left.-\sum_{j=2}^{\infty}\int_{\mathbb{R}^2\times\mathbb{R}^2} V_{1j}(x)\,K_0(k_j(\kappa_1)|x-x'|)\,V_{j1}(x')\,dx\,dx'\right\}\\ &+ \mathcal{O}(\lambda^{2+\gamma}) \end{aligned} \tag{vi.11}$$

with $\gamma := \min\{1,\delta/2\}$.

Proof: Inserting the identity

$$(I+\lambda M_\alpha)^{-1} = I - \lambda M_{\kappa_1} - \lambda(M_\alpha - M_{\kappa_1}) + \lambda^2 M_\alpha^2 (I+\lambda M_\alpha)^{-1},$$

into (vi.9) and employing Lemma vi.4(i-ii), we get the asymptotic expansion (vi.11). Note that its coefficients are well defined owing to ⟨a3⟩ ; in particular, for the second-order terms it is true since $(V^{\frac12}\chi_1, M_{\kappa_1}|V|^{\frac12}\chi_1)$ estimated by the Schwarz inequality is finite because of ⟨a3⟩ and Lemma vi.4(i). The sufficient and necessary condition (vi.10) follows from the fact that $E(\lambda)$ converges to κ_1^2 as $\lambda\to 0+$ because of Proposition vi.2, which corresponds to the situation that w goes to zero assuming *negative* values. In view of (vi.11) it is evident that this is the case if $\int V_{11}$ is strictly negative. We want to show that w is negative for small λ also if the first

term in the expansion vanishes. Suppose first that the potential projections $V_{jj'}$ belong to $L^2(\mathbb{R}^2)$. Then we have

$$\begin{aligned}
&\int_{\mathbb{R}^2\times\mathbb{R}^2} V_{1j}(x)\, K_0(k_j(\kappa_1)|x-x'|)\, V_{j1}(x')\, dx\, dx' \\
&\quad = (V_{1j}, K_0 * V_{j1}) = \left(\widehat{V_{1j}}, \widehat{K_0 * V_{j1}}\right) \\
&\quad = 2\pi \left(\widehat{V_{1j}}, \widehat{K_0}\widehat{V_{j1}}\right) = (2\pi)^2 \int_{\mathbb{R}^2} \frac{|\widehat{V_{1j}}(\omega)|^2}{|\omega|^2+\kappa_j^2-\kappa_1^2}\, d\omega > 0, \qquad \text{(vi.12)}
\end{aligned}$$

because $(2\pi)^{-1}K_0(k_j(\kappa_1)|\cdot|)$ is the Green function of $-\Delta + k_j(\kappa_1)^2$. At the same time, by Lemma vi.3(i) and the fact that we deal with the case $\int V_{00} = 0$ now,

$$\begin{aligned}
&-\int_{\mathbb{R}^2\times\mathbb{R}^2} V_{11}(x)\, \left(\gamma_{\mathrm{E}} + \ln\frac{|x-x'|}{2}\right)\, V_{11}(x')\, dx\, dx' \\
&\quad = \lim_{\varepsilon\to 0+} \int_{\mathbb{R}^2\times\mathbb{R}^2} V_{11}(x)\, \left(K_0(\varepsilon|x-x'|) + \ln\varepsilon\right)\, V_{11}(x')\, dx\, dx' \\
&\quad = \lim_{\varepsilon\to 0+} \int_{\mathbb{R}^2\times\mathbb{R}^2} V_{11}(x)\, K_0(\varepsilon|x-x'|)\, V_{11}(x')\, dx\, dx' \qquad \text{(vi.13)}
\end{aligned}$$

is also positive, which follows by the consecutive use of the Fourier transform trick (vi.12). For a general $V_{jj'} \notin L^2(\mathbb{R}^2)$ we can approximate the potential by the cut-off functions $V^N := \chi_{[-N,N]^2} \operatorname{sgn} V \min\{|V|, N\}$, where $\chi_{\mathcal{A}}$ denotes the characteristic function of a set $\mathcal{A}$. Then the expressions in the first line of (vi.12) and the last line of (vi.13) are approximated by sequences whose elements are positive by the above argument. Using the dominated convergence and the absolute continuity of the Lebesgue integral we find that the limits exist, and of course they are positive again. Together we get that the second-order term in the expansion (vi.11) is negative.

It remains to check that (vi.11) is the only solution of (vi.9) for λ small. This will be true if we prove it for a non-positive V since it represents a more attractive interaction; we thus replace V by $-|V|$ in the expression for F. Using the Schwarz and triangle inequalities together with Lemma vi.4(i), (iii), we arrive at the estimate

$$\begin{aligned}
&\left|\frac{\partial F}{\partial w}(\lambda, w)\right| \\
&\quad = \frac{\lambda}{2\pi}\left|\left(|V|^{\frac12}\chi_1, (I+\lambda M_{\alpha(w)})^{-1}\lambda\frac{dM_{\alpha(w)}}{dw}(I+\lambda M_{\alpha(w)})^{-1}|V|^{\frac12}\chi_1\right)\right| \\
&\quad \le \frac{\lambda^2}{2\pi}\left\||V|^{\frac12}\chi_1\right\|_2^2 \left\|\left(I+\lambda M_{\alpha(w)}\right)^{-1}\right\|^2 \left\|\frac{dM_{\alpha(w)}}{dw}\right\| \\
&\quad \le \frac{\lambda^2}{2\pi}\,(1-\lambda C_2)^{-2}\frac{C_4}{|w|}\,\||V|_{11}\|_1^2\,,
\end{aligned}$$

which holds for λ sufficiently small and strictly less than C_2^{-1}. The norm of the potential is finite by assumption ⟨a3⟩. Excluding the trivial case $V \equiv 0$ we note that there exists a $c' > 0$ such that the inequality $|w|^{-1} \le c'\lambda^{-1}$ is valid for any solution w of the implicit equation (vi.9) and λ small enough. So there is a $C_5 > 0$ such that the partial derivative of F w.r.t. w is bounded by $C_5\lambda$ for all sufficiently

small λ. Since any two solutions w_1, w_2 of the equation $w = F(\lambda, w)$ have to fulfill

$$|w_2 - w_1| = \left| \int_{w_1}^{w_2} \frac{\partial F}{\partial w}\, dw \right| \leq \left| \int_{w_1}^{w_2} \left| \frac{\partial F}{\partial w} \right| \, dw \right| \leq C_5 \lambda \, |w_2 - w_1|,$$

the uniqueness is ensured for $\lambda < C_5^{-1}$. □

vi.3.2 Proof of Lemma vi.4

A reader not interested in the following technical analysis of the operator M_α may skip this subsection. We recall that M_α is given by the sum of A_α and B_α, which are of a different nature. To prove the assertions of Lemma vi.4 we consider each of the operators separately.

Analysis of A_α

We show first that this operator is of the Hilbert-Schmidt class for $\alpha = \kappa_1$.

Lemma vi.6. *Asuume* ⟨a2⟩, ⟨a3⟩, *then* A_{κ_1} *is a Hilbert-Schmidt operator.*

Proof: Let us compute the HS-norm

$$\|A_{\kappa_1}\|_{HS}^2 = \frac{1}{4\pi^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |V|_{11}(x) \left| \gamma_{\mathrm{E}} + \ln \frac{|x - x'|}{2} \right|^2 |V|_{11}(x')\, dx\, dx'.$$

It can be estimated by a sum of two integrals. The first one will be finite if $|V|_{11} \in L^1(\mathbb{R}^2)$ which is true by ⟨a3⟩, so it remains to check that the integral

$$J := \int_{\mathbb{R}^2 \times \mathbb{R}^2} |V|_{11}(x)\, \ln^2 |x - x'|\, |V|_{11}(x')\, dx\, dx'$$

is finite. To estimate it, we divide the region of integration into two parts : if $|x - x'| \geq 1$, then for any $\delta > 0$ there is a $C_\delta > 0$ such that

$$\ln^2 |x - x'| \leq \ln^2(|x| + |x'|) \leq \ln^2(1 + |x|)(1 + |x'|) \leq C_\delta (1 + |x|^\delta)(1 + |x'|^\delta)$$

and the contribution to J is thus finite because of ⟨a3⟩. On the other hand, for $|x - x'| < 1$ we use the Hölder and Young inequalities

$$\begin{aligned} J &= \int_{\mathbb{R}^2} dx\, |V|_{11}(x) \int_{\mathbb{R}^2} dx' \chi_{[0,1]}(|x - x'|)\, \ln^2 |x - x'|\, |V|_{11}(x') \\ &\leq \| |V|_{11} \|_{1+\delta} \, \| \chi_{[0,1]} \ln^2 * |V|_{11} \|_{1+\delta^{-1}} \\ &\leq \| |V|_{11} \|_{1+\delta}^2 \, \| \chi_{[0,1]} \ln \|_r = \Gamma(r+1)^{\frac{1}{r}} \, \| |V|_{11} \|_{1+\delta}^2 \,, \end{aligned}$$

where $r := (1 + \delta^{-1})/2$, which yields a finite value owing to ⟨a2⟩. □

In a similar way we can estimate the HS-norm of $A_\alpha - A_{\kappa_1}$.

Lemma vi.7. *Assume* ⟨a3⟩, *then* $\|A_\alpha - A_{\kappa_1}\|_{HS} \leq C_6\, k_1(\alpha)^\delta$ *holds with a positive constant* C_6 *independent of* α.

PROOF: Using the decomposition of Lemma vi.3,

$$\begin{aligned}(A_\alpha - A_{\kappa_1})(x,y,x',y') \\ &= |V(x,y)|^{\frac{1}{2}}\,\chi_1(y)\,\Big\{[f(k_1(\alpha)|x-x'|) - f(0)]\ln k_1(\alpha)|x-x'| \\ &\quad + g(k_1(\alpha)|x-x'|) - g(0)\Big\}\,\chi_1(y')\,V(x',y')^{\frac{1}{2}},\end{aligned}$$

which yields the estimate $\|A_\alpha - A_{\kappa_1}\|_{HS}^2 \leq 2\,(J_1^2 + J_2^2)$, where

$$J_\ell := \int_{\mathbb{R}^2\times\mathbb{R}^2} |V|_{11}(x)\,h_\ell(k_1(\alpha)|x-x'|)\,|V|_{11}(x')\,dx\,dx', \quad \ell = 1,2\,,$$

with $h_1(u) := [(f(u)-f(0))\ln u]^2$ and $h_2(u) := [g(u)-g(0)]^2$. Since these functions are bounded, both integrals are finite under the assumption $|V|_{11} \in L^1(\mathbb{R}^2)$. Consequently, $\|A_\alpha - A_{\kappa_1}\|_{HS}$ has a bound independent of α. However, we want to prove in addition that A_α converges in HS-norm to A_{κ_1}, *i.e.*, the stated assertion. By virtue of Lemma vi.3, we have for any $\delta \in (0,2)$ the rough bounds $h_\ell(u) \leq c_\ell u^\delta$ for some constants $c_\ell > 0$. This bound together with $|x-x'|^\delta \leq \max\{1, 2^{\delta-1}\}\,(|x|^\delta + |x'|^\delta)$ and $|x|^\delta + |x'|^\delta \leq (1+|x|^\delta)(1+|x'|^\delta)$, yields the estimate

$$J_\ell \leq \tilde{C}_6\,k_1(\alpha)^\delta \left(\int_{\mathbb{R}^2} |V|_{11}(x)\,(1+|x|^\delta)\,dx\right)^2,$$

where $\tilde{C}_6 := \max\{1, 2^{\delta-1}\}\max\{c_1, c_2\}$. Since the integral is finite by ⟨a3⟩, we arrive at the sought result. □

It is now easy to check that the two preceding lemmas imply the claims (i) and (ii) of Lemma vi.4 for the operator A_α, since $\|\cdot\| \leq \|\cdot\|_{HS}$ and $k_1(\alpha) = \mathcal{O}(\lambda^{\frac{1}{2}})$ as it follows from Proposition vi.2.

It is also easy to see that $\alpha \mapsto A_\alpha$ considered as the operator-valued function is real-analytic in $[0,\kappa_1)$. It cannot be analytically continued to an open interval containing κ_1, however, if we consider instead the function $w \mapsto A_{\alpha(w)}$ with the auxiliary variable $w = (\ln k_1(\alpha))^{-1}$, this one can be continued to a complex region that includes $w = 0$, which is the point of our interest because it is obtained in the limit $\lambda \to 0$. We use this fact to estimate the norm of the derivative w.r.t. w, which establishes the claim (iii) of Lemma vi.4 for the operator $A_{\alpha(w)}$.

Lemma vi.8. *Assume* ⟨a2⟩ *and* ⟨a3⟩*, then for sufficiently small* w*,*

$$\left\|\frac{dA_{\alpha(w)}}{dw}\right\| < \frac{C_7}{|w|} \quad \textit{with some} \quad C_7 > 0.$$

PROOF: Let us choose the contour $\Gamma := \{z = w + we^{it} \;:\; t \in [0,2\pi)\}$ in the complex plane, where w is supposed to be negative and small enough so that $A_{\alpha(w)}$ is analytic in the interior of the curve. We can use the Cauchy integral formula to estimate the complex derivative

$$\left\|\frac{dA_{\alpha(w)}}{dw}\right\| = \left\|\frac{1}{2\pi i}\oint_\Gamma \frac{A_{\alpha(z)}}{(z-w)^2}\,dz\right\| \leq \frac{\sup_{z\in\Gamma}\|A_{\alpha(z)}\|}{|w|}.$$

It is straightforward to modify the proof of Lemma vi.7 (including the technical Lemma vi.3) in order to check the continuity of A_α in κ_1 w.r.t. to the HS-norm also for complex values of α. This yields the desired result. □

Analysis of B_α

Mimicking [BGRS, Lemma 2.2] and [BEGK, Lemma 2.3] we denote as $\mathcal{H}_1 \subset \mathcal{H}$ the subspace $L^2(\mathbb{R}^2)\otimes\{\chi_1\}$. Let $\mathcal{P}_1$ be the corresponding projection and $\mathcal{P}_1^\perp := I - \mathcal{P}_1$, then we can write $R_0^\perp(\alpha)$ defined in (vi.8) as $\mathcal{P}_1^\perp\, R_0(\alpha)\, \mathcal{P}_1^\perp$.

Lemma vi.9. *Assume* $\langle$a1$\rangle$*, then* $\alpha \mapsto B_\alpha$ *is uniformly bounded in the operator-norm topology on the interval* $[0, \kappa_2 - \varepsilon]$ *for any* $\varepsilon \in (0, \kappa_2]$.

Proof: Since the lowest point in the spectrum of $H_0\,\mathcal{P}_1^\perp \restriction \mathcal{P}_1^\perp\mathcal{H}$ is κ_2^2, the operator-valued function $R_0^\perp(\cdot)$ has an analytic continuation into the region $\{\alpha \in \mathbb{C} \mid \alpha^2 \in \mathbb{C}\setminus[\kappa_2^2, \infty)\}$. In particular, this region includes the interval $[0, \kappa_1]$ actually considered, where one has the following estimate on the norm

$$\left\| R_0^\perp(\alpha) \right\| = \sup_{j=2,3,\ldots} (\kappa_j^2 - \alpha^2)^{-1} = (\kappa_2^2 - \alpha^2)^{-1} < (\kappa_2^2 - \kappa_1^2)^{-1}.$$

If V was essentially bounded then this result would be sufficient for the boundedness of B_α because $\|B_\alpha\| \leq \|V^{\frac12}\|_\infty \|R_0^\perp(\alpha)\|\, \|V^{\frac12}\|_\infty$. In order to accommodate the extra factors $|V|^{\frac12}, V^{\frac12}$ under our weaker assumption $\langle$a1$\rangle$, we introduce the quadratic form

$$b_\alpha(\phi,\psi) := (\phi, B_\alpha\psi) = \left(R_0^\perp(\alpha)^{\frac12}\, \mathcal{P}_1^\perp\, |V|^{\frac12}\phi, R_0^\perp(\alpha)^{\frac12}\, \mathcal{P}_1^\perp\, V^{\frac12}\psi \right)$$

with α supposed to be a real number from an interval $[0, \kappa_2 - \varepsilon]$. To check boundedness of this form, it is sufficient to verify that $R_0^\perp(\alpha)^{\frac12}\, \mathcal{P}_1^\perp\, |V|^{\frac12}$ is a bounded operator, *i.e.*, that $|V|^{\frac12}$ is $(R_0^\perp(\alpha)^{-\frac12}\, \mathcal{P}_1^\perp)$-bounded, which is equivalent to the statement that there exist $c_1, c_2 \geq 0$ such that

$$\forall \psi \in \mathrm{Dom}\, Q_0 : \quad \left\| V^{\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 \leq c_1\, \|\psi\|^2 + c_2 \left\| R_0^\perp(\alpha)^{-\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 .$$

However,

$$\begin{aligned} \left\| V^{\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 &= \left(\mathcal{P}_1^\perp\, \psi, |V|\, \mathcal{P}_1^\perp\, \psi \right) \leq \left\| \mathcal{P}_1^\perp\, \psi \right\| \, \left\| V\, \mathcal{P}_1^\perp\, \psi \right\| \\ &\leq \left\| \mathcal{P}_1^\perp\, \psi \right\| \left(a \left\| \mathcal{P}_1^\perp\, \psi \right\| + b \left\| H_0^{\frac12}\, \mathcal{P}_1^\perp\, \psi \right\| \right) \\ &\leq \left(a + \frac{b}{2} \right) \|\psi\|^2 + \frac{b}{2} \left\| H_0^{\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 . \end{aligned}$$

In the first step we have used the Schwarz inequality, in the second our hypothesis $\langle$a1$\rangle$, and finally the inequality between the geometric and arithmetic means together with $\| \mathcal{P}_1^\perp\, \psi\| \leq \|\psi\|$. At the same time,

$$\left\| R_0^\perp(\alpha)^{-\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 = \left(\mathcal{P}_1^\perp\, \psi, (H_0 - \alpha^2)\, \mathcal{P}_1^\perp\, \psi \right) \geq \left\| H_0^{\frac12}\, \mathcal{P}_1^\perp\, \psi \right\|^2 ,$$

so we can identify $c_1 := a + b/2$ and $c_2 := b/2$ which completes our proof. □

This establishes Lemma vi.4(i) for the operator B_α. Since $k_1(\alpha)^2 \leq c\lambda$ owing to Proposition vi.2, the property (ii) is included in the following result.

Lemma vi.10. *Assume* $\langle$a1$\rangle$*, then there exists* $C_7 > 0$ *such that*

$$\|B_\alpha - B_{\kappa_1}\| \leq C_7\, k_1(\alpha)^2.$$

PROOF: Using the first resolvent identity [Wei, Thm. 5.13], we infer

$$\begin{aligned}\|B_\alpha - B_{\kappa_1}\| &= |\alpha-\kappa_1| \left\| |V|^{\frac{1}{2}} R_0^\perp(\alpha) R_0^\perp(\kappa_1) V^{\frac{1}{2}} \right\| \\ &\leq |\alpha-\kappa_1| \left\| |V|^{\frac{1}{2}} R_0^\perp(\alpha)^{\frac{1}{2}} \right\| \left\| R_0^\perp(\alpha)^{\frac{1}{2}} \right\| \left\| R_0^\perp(\kappa_1)^{\frac{1}{2}} \right\| \left\| R_0^\perp(\kappa_1)^{\frac{1}{2}} V^{\frac{1}{2}} \right\| .\end{aligned}$$

However, $|\kappa_1 - \alpha| \leq \kappa_1^{-1} k_1(\alpha)^2$ and it is clear from the proof of Lemma vi.9 that the remaining factors at the r.h.s. of the above estimate are finite. □

Similarly to the operator A_α, we need also a bound on the derivative of $B_{\alpha(w)}$ w.r.t. w. However, the situation in the present case is simpler because $R_0^\perp(\alpha)$ itself is analytic in an open complex set containing $\alpha = \kappa_1$.

Lemma vi.11. *Assume* ⟨a1⟩*, then for sufficiently small* w*,*

$$\left\| \frac{dB_{\alpha(w)}}{dw} \right\| \leq C_8 \quad \textit{with some} \quad C_8 > 0.$$

PROOF: Since

$$\frac{dB_{\alpha(w)}}{dw} = \frac{dB_\alpha}{d\alpha}\frac{d\alpha}{dw} = 2\frac{e^{2w^{-1}}}{w^2} |V|^{\frac{1}{2}} R_0^\perp(\alpha(w))^2 V^{\frac{1}{2}}$$

and the prefactor function $w^{-2}e^{2w^{-1}}$ is uniformly bounded in $(-\infty, 0)$, we can employ the Schwarz inequality to get the estimate

$$\left\| |V|^{\frac{1}{2}} R_0^\perp(\alpha)^2 V^{\frac{1}{2}} \right\| \leq \left\| |V|^{\frac{1}{2}} R_0^\perp(\alpha)^{\frac{1}{2}} \right\| \left\| R_0^\perp(\alpha) \right\| \left\| R_0^\perp(\alpha) V^{\frac{1}{2}} \right\| .$$

It is clear from the proof of Lemma vi.9 that the right hand side of this inequality is uniformly bounded in $[0, \kappa_2 - \varepsilon]$ for any $\varepsilon \in (0, \kappa_2]$. The former interval contains a neighbourhood of κ_1 in which w is well defined. □

This yields the remaining assertion (iii) of Lemma vi.4 for $|w| < 1$.

vi.4 Mildly Curved Layers

Our strategy in proving the ground-state asymptotic expansion in mildly curved layers Ω_ε will be to estimate the corresponding Hamiltonian $-\Delta_D^{\Omega_\varepsilon}$ by an operator of the form $-\Delta - \Delta_D^I + \varepsilon V$ and to apply Theorem vi.5 to the latter. Here $-\Delta$ is the Laplacian in the plane, $-\Delta_D^I$ is the transverse operator which is the particular case of $-\Delta_D^M$ discussed in the preceding section, and V is an effective potential given by curvatures of Σ_ε.

vi.4.1 The Geometry

The family of metric tensors for the surfaces given by (vi.1) has the form

$$g_{\mu\nu}(\varepsilon) = \delta_{\mu\nu} + \varepsilon^2 \eta_{\mu\nu} \qquad \text{with} \qquad (\eta_{\mu\nu}) := \begin{pmatrix} f_{,1}{}^2 & f_{,1}f_{,2} \\ f_{,1}f_{,2} & f_{,2}{}^2 \end{pmatrix},$$

where the symbol $\delta_{\mu\nu}$ (as well as $\delta^{\mu\nu}$) has to be understood as the identity matrix. Since $\det(\eta_{\mu\nu}) = 0$ we get immediately

$$g(\varepsilon) := \det(g_{\mu\nu}) = 1 + \varepsilon^2 \operatorname{tr}(\eta_{\mu\nu}) = 1 + \varepsilon^2 (f_{,1}{}^2 + f_{,2}{}^2) \tag{vi.14}$$

together with the expression for the inverse matrix

$$g^{\mu\nu}(\varepsilon) = g(\varepsilon)^{-1}(\delta^{\mu\nu} + \varepsilon^2\tilde{\eta}^{\mu\nu}) \qquad \text{with} \qquad (\tilde{\eta}^{\mu\nu}) := \begin{pmatrix} {f_{,2}}^2 & -f_{,1}f_{,2} \\ -f_{,1}f_{,2} & {f_{,1}}^2 \end{pmatrix}.$$

In particular, the Jacobian $g^{\frac{1}{2}}$ defines through $d\Sigma_\varepsilon := g^{\frac{1}{2}}dx$ the invariant surface element. We will suppose that the matrix function $\eta_{\mu\nu}$ is bounded. Since its eigenvalues are 0 and ${f_{,1}}^2 + {f_{,2}}^2$, this will be true provided the second eigenvalue is a bounded function in $\mathbb{R}^2$, *i.e.*, if we adopt the assumption $\langle$d1$\rangle$. Denote the bound of $\eta_{\mu\nu}$ by η_∞. Then it follows that $g_{\mu\nu}(\varepsilon)$ is uniformly elliptic for sufficiently small ε because

$$c_-\delta_{\mu\nu} \le g_{\mu\nu}(\varepsilon) \le c_+\delta_{\mu\nu} \qquad \text{with} \qquad c_\pm := 1 \pm \varepsilon^2\eta_\infty. \tag{vi.15}$$

At the same time, the vector $n(\varepsilon) = g(\varepsilon)^{-\frac{1}{2}}(-\varepsilon f_{,1}, -\varepsilon f_{,2}, 1)$ represents the surface normal and therefore the second fundamental form is given by

$$h_{\mu\nu}(\varepsilon) = \varepsilon g(\varepsilon)^{-\frac{1}{2}}\theta_{\mu\nu} \qquad \text{with} \quad (\theta_{\mu\nu}) := \begin{pmatrix} f_{,11} & f_{,12} \\ f_{,21} & f_{,22} \end{pmatrix}.$$

We can construct now the Weingarten tensor [Kli, Def. 3.3.4 & Prop. 3.5.5]

$$h_\mu{}^\nu(\varepsilon) := h_{\mu\rho}g^{\rho\nu} = \varepsilon g(\varepsilon)^{-\frac{3}{2}}\left(\theta_{\mu\rho}\delta^{\rho\nu} + \varepsilon^2\theta_{\mu\rho}\tilde{\eta}^{\rho\nu}\right),$$

which determines respectively the Gauss curvature K and the mean curvature M of the surface Σ_ε :

$$\begin{aligned} K(\varepsilon) &= \varepsilon^2 g(\varepsilon)^{-2}k_0 \qquad\qquad \text{with} \quad k_0 := \det(\theta_{\mu\nu}) = f_{,11}f_{,22} - {f_{,12}}^2, \\ M(\varepsilon) &= \varepsilon g(\varepsilon)^{-\frac{3}{2}}\left(m_0 + \varepsilon^2 m_1\right) \text{ with} \quad m_0 := \frac{1}{2}\operatorname{tr}(\theta_{\mu\nu}) = \frac{1}{2}\left(f_{,11} + f_{,22}\right) \\ &\text{and} \quad m_1 := \frac{1}{2}\operatorname{tr}(\theta_{\mu\rho}\tilde{\eta}^{\rho\nu}) = \frac{1}{2}\left({f_{,1}}^2 f_{,22} + {f_{,2}}^2 f_{,11} - 2f_{,1}f_{,2}f_{,12}\right). \end{aligned} \tag{vi.16}$$

Since we are interested in the case when Σ_ε is asymptotically planar [DEK2], *i.e.*, when $K, M \to 0$ as $|x| \to \infty$, we assume $\langle$d2$\rangle$.

It is clear from the definition (vi.2) that the metric tensor of the layer Ω_ε as a manifold in $\mathbb{R}^3$ has the block form

$$(G_{ij}) = \begin{pmatrix} (G_{\mu\nu}) & 0 \\ 0 & 1 \end{pmatrix} \quad \text{with} \quad G_{\nu\mu} = (\delta^\sigma_\nu - uh_\nu{}^\sigma)(\delta^\rho_\sigma - uh_\sigma{}^\rho)g_{\rho\mu}, \tag{vi.17}$$

and thus $G := \det(G_{ij}) = g(1 - 2Mu + Ku^2)^2$. Following [DEK2], one should make sure that the layer mapping $\mathcal{L}$ is a diffeomorphism. However, this is automatically fulfilled for an arbitrary a provided ε is small enough and the layer is built over surfaces of the special form (vi.1). At the same time, $G_{\mu\nu}$ can be estimated by the surface metric,

$$C_-g_{\mu\nu} \le G_{\mu\nu} \le C_+g_{\mu\nu} \qquad \text{with} \qquad C_\pm := \left(1 \pm a\rho_m^{-1}\right)^2, \tag{vi.18}$$

where $\rho_m^{-1} := \max\{\|k_1\|_\infty, \|k_2\|_\infty\} = \mathcal{O}(\varepsilon)$ and k_1, k_2 are the principal curvatures of Σ_ε, *i.e.*, the eigenvalues of $h_\mu{}^\nu$.

vi.4.2 The Hamiltonian

In the beginning we have identified the particle Hamiltonian with $-\Delta_D^{\Omega_\varepsilon}$. We want to replace it by a Schrödinger-type operator which would allow us to employ the result of the previous section. This is achieved by means of the unitary transformation

$$U : L^2(\Omega_\varepsilon) \to L^2(\Omega_0, g^{\frac{1}{2}} dx\, du) : \{\psi \mapsto U\psi := (1 - 2Mu + Ku^2)^{\frac{1}{2}}\, \psi \circ \mathcal{L}\},$$

which leads to the unitarily equivalent operator

$$\begin{aligned} H &:= U(-\Delta_D^{\Omega_\varepsilon})U^{-1} = -g^{-\frac{1}{2}} \partial_i g^{\frac{1}{2}} G^{ij} \partial_j + V \\ V &= g^{-\frac{1}{2}} (g^{\frac{1}{2}} G^{ij} J_{,j})_{,i} + J_{,i} G^{ij} J_{,j} \qquad \text{with} \quad J := \ln \sqrt{1 - 2Mu + Ku^2}. \end{aligned}$$

It makes sense since we suppose that the surface is C^4-smooth. Using the block form (vi.17) of G_{ij}, we can split H into a sum, $H = H_1 + H_2$. For the first operator which is given by the part of H where one sums over the Greek indices (referring to the longitudinal coordinates) we have owing to (vi.18) the estimate

$$(C_-/C_+^2)\,(-\Delta_g + v_1) \le H_1 \le (C_+/C_-^2)\,(-\Delta_g + v_1) \tag{vi.19}$$

which holds in $L^2(\mathbb{R}^2 \times I, g^{\frac{1}{2}} dx\, du)$ in the form sense. Here $-\Delta_g$ denotes the surface Laplace-Beltrami operator which can be written in the component form as $-g^{-\frac{1}{2}} \partial_\mu g^{\frac{1}{2}} g^{\mu\nu} \partial_\nu$, and

$$v_1 := -\frac{|u^2 \nabla_g K - 2u \nabla_g M|_g^2}{4(1 - 2Mu + Ku^2)^2} + \frac{u^2 \Delta_g K - 2u \Delta_g M}{2(1 - 2Mu + Ku^2)}\,, \tag{vi.20}$$

where $|\cdot|_g$ and ∇_g mean respectively the norm and the gradient operator induced by the metric $g_{\mu\nu}$. On the other hand,

$$H_2 = -\partial_3^2 + V_2\,, \qquad V_2 = \frac{K - M^2}{(1 - 2Mu + Ku^2)^2}\,, \tag{vi.21}$$

where the potential V_2 is attractive because $K - M^2$ can be rewritten by means of the principal curvatures as $-\frac{1}{4}(k_1 - k_2)^2$.

In the second step one uses the inequalities (vi.15), which are a consequence of $\langle$d1$\rangle$, in order to get the bounds

$$(c_-^2/c_+^3)\,(-\Delta) \le -\Delta_g \le (c_+^2/c_-^3)\,(-\Delta) \qquad \text{in} \quad L^2(\mathbb{R}^2, g^{\frac{1}{2}} dx).$$

It remains to realize that – as another consequence of the uniform ellipticity of the metric – one can identify $L^2(\mathbb{R}^2, g^{\frac{1}{2}} dx) = L^2(\mathbb{R}^2)$, and also $L^2(\mathbb{R}^2 \times I, g^{\frac{1}{2}} dx\, du) = L^2(\mathbb{R}^2 \times I)$ as sets. If we rescale the longitudinal variable by means of $x \mapsto \sigma_\pm x$ with $\sigma_\pm^2 := c_\mp^3 C_\mp^2/(c_\pm^2 C_\pm)$, we obtain finally the above indicated bounds

$$H_- \le H \le H_+ \qquad \text{with} \qquad H_\pm := -\Delta - \partial_3^2 + \varepsilon V_\pm, \tag{vi.22}$$

where

$$V_\pm(x, u) := \frac{1}{\varepsilon} \left(\frac{C_\pm}{C_\mp^2}\, v_1 + V_2 \right) (x/\sigma_\pm, u)\,.$$

We notice that since v_1 and V_2 are ε-dependent – *cf.* (vi.16) and the explicit formulae for the potentials (vi.20) and (vi.21) – the potentials $V_\pm$ are well defined for $\varepsilon = 0$.

vi.4.3 The Ground State Asymptotics

Suppose that each of the operators $H_\pm$ has for all sufficiently small ε just one eigenvalue $E_\pm(\varepsilon)$. Since H_- is below bounded, the minimax principle tells us that the same is true for H and

$$E_-(\varepsilon) \leq E(\varepsilon) \leq E_+(\varepsilon). \tag{vi.23}$$

If we identify ε with λ of the previous section, we see that under our assumptions the operators $H_\pm$ are well suited for application of Theorem vi.5.

Indeed, the decay requirements $\langle$d1–4$\rangle$ yield that $K, M, |\nabla_g K|_g, |\nabla_g M|_g$ and $\Delta_g K$ tend to zero at infinity, and consequently, $(V_\pm)_{11} \to 0$ as $|x| \to \infty$. Notice that we do not assume a decay of $\Delta_g M$ at infinity which would require $f_{,\mu\nu\rho\sigma} \to 0$ as $|x| \to \infty$. The reason is that the term $u\Delta_g M$ itself in the potential (vi.20) vanishes when projected onto the first transverse mode χ_1. One can thus take $\psi_n(x,u) := \varphi_n(x)\chi_1(u)$, where φ_n with $\|\varphi_n\| = 1$ is a sequence of functions with increasing supports which move towards infinity as $n \to \infty$. If φ_n is properly chosen such ψ_n form a Weyl sequence for $H_\pm$ and any $\kappa_1^2 + \alpha$ with $\alpha \in \mathbb{R}^+$. Using then a Neumann bracketing argument, as mentioned in Section vi.2, in order to show that no $\kappa_1^2 + \alpha$ with $\alpha < 0$ can belong to the essential spectrum, we conclude that $\sigma_{\mathrm{ess}}(H_\pm) = [\kappa_1^2, \infty)$. This verifies $\langle$a0$\rangle$ of Theorem vi.5. Furthermore, using this result together with (vi.22) and the minimax principle, we infer that $\inf \sigma_{\mathrm{ess}}(H) = \kappa_1^2$.

The requirement $\langle$a1$\rangle$ holds trivially true because $V_\pm$ are essentially bounded due to the surface regularity assumption and $\langle$d1–4$\rangle$. Under $\langle$r1–3$\rangle$, explicit expressions for the covariant derivatives of K and M in terms of the partial derivatives of the function f show that even $\sup\{V_\pm(\cdot,u)|\, u \in I\}$ belongs to $L^1(\mathbb{R}^2, (1+|x|^\delta)\,dx)$ which gives $\langle$a3$\rangle$. Let us remark that we require the L^1-integrability in $\langle$r3$\rangle$, which is a stronger condition than the L^2-integrability required for the second and third derivatives of f. The assumption $\langle$a2$\rangle$ is a consequence of $\langle$a3$\rangle$ and the boundedness of $V_\pm$.

On the other hand, there is a difference between the Hamiltonian (vi.5) and our operators $H_\pm$ because the potentials $V_\pm$ depend themselves on ε. Inspecting the proof of Theorem vi.5 we see that one can modify it to get the expansion (vi.11) using $\varepsilon \mapsto V_\pm(\varepsilon)$ as well. However, expanding the latter in terms of ε, the final expansion resulting from (vi.11) changes and to ensure that it represents an eigenvalue it is necessary that the lowest-order term in this expansion is not only non-positive but rather strictly negative. Recall that one can find (physically interesting) examples of situations when the potential depends on the coupling parameter in a nonlinear way and a bound state in the critical zero-mean case may or may not exist [BCEZ].

Hence one has to examine carefully the behaviour with respect to powers of ε in the expansion obtained from (vi.11) by an appropriate change of the integration

variables,

$$\begin{aligned} w_\pm(\varepsilon) &= \frac{\varepsilon}{2\pi}\,\sigma_\pm^2 \int_{\mathbb{R}^2} (V_\pm)_{11}(\sigma_\pm x;\varepsilon)\,dx \\ &+ \left(\frac{\varepsilon}{2\pi}\right)^2 \sigma_\pm^4 \Bigg\{ \int_{\mathbb{R}^2\times\mathbb{R}^2} (V_\pm)_{11}(\sigma_\pm x;\varepsilon)\left(\gamma_{\rm E} + \ln\frac{\sigma_\pm|x-x'|}{2}\right) \\ &\qquad \times (V_\pm)_{11}(\sigma_\pm x';\varepsilon)\,dx\,dx' \\ &- \sum_{j=2}^{\infty} \int_{\mathbb{R}^2\times\mathbb{R}^2} (V_\pm)_{1j}(\sigma_\pm x;\varepsilon)\,K_0\left(k_j(\kappa_1)\sigma_\pm|x-x'|\right) \\ &\qquad \times (V_\pm)_{j1}(\sigma_\pm x';\varepsilon)\,dx\,dx' \Bigg\} + \mathcal{O}(\varepsilon^{2+\gamma}), \end{aligned}$$

which determines the possible eigenvalues of $H_\pm$ via $E_\pm = \kappa_1^2 - \exp(2w_\pm^{-1})$. By virtue of (vi.16) we can write

$$\varepsilon^{-1}V_2(x,u;\varepsilon) = \varepsilon\left(k_0(x) - m_0(x)^2\right) + r_2(x,u;\varepsilon),$$

where r_2 is an integrable function collecting the terms of order ε^2 and higher. Hence

$$\forall j\in\mathbb{N}: \quad \varepsilon^{-1}(V_2)_{1j}(x;\varepsilon) = \left[\varepsilon\left(k_0(x) - m_0(x)^2\right) + \mathcal{O}(\varepsilon^2)\right]\delta_{1j},$$

where we abuse the notation a little because the error term depends on x as well. The expansion of $\varepsilon^{-1}v_1$ requires more attention because $\varepsilon^{-1}\Delta_g M$ in the second term of (vi.20) is of order one. First of all, we can write

$$\begin{aligned} v_1(x,u;\varepsilon) &= -u(\Delta_g M)(x;\varepsilon) \\ &\quad + u^2\left(\frac{1}{2}\Delta_g K - |\nabla_g M|_g^2 - 2M\Delta_g M\right)(x;\varepsilon) + r_1(x,u;\varepsilon), \end{aligned}$$

where r_1 is an integrable function of order $\mathcal{O}(\varepsilon^3)$. This does not mean, of course, that the first two terms constitute a quadratic polynomial in ε, because $|\cdot|_g$, ∇_g and Δ_g expand as well. Since the first term in the above expansion of v_1 is an odd function of u, it does not contribute to $(V_\pm)_{11}$. On the other hand, it plays an important role in the higher modes :

$$\begin{aligned} (v_1)_{11}(x;\varepsilon) &= \|u\chi_1\|_I^2\left(\frac{1}{2}\Delta_g K - |\nabla_g M|_g^2 - 2M\Delta_g M\right)(x;\varepsilon) + \mathcal{O}(\varepsilon^3), \\ (v_1)_{1j}(x;\varepsilon) &= -(\chi_1, u\chi_j)_I\,(\Delta_g M)(x;\varepsilon) + \mathcal{O}(\varepsilon^2) \quad \text{if} \quad j\in\mathbb{N}\setminus\{1\}. \end{aligned}$$

Notice that the inner product in the second line is non-zero for even j only. Now we use the relations

$$|\nabla_g M|_g^2 = |\nabla M|^2 + \varepsilon^2 M_{,\mu}\tilde\eta^{\mu\nu}M_{,\nu} \qquad \text{and} \qquad -\Delta_g = -\Delta + \varepsilon^2 L(\varepsilon),$$

where $L(\varepsilon)$ is a second-order differential operator with coefficients which expand as $\mathcal{O}(1)$. This together with (vi.16) yields

$$\begin{aligned} \varepsilon^{-1}(v_1)_{11}(x;\varepsilon) &= \varepsilon\,\|u\chi_1\|_I^2\left(\frac{1}{2}\Delta k_0 - |\nabla m_0|^2 - 2m_0\Delta m_0\right)(x) + \mathcal{O}(\varepsilon^2) \\ \varepsilon^{-1}(v_1)_{1j}(x;\varepsilon) &= -(\chi_1, u\chi_j)_I\,(\Delta m_0)(x) + \mathcal{O}(\varepsilon). \end{aligned}$$

Since $C_\pm/C_\mp^2$ and $\sigma_\pm$ expand like $1+\mathcal{O}(\varepsilon)$, we arrive at

$$\begin{aligned} w_\pm(\varepsilon) &= \frac{\varepsilon^2}{2\pi}\Bigg\{ \int_{\mathbb{R}^2} \left(k_0 - m_0^2\right)(x)\, dx \\ &+ \|u\chi_1\|_I^2 \int_{\mathbb{R}^2} \left(\frac{1}{2}\Delta k_0 - |\nabla m_0| - 2m_0\Delta m_0\right)(x)\, dx \\ &- \frac{1}{2\pi}\sum_{j=2}^{\infty}(\chi_1, u\chi_j)_I^2 \int_{\mathbb{R}^2\times\mathbb{R}^2} (\Delta m_0)(x)\, K_0\left(k_j(\kappa_1)\sigma_\pm|x-x'|\right) \\ &\qquad \times\ (\Delta m_0)(x')\, dx\, dx' \Bigg\} + \mathcal{O}(\varepsilon^{2+\gamma}), \end{aligned} \tag{vi.24}$$

where the sum runs in fact over even j only.

This expression can be further simplified. By a double integration by parts where one uses the fact that $f_{,\mu}f_{,\nu\rho} \to 0$ as $|x| \to \infty$ due to $\langle \mathsf{d1}\rangle$ and $\langle \mathsf{d2}\rangle$, we get that the integral of k_0 is equal to zero. We note in this connection that it follows then from (vi.14) and (vi.16) that the total Gauss curvature, $\mathcal{K} := \int_{\Sigma_\varepsilon} K d\Sigma_\varepsilon$, behaves as $\mathcal{O}(\varepsilon^4)$. Using the divergence theorem and the assumptions $\langle \mathsf{d1}\rangle$, $\langle \mathsf{d2}\rangle$ and $\langle \mathsf{d3}\rangle$ by which $\nabla K \to 0$ as $|x| \to \infty$, we find that the integral of Δk_0 does not contribute as well. A similar argument employing the Green formula gives

$$\int_{\mathbb{R}^2} (m_0\Delta m_0)(x)\, dx = -\int_{\mathbb{R}^2} |\nabla m_0|^2(x)\, dx. \tag{vi.25}$$

It is convenient to rewrite the integral part of the last term in (vi.24) by means of a convolution

$$\begin{aligned} &\frac{1}{2\pi}\int_{\mathbb{R}^2\times\mathbb{R}^2} (\Delta m_0)(x)\, K_0\left(k_j(\kappa_1)\sigma_\pm|x-x'|\right)\, (\Delta m_0)(x')\, dx\, dx' \\ &\qquad\qquad = \left(\Delta m_0, G_k * \Delta m_0\right), \end{aligned}$$

where $G_k(\cdot) := (2\pi)^{-1} K_0(k|\cdot|)$ and k abbreviates $k_j(\kappa_1)\sigma_\pm$. Since G_k is the fundamental solution of the distributional equation $(-\Delta + k^2)G_k = \delta$, we get

$$\begin{aligned} &\left(\Delta m_0, G_k * \Delta m_0\right) = \left(\Delta m_0, \Delta G_k * m_0\right) = \left(\Delta m_0, (k^2 G_k - \delta) * m_0\right) \\ &\quad = k^2\left(\Delta m_0, G_k * m_0\right) - \left(\Delta m_0, m_0\right) = k^2\left(G_k * \Delta m_0, m_0\right) + \|\nabla m_0\|^2 \\ &\quad = k^2\left(\Delta G_k * m_0, m_0\right) + \|\nabla m_0\|^2 = k^2\left((k^2 G_k - \delta) * m_0, m_0\right) + \|\nabla m_0\|^2 \\ &\quad = k^4\left(m_0, G_k * m_0\right) - k^2\|m_0\|^2 + \|\nabla m_0\|^2. \end{aligned} \tag{vi.26}$$

In the second line we have employed the identity (vi.25). If we insert the obtained expression into the expansion (vi.24) and use, in addition, the Parseval identity,

$$\|u\chi_1\|_I^2 = \sum_{j=1}^{\infty}(\chi_1, u\chi_j)_I^2, \tag{vi.27}$$

we find that the terms containing $\|\nabla m_0\|$ cancel, hence we arrive at

$$\begin{aligned} w_\pm(\varepsilon) &= -\frac{\varepsilon^2}{2\pi}\left\{ \|m_0\|^2 + \sum_{j=2}^{\infty}(\chi_1, u\chi_j)_I^2\, k^2\left[k^2\left(m_0, G_k * m_0\right) - \|m_0\|^2\right]\right\} \\ &\quad + \mathcal{O}(\varepsilon^{2+\gamma}), \end{aligned}$$

where, of course, k expands as $k_j(\kappa_1) + \mathcal{O}(\varepsilon)$. Since

$$\sum_{j=2}^{\infty} (\chi_1, u\chi_j)_I^2 \, k_j(\kappa_1)^2 = \|u\,\partial_3\chi_1\|_I^2 - \kappa_1^2 \|u\chi_1\|_I^2 = 1,$$

we see that also the terms containing $\|m_0\|$ cancel. Using finally the Fourier transformation as in (vi.12), we obtain

$$w_\pm(\varepsilon) = -\varepsilon^2 \sum_{j=2}^{\infty} (\chi_1, u\chi_j)_I^2 \, k_j(\kappa_1)^4 \int_{\mathbb{R}^2} \frac{|\widehat{m_0}(\omega)|^2}{|\omega|^2 + \kappa_j^2 - \kappa_1^2} \, d\omega + \mathcal{O}(\varepsilon^{2+\gamma}),$$

where we have also expanded the remaining k from G_k w.r.t. ε and included the higher orders into the error term .

We note that m_0 (and therefore $\widehat{m_0}$) cannot be identically zero once Σ_1 is not a plane. It can be seen from the formulae (vi.16) : suppose that $m_0 \equiv 0$. Then $f_{,11} \equiv -f_{,22}$, which yields $k_0 = -({f_{,11}}^2 + {f_{,12}}^2)$ and consequently $k_0 \equiv 0$ because we have shown that $\int_{\mathbb{R}^2} k_0(x)\,dx = 0$. Hence $K \equiv 0$. At the same time, $f_{,\mu\nu} \equiv 0$, which gives $m_1 \equiv 0$ and therefore $M \equiv 0$. If we thus exclude the trivial planar case, the lowest-order term in the expansion is strictly negative. Since it is identical for both w_+ and w_-, it follows by (vi.23) that it is the same also for the expansion of $w(\varepsilon)$ in the ground-state energy $E = \kappa_1^2 - e^{2w^{-1}}$ of the Hamiltonian H. This concludes the proof of Theorem vi.1.

Remark. The surface Σ_1 is not planar if the matrix $\theta_{\mu\nu}$ is not identically zero, *i.e.*, if $f_{,\mu\nu} \not\equiv 0$. This can be seen as follows. Suppose that $f_{,\mu\nu} = 0$ identically. Solving this as a system of differential equations, we get $f(x) = c_\mu x^\mu$, where c_μ is a constant vector, which is exactly a plane parametrization.

vi.4.4 The Thin Layer Limit

We say that the layer Ω_ε is thin if $a \ll \rho_m$. Since the minimum curvature radius introduced in (vi.18) explodes as $\varepsilon \to 0$ this condition is eventually always satisfied. It is useful, however, to consider also a "true" thin-layer limit in which we start with a mildly curved layer with a fixed ε which is already in the asymptotic regime, and make its width d small. To this aim we rewrite the formula for w_1 in the expansion $w(\varepsilon) =: \varepsilon^2 w_1 + \mathcal{O}(\varepsilon^{2+\gamma})$ of Theorem vi.1 in a different way. For this we go back to the intermediate expansion (vi.24). We simplify it as above, however, do not use (vi.26) and (vi.27). Instead we apply the transformation (vi.12) directly to $(\Delta m_0, G_k * \Delta m_0)$, expand k in terms of ε obtaining thus

$$w_1 = -\frac{1}{2\pi}\,\|m_0\|^2 + \frac{\|u\chi_1\|_I^2}{2\pi}\,\|\nabla m_0\|^2 - \sum_{j=2}^{\infty} (\chi_1, u\chi_j)_I^2 \int_{\mathbb{R}^2} \frac{|\widehat{\Delta m_0}(\omega)|^2}{|\omega|^2 + k_j(\kappa_1)^2}\, d\omega.$$

An explicit calculation yields $\|u\chi_1\|_I^2 = (\pi^2 - 6)/(12\kappa_1^2)$, so the second term in the expression for w_1 is proportional to d^2 by the definition of κ_1. On the other hand, using the estimate $|\omega|^2 + k_j(\kappa_1)^2 \geq k_j(\kappa_1)^2 \geq \kappa_2^2 - \kappa_1^2 = 3\kappa_1^2$ together with (vi.27) and the above explicit result, we see that the third term is $\mathcal{O}(d^4)$. Note that this makes sense because $\|\widehat{\Delta m_0}\| = \|\Delta m_0\|$ is finite due to $\langle$r3$\rangle$. Summing up the argument, we obtain the expansion (vi.4).

This formula has a transparent structure. By virtue of (vi.16), (vi.14), and the fact that $\int_{\mathbb{R}^2} k_0(x)\,dx = 0$, we get the behaviour

$$\int_{\Sigma_\varepsilon} \left(K - M^2\right) d\Sigma_\varepsilon = -\varepsilon \left(\|m_0\|^2 + \mathcal{O}(\varepsilon^2)\right).$$

Hence the first term of (vi.4) comes from the surface attractive potential $K - M^2$ which dominates the picture for thin layers. The last claim follows from (vi.20) and (vi.21), because $v_1 \to 0$ and the leading term of V_2 is $K - M^2$ in the limit $u \to 0$, which one can do as soon as $d \to 0$. At the same time, $C_\pm \to 1$, which in view of (vi.19) leads to the "limiting" Hamiltonian $-\Delta_g - \partial_3^2 + K - M^2$. Such a limit is, of course, only formal since the transverse spectrum explodes, which classically corresponds to increasingly rapid oscillations in the transverse direction. Nevertheless, a similar limit with the confinement realized by a harmonic potential transverse to a compact curved surface was discussed recently in a rigorous way in [FH] and led to the same tangential operator $-\Delta_g + K - M^2$.

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Chapitre vii

Les bosses et les creux

Résumé

Nous considérons les laplaciens Dirichlet dans l'espace délimité par deux lignes droites parallèles dans $\mathbb{R}^2$ ou par deux plans parallèles dans $\mathbb{R}^3$ avec une déformation faible locale. Premièrement, nous généralisons le résultat de Bulla *et al.* en dimension trois en montrant que des états liés du couplage faible existent si le changement de volume dû à la déformation est positif; nous dérivons en même temps l'ordre principal dans le développement asymptotique de la valeur propre par rapport au paramètre décrivant ce couplage faible. A l'aide des propriétés analytiques de la valeur propre, nous proposons une méthode alternative permettant d'établir le terme suivant dans le développement limité pour les cas des dimensions deux et trois. En particulier, ceci fournit un critère d'existence d'états liés dans le cas critique où le volume de déformation est égal à zéro.

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Bound states in weakly deformed strips and layers

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Abstract. We consider Dirichlet Laplacians on straight strips in $\mathbb{R}^2$ or layers in $\mathbb{R}^3$ with a weak local deformation. First we generalize a result of Bulla *et al.* to the three-dimensional situation showing that weakly coupled bound states exist if the volume change induced by the deformation is positive; we also derive the leading order of the weak-coupling asymptotics. With the knowledge of the eigenvalue analytic properties, we demonstrate then an alternative method which makes it possible to evaluate the next term in the asymptotic expansion for both the strips and layers. It gives, in particular, a criterion for the bound-state existence in the critical case when the added volume is zero.

vii.1 Introduction

Spectra of Dirichlet Laplacians in infinitely stretched regions such as a planar strip or a layer of a fixed width have attracted a lot of attention recently. Of course, the problem is trivial as long as the strip or layer is straight because then one can employ separation of variables. However, already a local perturbation such as bending, deformation, or a change of boundary conditions can produce a non-empty discrete spectrum.

This effect was studied intensively in the last decade, first because it had applications in condensed matter physics, and also because it was itself an interesting mathematical problem. A particular aspect we will be concerned with here is the behaviour in the weak-coupling regime, *i.e.*, the situation when the perturbation is gentle.

Recall that the answer to this question depends on the type of the perturbation. For bend strips, *e.g.*, one can perform the Birman-Schwinger analysis which yields the first term in the asymptotic expansion for the gap between the eigenvalue and the threshold of the essential spectrum [DE]. It is proportional to the fourth power of the bending angle and always positive, since any nontrivial (local) bending induces a non-empty discrete spectrum. A local switch of the boundary condition from Dirichlet to Neumann has a similar effect. Here the weak-coupling behaviour was determine variationally to be governed by the fourth power of the "window width" [EV1] and the exact asymptotics was derived formally in [Po] by a direct application of the technique developed in [Il, Ga]. Notice that this asymptotics differs substantially from that corresponding to a local change in the *mixed* boundary conditions, where the Birman-Schwinger technique is applicable and the leading term is a multiple of the *square* of the said parameter [EK]. Recall also that analogous results can be derived for layers with locally perturbed boundary conditions where, however, the asymptotics is exponential rather that powerlike [EV2].

The present paper deals with the case of a local *deformation* of the strip or layer, which is more subtle than the bending or boundary-condition modification. The main difference is that the effective interaction induced by a deformation can

be of different signs, both attractive and repulsive. It is easy to see by bracketing that a bulge on a strip or layer does create bound states while a squeeze does not. The answer is less clear for more complicated deformations where the width change does not have a definite sign.

The first rigorous treatment of this problem was presented in the work of Bulla *et al* [BGRS] dealing with a local one-sided deformation (characterized by a function λv) of a straight strip of a constant width d. The authors found that the added volume was decisive : a bound state exists for small positive λ if the area change $\lambda d\langle v\rangle$ is positive, and in that case the ground-state eigenvalue has the following weak-coupling expansion,

$$E(\lambda) = \kappa_1^2 - \lambda^2\kappa_1^4\langle v\rangle^2 + \mathcal{O}(\lambda^3)\,, \tag{vii.1}$$

where $\kappa_1 = \frac{\pi}{d}$ is the square root of the first transverse eigenvalue.[1] On the other hand, the discrete spectrum is empty if $\langle v\rangle < 0$. A problem arises in the critical case, $\langle v\rangle = 0$, when the areas of the outward and inward deformation coincide. The authors of [BGRS] suggested that the analogy with one-dimensional Schrödinger operators by which bound states should exist again may be misleading due to the presence of the higher transverse modes.

This suspicion was confirmed in [EV3] where it was shown that this is true only if the deformation was "smeared" enough. More specifically, the discrete spectrum is empty if

$$d > \frac{4}{\sqrt{3}}\, b \tag{vii.2}$$

provided $\operatorname{supp} v \subset [-b, b]$. On the other hand, a weakly bound state exists if

$$\frac{\|v'\|^2}{\|v\|^2} < \frac{6\kappa_1^2}{9 + \sqrt{90 + 12\pi^2}}\,, \tag{vii.3}$$

and in that case there are positive c_1, c_2 such that

$$-c_1\lambda^4 \le E(\lambda) - \kappa_1^2 \le -c_2\lambda^4\,. \tag{vii.4}$$

These results have been obtained by a variational method and they are certainly not optimal, because there are deformed strips which fulfill neither of the conditions (vii.2), (vii.3).

A way to improve the above conclusions would be to compute the Birman-Schwinger expansion employed in [BGRS] to the second order which becomes the leading one when the term linear in λ^2 in (vii.1) is absent, and the asymptotics is governed by λ^4 in correspondence with (vii.4). This is not easy, however. The standard technique in these situations is to map the strip in question onto a straight one by means of suitable curvilinear coordinates. In distinction to the bent-strip case [DE] these coordinates typically are not locally orthogonal. Hence the transformed Laplacian contains numerous terms which make the computation extremely cumbersome.

After this introduction, let us describe the aim and the scope of the present paper. The aim is twofold. First we are going to consider an extension of the result

[1] In fact, they assumed $d = 1$, but it is easy to restore the strip width in their expression obtaining eq. (vii.1).

of [BGRS] to the case of a locally deformed layer. The result is summarized in Theorem vii.4. In particular, we derive a weak-coupling expansion of the ground-state eigenvalue,

$$E(\lambda) = \kappa_1^2 - \exp\left[2\left(-\lambda\frac{\kappa_1^2}{\pi}\langle v\rangle + \mathcal{O}(\lambda^2)\right)^{-1}\right] \tag{vii.5}$$

and show the analytical properties of the round-bracket expression w.r.t. λ. This is done in Section vii.2; the results again say nothing about the behaviour in the critical case.

Instead of attempting to proceed further by the Birman-Schwinger method, we demonstrate in Section vii.3 a different approach to the weak-coupling problem. It is based on constructing the asymptotics of a particular boundary value problem, and requires as a prerequisite the analyticity of the function $E(\cdot)$ itself in dimension two, and of its above mentioned constituent in dimension three. In the present case, however, these properties are guaranteed by [BGRS] and the results of Section vii.2. The methods allows us to recover the expansions (vii.1) and (vii.5) in a different way. What is more, we are also able to compute higher terms, in principle of any order. We perform the explicit computation for the second-order terms which play role in the critical case. In particular, we made in this way more precise the result expressed by (vii.2) and (vii.3) about the critical bound-state existence for smeared perturbations, and derive its analog in the deformed-layer case.

vii.2 Locally deformed layers

vii.2.1 The curvilinear coordinates

Let $x = (x^1, x^2) \in \mathbb{R}^2$ and $(x, u) \in \Omega_0 := \mathbb{R}^2 \times (0, d)$ with $d > 0$. Given a function $v \in \boldsymbol{C}_0^\infty(\mathbb{R}^2)$ we define the mapping

$$\phi : \Omega_0 \to \mathbb{R}^3 : \big\{(x, u) \mapsto \phi(x, u) := \big(x^1, x^2, (1 + \lambda v(x))\, u\big)\big\} \tag{vii.6}$$

for $\lambda > 0$, which defines our deformed layer $\Omega_\lambda := \phi(\Omega_0)$.

To make use of the curvilinear coordinates defined by the mapping ϕ we need the metric tensor $G_{ij} := \phi_{,i}.\phi_{,j}$ of the deformed layer. It can be seen easily to be of the form

$$(G_{ij}) = \begin{pmatrix} 1 + \lambda^2 v_{,1}^2 u^2 & \lambda^2 v_{,1} v_{,2} u^2 & \lambda v_{,1}(1 + \lambda v) u \\ \lambda^2 v_{,1} v_{,2} u^2 & 1 + \lambda^2 v_{,2}^2 u^2 & \lambda v_{,2}(1 + \lambda v) u \\ \lambda v_{,1}(1 + \lambda v) u & \lambda v_{,2}(1 + \lambda v) u & (1 + \lambda v)^2 \end{pmatrix}, \tag{vii.7}$$

where $v_{,\mu}$ means the derivative w.r.t. x^μ, and its determinant is $G := \det(G_{ij}) = (1 + \lambda v)^2$.

In view of the inverse function theorem, the mapping ϕ defining the layer will be diffeomorphism provided $\lambda \|v_-\|_\infty < 1$, where we put conventionally $v_- := \max\{0, -v\}$. For a sign-changing v, this is a nontrivial restriction which is satisfied, however, when λ is small enough. That is just the case we are interested in.

We will also need the contravariant metric tensor, in other words the inverse matrix

$$(G^{ij}) = \begin{pmatrix} 1 & 0 & -\frac{\lambda v_{,1} u}{1+\lambda v} \\ 0 & 1 & -\frac{\lambda v_{,2} u}{1+\lambda v} \\ -\frac{\lambda v_{,1} u}{1+\lambda v} & -\frac{\lambda v_{,2} u}{1+\lambda v} & \frac{1+\lambda^2 |\nabla v|^2 u^2}{(1+\lambda v)^2} \end{pmatrix} \tag{vii.8}$$

and the following contraction identities

$$G^{\mu j}_{\ \ ,j} = -\frac{\lambda v_{,\mu}}{1+\lambda v}, \qquad G^{3j}_{\ \ ,j} = -\frac{\lambda \Delta v\, u}{1+\lambda v} + \frac{3\lambda^2 |\nabla v|^2 u}{(1+\lambda v)^2}, \tag{vii.9}$$

where conventionally summation is performed over repeated indices, and we denote $|\nabla v|^2 := v_{,1}^2 + v_{,2}^2$ and $\Delta v := v_{,11} + v_{,22}$. Another convention concerns the range of the indices, which is $1, 2$ for Greek and $1, 2, 3$ for Latin indices. The indices are at that associated with the above coordinates by $(1, 2, 3) \leftrightarrow (x^1, x^2, u)$.

vii.2.2 The straightening transformation

As mentioned in the introduction the main object of our study is the Dirichlet Laplacian $-\Delta_D^{\Omega_\lambda}$ on $\boldsymbol{L}^2(\Omega_\lambda)$. If we think of a quantum particle living in the region Ω_λ with hard walls and exposed to no other interaction, $-\Delta_D^{\Omega_\lambda}$ will be its Hamiltonian up to a multiplicative constant; we can get rid of the latter by setting the Planck's constant $\hbar = 1$ and the effective mass $m_* = \frac{1}{2}$. Mathematically speaking, $-\Delta_D^{\Omega_\lambda}$ is defined for an open set $\Omega_\lambda \subset \mathbb{R}^3$ as the Friedrichs extension of the free Laplacian with the domain $\boldsymbol{C}_0^\infty(\Omega)$ – *cf.* [RS, Sec. XIII.15]. Moreover, since the smooth boundary of Ω_λ has the segment property, $-\Delta_D^{\Omega_\lambda}$ acts simply as $\psi \mapsto -\psi_{,jj}$ with the Dirichlet b.c. at $\partial\Omega_\lambda$.

A natural way to investigate the Hamiltonian is to introduce the unitary transformation $U : \boldsymbol{L}^2(\Omega_\lambda) \to \boldsymbol{L}^2(\Omega_0) : \{\psi \mapsto U\psi := G^{\frac{1}{4}} \psi \circ \phi\}$ and to investigate the unitarily equivalent operator

$$H_\lambda := U(-\Delta_D^{\Omega_\lambda})U^{-1} = -G^{-\frac{1}{4}} \partial_i G^{\frac{1}{2}} G^{ij} \partial_j G^{-\frac{1}{4}} \tag{vii.10}$$

with the form domain $Q(H_\lambda) = \boldsymbol{W}_0^{1,2}(\Omega_0)$ instead of $-\Delta_D^{\Omega_\lambda}$. As usual in such situations, the "straightened" region is geometrically simpler and the price we pay is a more complicated form of the operator (vii.10).

To make it more explicit, put $F := \ln G^{\frac{1}{4}}$. Commuting $G^{-\frac{1}{4}}$ with the gradient components, we cast the operator (vii.10) into a form which has a simpler kinetic part,

$$H_\lambda = -\partial_i G^{ij} \partial_j + V = -G^{ij} \partial_i \partial_j - G^{ij}_{\ \ ,j} \partial_i + V,$$

but contains an effective potential,

$$V := (G^{ij} F_{,j})_{,i} + F_{,i} G^{ij} F_{,j} = G^{ij} F_{,ij} + G^{ij}_{\ \ ,j} F_{,i} + G^{ij} F_{,i} F_{,j}.$$

If we now employ the particular form (vii.7) of the metric tensor together

with (vii.8), (vii.9), we can write

$$\begin{aligned} H_\lambda &= -\partial_1^2 - \partial_2^2 - \frac{1+\lambda^2|\nabla v|^2 u^2}{(1+\lambda v)^2}\partial_3^2 + \frac{2\lambda v_{,1} u}{1+\lambda v}\partial_1\partial_3 + \frac{2\lambda v_{,2} u}{1+\lambda v}\partial_2\partial_3 \\ &\quad + \frac{\lambda v_{,1}}{1+\lambda v}\partial_1 + \frac{\lambda v_{,2}}{1+\lambda v}\partial_2 + \left(\frac{\lambda \Delta v\, u}{1+\lambda v} - \frac{3\lambda^2|\nabla v|^2 u}{(1+\lambda v)^2}\right)\partial_3 + V \end{aligned}$$

with

$$V = \frac{\lambda \Delta v}{2} - \frac{\lambda^2 v \Delta v}{2(1+\lambda v)} - \frac{3\lambda^2|\nabla v|^2}{4(1+\lambda v)^2}.$$

For our purpose it useful to rewrite this expression further in a form sorted w.r.t. to the powers of λ :

$$\begin{aligned} H_\lambda = -\Delta_D^{\Omega_0} &+ \lambda\Big[2v\partial_3^2 + 2v_{,1}u\partial_1\partial_3 + 2v_{,2}u\partial_2\partial_3 + v_{,1}\partial_1 + v_{,2}\partial_2 \\ &\quad + (\Delta v)\, u\partial_3 + \frac{\Delta v}{2}\Big] \\ -\lambda^2 &\left[\frac{3v^2 + |\nabla v|^2 u^2 + 2\lambda v^3}{(1+\lambda v)^2}\,\partial_3^2 + \frac{2vv_{,1}u}{1+\lambda v}\,\partial_1\partial_3 + \frac{2vv_{,2}u}{1+\lambda v}\,\partial_2\partial_3\right. \\ &\quad + \frac{vv_{,1}}{1+\lambda v}\,\partial_1 + \frac{vv_{,2}}{1+\lambda v}\,\partial_2 + \left(\frac{v(\Delta v)\, u}{1+\lambda v} + \frac{3|\nabla v|^2 u}{(1+\lambda v)^2}\right)\partial_3 \\ &\quad \left. + \frac{v\Delta v}{2(1+\lambda v)} + \frac{3|\nabla v|^2}{4(1+\lambda v)^2}\right] \end{aligned}$$

In analogy with [BGRS], we thus get the following formula for the "straightened" operator,

$$H_\lambda = H_0 + \lambda \sum_{n=1}^{3} A_n^* B_n + \lambda^2 \sum_{n=4}^{7} A_n^* B_n, \tag{vii.11}$$

where each of the A_n's and B_n's is a first-order differential operator with compactly supported coefficients and

$$\begin{aligned} A_1^* &:= 2v\partial_3 & B_1 &:= \omega\partial_3 \\ A_2^* &:= \Delta v & B_2 &:= \omega\left(u\partial_3 + \frac{1}{2}\right) \\ A_3^* &:= (2u\partial_3 + 1)\,\omega & B_3 &:= v_{,1}\partial_1 + v_{,2}\partial_2 \\ A_4^* &:= -\frac{3v^2 + |\nabla v|^2 u^2 + 2\lambda v^3}{(1+\lambda v^3)}\,\partial_3 & B_4 &:= \omega\partial_3 \\ A_5^* &:= -\frac{v\Delta v}{1+\lambda v} & B_5 &:= \omega\left(u\partial_3 + \frac{1}{2}\right) \\ A_6^* &:= -\frac{3|\nabla v|^2}{(1+\lambda v)^2} & B_6 &:= \omega\left(u\partial_3 + \frac{1}{4}\right) \\ A_7^* &:= -\frac{2u\partial_3 + 1}{1+\lambda v}\, v & B_7 &:= v_{,1}\partial_1 + v_{,2}\partial_2 \end{aligned}$$

with $\omega \in \boldsymbol{C}_0^\infty(\mathbb{R}^2)$ such that $\omega \equiv 1$ on $\operatorname{supp} v$. We define a pair of operators $C_\lambda, D : \boldsymbol{L}^2(\Omega_0) \to \boldsymbol{L}^2(\Omega_0) \otimes \mathbb{C}^7$ by

$$\varphi \mapsto (C_\lambda \varphi)_n := \begin{cases} A_n \varphi & n = 1,2,3 \\ \lambda A_n \varphi & n = 4,\dots,7 \end{cases}$$

$$\varphi \mapsto (D\varphi)_n := B_n \varphi \quad n = 1,\dots,7$$

then (vii.11) finally becomes $H_\lambda = H_0 + \lambda C_\lambda^* D$.

vii.2.3 Weak coupling analysis

First we note that since the our layer is deformed only locally, we have

$$\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_\lambda}) = \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_0}) = [\kappa_1^2, \infty)\,.$$

This is easy to see, for instance, by using a bracketing to show that $\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega_\lambda}) = \kappa_1^2$ – *cf.* [DEK] – while the opposite inclusion is obtained by constructing an appropriate Weyl sequence. We use the notation $\kappa_j^2 := (\frac{\pi}{d} j)^2$ for the eigenvalues of the transverse operator $(-\partial_3^2)_D$; the corresponding eigenfunctions are denoted by χ_j, and their explicit form is

$$\chi_j(u) = \sqrt{\frac{2}{d}}\, \sin \kappa_n u\,.$$

Next we define $K_\lambda^\alpha := \lambda D(H_0 - \alpha^2)^{-1} C_\lambda^*$. We are interested in (positive) eigenvalues $E(\lambda) =: \alpha^2$ of H_λ below the lowest transverse mode, hence we choose $\alpha \in [0, \kappa_1)$. Our basic tool is the following classical result – *cf.* [BGRS, Lemma 2.1] :

Proposition vii.1 (Birman-Schwinger principle).

$$\alpha^2 \in \sigma_{\mathrm{disc}}(H_\lambda) \iff -1 \in \sigma_{\mathrm{disc}}(K_\lambda^\alpha)$$

Proof. If $K_\lambda^\alpha \psi = -\psi$, then $\varphi := -\lambda(H_0 - \alpha^2)^{-1} C_\lambda^* \psi$ is easily checked to satisfy $H_\lambda \varphi = \alpha^2 \varphi$. Conversely, if $H_\lambda \varphi = \alpha^2 \varphi$, we have $\varphi \in Q(H_\lambda) \subset D(D)$, so $\psi := D\varphi$ is in $\boldsymbol{L}^2(\Omega_0)$ and $K_\lambda^\alpha \psi = -\psi$. □

To make use of the above equivalence, we have to analyze the structure of K_λ^α. Let $R_0(\alpha) := (H_0 - \alpha^2)^{-1}$ be the free resolvent corresponding to H_0. Using the transverse-mode decomposition and the fact that $H_0 = -\Delta^{\mathbb{R}^2} \otimes I_1 + I_2 \otimes (-\partial_3^2)^D$, we can express the integral kernel of R_0,

$$R_0(x,u,x',u';\alpha) = \sum_{j=1}^\infty \chi_j(u)\, r_j(x,x';\alpha)\, \chi_j(u')$$

where $r_j(x,x';\alpha)$ is the kernel of $(-\Delta^{\mathbb{R}^2} + \kappa_j^2 - \alpha^2)^{-1}$ in $\boldsymbol{L}^2(\mathbb{R}^2)$. We define $k_j(\alpha)^2 := \kappa_j^2 - \alpha^2$. The free kernel r_j can be expressed in terms of Hankel's functions – *cf.* [AGH, Chap. I.5] – which are related to Macdonald's functions by [AS, 9.6.4], so finally we arrive at the formula

$$R_0(x,u,x',u';\alpha) = \frac{1}{2\pi} \sum_{j=1}^\infty \chi_j(u)\, K_0\left(k_j(\alpha)|x - x'|\right)\, \chi_j(u')\,.$$

Now we want to split the singular part of R_0^α ; we write $K_\lambda^\alpha = \hat{L}_\lambda + \hat{M}_\lambda$ where $\hat{L}_\lambda := \lambda D L_\alpha C_\lambda^*$ contains the singularity :

$$L_\alpha(x,u,x',u') := -\frac{1}{2\pi}\,\chi_1(u)\,\ln k_1(\alpha)\,\chi_1(u')$$

diverges logarithmically as $\alpha \to \kappa_1-$. The regular part $\hat{M}_\lambda = \lambda D M_\alpha C_\lambda^*$ consists of two terms, $M_\alpha = N_\alpha + R_0^\perp(\alpha)$, where the operator $R_0^\perp$ is defined as the projection of the resolvent on higher transverse modes

$$R_0^\perp(x,u,x',u';\alpha) := \frac{1}{2\pi}\sum_{j=2}^{\infty}\chi_j(u)\,K_0(k_j(\alpha)|x-x'|)\,\chi_j(u'),$$

and the remaining term is therefore

$$N_\alpha(x,u,x',u') := \frac{1}{2\pi}\chi_1(u)\,\Big(K_0(k_1(\alpha)|x-x'|) + \ln k_1(\alpha)\Big)\,\chi_1(u').$$

Put $w^{-1} := \ln k_1(\alpha)$. The next step in the BS method is to show the boundedness and the analyticity (w.r.t. w) of the regular part of K_λ^α. A more difficult part of this task concerns the operator containing N_α where we have to take a different route than that used in [BGRS].

First we note that while the Hilbert-Schmidt norm is suitable for estimating the operator N_α, it fails when the latter is sandwiched between λD and C_λ^*. More specifically, using the regularity and compact support of the functions involved one could transform $\lambda D N_\alpha C_\lambda^*$ into an integral operator via integration by parts, but the obtained kernel has a singularity which is not square integrable. Hence we use instead the "continuous" version of the *Schur-Holmgren bound.* Since it seems to be less known than its discrete analogue [AGH, Lemma C.3], [Mad, Thm. 7.1.9], we present it here with the proof.

Lemma vii.2. *Suppose that M is an open subset of $\mathbb{R}^n$ and let $K : \boldsymbol{L}^2(M) \to \boldsymbol{L}^2(M)$ be an integral operator with the kernel $K(\cdot,\cdot)$. Then*

$$\|K\| \le \|K\|_{\mathrm{SH}} := \left(\sup_{x\in M}\int_M |K(x,x')|dx' \;\sup_{x'\in M}\int_M |K(x,x')|dx\right)^{\frac{1}{2}}.$$

Proof. The claim follows from the inequality

$$\|K\|_{p,p} \le \|K\|_{1,1}^{1/p}\,\|K\|_{\infty,\infty}^{1/q}\,, \tag{vii.12}$$

where K is now an integral operator on $\boldsymbol{L}^p(M)$, $p^{-1}+q^{-1}=1$, and

$$\|K\|_{\infty,\infty} := \sup_{x\in M}\int_M |K(x,x')|\,dx', \quad \|K\|_{1,1} := \sup_{x'\in M}\int_M |K(x,x')|\,dx.$$

If K is bounded for $p=1,\infty$, we can prove (vii.12) for the other p by an interpolation argument adapted from the discrete case [Mad]. By Hölder's inequality

$$\begin{aligned}\left|\int_M K(x,x')\psi(x')dx'\right| &\le \int_M |K(x,x')|^{\frac{1}{p}}|K(x,x')|^{\frac{1}{q}}|\psi(x')|\,dx' \\ &\le \left(\int_M |K(x,x')||\psi(x')|^p dx'\right)^{\frac{1}{p}}\int_M |K(x,x')|\,dx'\,,\end{aligned}$$

so we can easily estimate the $\boldsymbol{L}^p$-norm of $K\psi$,

$$\begin{aligned}
\|K\psi\|_p^p &= \int_M dx \left| \int_M K(x,x')\psi(x')\,dx' \right|^p \\
&\leq \|K\|_{\infty,\infty}^{p/q} \int_M dx \int_M |K(x,x')||\psi(x')|^p\,dx' \\
&\leq \|K\|_{\infty,\infty}^{p/q} \int_M dx' \,|\psi(x')|^p \int_M dx\,|K(x,x')| \\
&\leq \|K\|_{\infty,\infty}^{p/q} \|K\|_{1,1} \|\psi\|_p^p\,,
\end{aligned}$$

which yields the result. □

Recall that $\|\cdot\|_{\mathrm{SH}}$ is *not* a norm and that it simplifies for the symmetric kernels, $\|K\|_{\mathrm{SH}} = \sup_{x\in M} \int_M |K(x,x')|\,dx'$. We are now ready to prove the following key result.

Lemma vii.3. *$w \mapsto \hat{M}(\alpha(w))$ is a bounded and analytic operator-valued function, which can be continued from $\{w \in \mathbb{C} \,|\, \mathrm{Re}\, w < 0\}$ to a region that includes $w = 0$.*

Proof. As in [BGRS, Lemma 2.2], let $\mathcal{H}_1 \subset \boldsymbol{L}^2(\Omega_0)$ be the space of $\boldsymbol{L}^2(\Omega_0)$ functions of the form $\varphi\chi_1$, where $\varphi \in \boldsymbol{L}^2(\mathbb{R}^2)$. Let further $\mathcal{P}_1$ be the projection onto this subspace, and $\mathcal{P}_1^\perp := I - \mathcal{P}_1$ the projection onto its orthogonal complement in $\boldsymbol{L}^2(\Omega_0)$. Then $R_0^\perp(\alpha) \equiv R_0(\alpha)\mathcal{P}_1^\perp$ has an analytic continuation into the region $\{\alpha \in \mathbb{C} \,|\, \alpha^2 \in \mathbb{C}\setminus[\kappa_2^2,\infty)\}$ since the lowest point in the spectrum of $H_0\mathcal{P}_1^\perp \restriction \mathcal{P}_1^\perp \boldsymbol{L}^2(\Omega_0)$ is κ_2^2. This region includes the domain $[0,\kappa_1)$ actually considered. To accommodate the extra factors D, C_λ^*, we introduce the quadratic form

$$b_\alpha(\phi,\psi) := (\phi, DR_0^\perp(\alpha)C_\lambda^*\psi) = (R_0^\perp(\alpha)^{\frac{1}{2}}\mathcal{P}_1^\perp D^*\phi, R_0^\perp(\alpha)^{\frac{1}{2}}\mathcal{P}_1^\perp C_\lambda\psi)\,.$$

To check boundedness of this form, it is therefore sufficient to verify that $R_0^\perp(\alpha)^{\frac{1}{2}}\mathcal{P}_1^\perp D^*$ and $R_0^\perp(\alpha)^{\frac{1}{2}}\mathcal{P}_1^\perp C_\lambda^*$ are bounded operators. We shall check it for their adjoints. To this purpose, it is enough to show that $C_\lambda\mathcal{P}_1^\perp$ and $D\mathcal{P}_1^\perp$ are $(R_0^\perp(\alpha)^{-\frac{1}{2}}\mathcal{P}_1^\perp)$ -bounded, *i.e.*, that there exist positive a, b such that

$$\forall\psi \in Q(H_\lambda): \qquad \|C_\lambda\mathcal{P}_1^\perp\psi\| \leq a\|R_0^\perp(\alpha)^{-\frac{1}{2}}\mathcal{P}_1^\perp\psi\| + b\|\psi\|\,,$$

and similarly for $D\mathcal{P}_1^\perp$. However,

$$\begin{aligned}
\|\nabla\mathcal{P}_1^\perp\psi\|^2 &= \|(H_0+1)^{\frac{1}{2}}\mathcal{P}_1^\perp\psi\|^2 - \|\mathcal{P}_1^\perp\psi\|^2 \\
\|(H_0+1)^{\frac{1}{2}}\mathcal{P}_1^\perp\psi\| &\leq \|(H_0-\alpha^2)^{\frac{1}{2}}\mathcal{P}_1^\perp\psi\| + \sqrt{1+\alpha^2}\|\mathcal{P}_1^\perp\psi\| \\
&\leq \|R_0^\perp(\alpha)^{-\frac{1}{2}}\mathcal{P}_1^\perp\psi\| + \sqrt{1+\alpha^2}\|\psi\|\,.
\end{aligned}$$

Here ∇ means the gradient in the variables (x,u) through which all the actions of C_λ, D can be estimated, *e.g.*, $|(C_\lambda\psi)_1| \equiv |A_1\psi| \leq 2\|v\|_\infty|\nabla\psi|$, *etc.* In the same way, one verifies the analyticity of the operator-valued function $DR_0^\perp(\alpha)C_\lambda^*$, which is equivalent to the analyticity of the complex-valued function $\alpha \mapsto b_\alpha(\cdot,\cdot)$.

Consider next the regular part of $R_0(\alpha)\mathcal{P}_1$ containing the operator N_α. Let h be a $\boldsymbol{C}^\infty$-function of compact support in $\mathbb{R}^2$. As pointed out above, using integration by parts and the explicit form of the operators C_λ, D one sees that it is sufficient

to check the boundedness and analyticity of $hn_\alpha h$ and $hn_{\alpha,\mu}h$, where

$$\begin{aligned} n_\alpha(x,x') &:= \frac{1}{2\pi}K_0(k_1(\alpha)|x-x'|) + \ln k_1(\alpha)\,, \\ n_{\alpha,\mu}(x,x') &= -\frac{1}{2\pi}\,\frac{x^\mu - x'^\mu}{|x-x'|}\,k_1(\alpha)K_1(k_1(\alpha)|x-x'|)\,; \end{aligned}$$

recall that $_{,\mu}$ means the derivative w.r.t. x^μ and $K_0' = -K_1$ holds true – *cf.* [AS, 9.6.27]. We will use the following estimates which are valid for the Macdonald functions [AS, 9.6–7] with any $z \in (0,\infty)$:

$$\begin{aligned} |(K_0(z)+\ln z)e^{-z}| \le c_1\,, \qquad & |K_1(z) - z^{-1}| \le c_2\,, \\ |[K_1(z) - z(K_0(z)+K_2(z))/2]| \le c_3\,, \qquad & |zK_1(z)| \le 1\,. \end{aligned}$$

Passing to the polar coordinates,

$$x^\mu - x'^\mu = (\rho\cos\varphi, \rho\sin\varphi)\,, \quad \rho_m := \sup_{x,x'\in\operatorname{supp} h} |x-x'|\,,$$

we check the finiteness of the Schur-Holmgren bounds :

$$\begin{aligned} \|hn_\alpha h\|_{\mathrm{SH}} &= \sup_{x\in\mathbb{R}^2} |h(x)| \int_{\mathbb{R}^2} |m_1(x,x';\alpha)h(x')|\,dx' \\ &\le c_1\|h\|_\infty^2 \int_0^{\rho_m} e^{k_1(\alpha)\rho}\,\rho\,d\rho + \int_0^{\rho_m} |\ln\rho|\,\rho\,d\rho \\ &\le c_1\|h\|_\infty^2\,\rho_m\left(\rho_m e^{\kappa_1\rho_m} + \max\{e^{-1}, \rho_m\ln\rho_m\}\right)\,, \\ \|hn_{\alpha,\mu}h\|_{\mathrm{SH}} &\le \|h\|_\infty^2 \int_0^{\rho_m} \frac{\rho\,d\rho}{\rho} = \|h\|_\infty^2\,\rho_m. \end{aligned}$$

Concerning the analyticity, one should investigate the complex-valued functions $w \mapsto \big(\phi, hn_{\alpha(w)}h\,\psi\big)$ and $w \mapsto \big(\phi, hn_{\alpha(w),\mu}h\,\psi\big)$, where ϕ, ψ are arbitrary vectors of $\boldsymbol{L}^2(\Omega_0)$. Using the Schwarz inequality, it is sufficient to check the finiteness of norms of the complex derivative w.r.t. w of the corresponding operator-valued functions. Since $K_1' = -(K_0+K_2)/2$ by [AS, 9.6.29] and $k_1(\alpha(w)) = e^{w^{-1}}$, we put $z := k_1(\alpha(w))|x-x'|$ and write

$$\begin{aligned} \frac{dn_{\alpha(w)}}{dw}(x,x') &= \frac{1}{2\pi}\frac{z}{w^2}\left(K_1(z) - \frac{1}{z}\right)\,, \\ \frac{dn_{\alpha(w),\mu}}{dw}(x,x') &= \frac{1}{2\pi}\frac{x^\mu - x'^\mu}{|x-x'|}\frac{e^{w^{-1}}}{w^2}\left[K_1(z) - \frac{z}{2}\big(K_0(z)+K_2(z)\big)\right]\,. \end{aligned}$$

Using now the inequality $w^{-2}e^{w^{-1}} \le c_4$ for $w \in (-\infty, 0)$, we are able to estimate the Schur-Holmgren bounds :

$$\left\| h\frac{dn_{\alpha(w)}}{dw}h\right\|_{\mathrm{SH}} \le c_2c_4\|h\|_\infty^2\,\rho_m^2\,, \quad \left\| h\frac{dn_{\alpha(w),\mu}}{dw}h\right\|_{\mathrm{SH}} \le c_3c_4\|h\|_\infty^2\,\rho_m^2\,.$$

Thus the derivatives are bounded for $w \in (-\infty, 0)$, and since the limits as w tends to zero make sense, we can continue the function analytically to $w = 0$. □

Now we are in position to follow the standard Birman-Schwinger scheme to derive the weak-coupling expansion. Eigenvalues of H_λ correspond to singularities of the operator-valued function $(I + K_\lambda^\alpha)^{-1}$ which we can express as

$$(I + K_\lambda^\alpha)^{-1} = \left[I + (I + \hat{M}_\lambda)^{-1}\hat{L}_\lambda\right]^{-1} (I + \hat{M}_\lambda)^{-1}. \qquad \text{(vii.13)}$$

Owing to Lemma vii.3, $\|\hat{M}_\lambda\|$ is finite and we can choose λ sufficiently small to have $\|\hat{M}_\lambda\| < 1$; then the second term at the *r.h.s.* of (vii.13) is a bounded operator. On the other hand, $(I + \hat{M}_\lambda)^{-1}\hat{L}_\lambda$ is a rank-one operator of the form $(\psi, \cdot)\varphi$, where

$$\begin{aligned} \bar{\psi}(x,u) &:= -\frac{\lambda}{2\pi} \ln k_1(\alpha)\, \chi_1(u) C_\lambda^*\,, \\ \varphi(x,u) &:= \left[(I + \hat{M}_\lambda)^{-1} D\, \chi_1\right](x,u)\,, \end{aligned}$$

so it has just one eigenvalue which is

$$(\psi, \varphi) = -\frac{\lambda}{2\pi} \ln k_1(\alpha) \int_0^d \int_{\mathbb{R}^2} \chi_1(u)\, C_\lambda^* \left[(I + \hat{M}_\lambda)^{-1} D\, \chi_1\right](x,u)\, dx\, du\,.$$

Putting it equal -1 we get an implicit equation, $F(\lambda, w) = 0$, with

$$F(\lambda, w) := w - \frac{\lambda}{2\pi} \int_0^d \int_{\mathbb{R}^2} \chi_1(u)\, C_\lambda^* \left[(I + \hat{M}_\lambda)^{-1} D\, \chi_1\right](x,u)\, dx\, du\,, \qquad \text{(vii.14)}$$

where $\hat{M}_\lambda$ has to be understood as a function both of λ and w. Expanding $(I + \hat{M}_\lambda)^{-1}$ into the Neumann series we find

$$F_{,w}(0,0) = 1 \neq 0\,, \qquad F_{,\lambda}(0,0) = -\frac{1}{2\pi}\,(\chi_1, C_0^* D\, \chi_1)\ ,$$

and by Lemma vii.3 we know that $F(\lambda, w)$ is jointly analytic in λ, w. In view of the implicit function theorem $w = w(\lambda)$ is then an analytic function and we can compute the first term in its Taylor expansion :

$$\frac{dw}{d\lambda}(0) = -\frac{F_{,\lambda}(0,0)}{F_{,w}(0,0)} = \frac{1}{2\pi}\,(\chi_1, C_0^* D\, \chi_1)\ .$$

But $(C_0)_n = 0$ for $n = 4, \ldots, 7$, $B_3\chi_1 = 0$, and $(A_2\chi_1, B_2\chi_1) = 0$ since $\int_{\mathbb{R}^2} \Delta v = 0$. It follows that

$$\frac{dw}{d\lambda}(0) = \frac{1}{2\pi}\,(A_1\chi_1, B_1\chi_1) = -\frac{1}{\pi} \int_0^d \chi_1'(u)^2\, du \int_{\mathbb{R}^2} v(x)\, dx = -\frac{\kappa_1^2}{\pi}\,\langle v\rangle, \qquad \text{(vii.15)}$$

where we have employed the symbol $\langle v\rangle := \int_{\mathbb{R}^2} v(x)\, dx$.

We note that $\alpha^2 \to \kappa_1^2-$ holds as $\lambda \to 0+$, and consequently, $k_1(\alpha) \to 0+$. Thus $w(0) = 0$ is well defined because $w = (\ln k_1(\alpha))^{-1}$ by definition. Furthermore, the solution α^2 clearly represents an eigenvalue if and only if w is strictly negative for λ small. A sufficient condition for that is that the first term of the expansion of $w(\lambda)$ is strictly negative; due to (vii.15) it happens if $\langle v\rangle$ is strictly positive. Summing up the discussion, we get the announced three-dimensional analogue to Theorem 1.2 in [BGRS] :

Theorem vii.4. *Let* Ω_λ *be given by* (vii.6)*, where* $v \in \boldsymbol{C}_0^\infty(\mathbb{R}^2)$ *satisfies* $\langle v\rangle > 0$*. Then for all sufficiently small positive* λ*,* $-\Delta_D^{\Omega_\lambda}$ *has a unique eigenvalue* $E(\lambda)$ *in* $[0,\kappa_1^2)$*, which is simple and can be expressed as* $E(\lambda) = \kappa_1^2 - e^{2w(\lambda)^{-1}}$*, where* $\lambda \mapsto w(\lambda)$ *is an analytic function. Moreover, the following asymptotic expansion is valid :*

$$w(\lambda) = -\lambda\,\frac{\kappa_1^2}{\pi}\,\langle v\rangle + \mathcal{O}(\lambda^2)\,.$$

vii.3 An alternative method

Now we will derive the weak-coupling expansion by constructing the asymptotics for singularities in a particular boundary value problem. This approach enables us to derive easily higher terms of the expansion. At the same time it allows a unified treatment for different dimensions ; in this way we will be able to amend the existing results concerning deformed strips.

First we introduce a unifying notation. Let $n = 2, 3$ be the dimension of the considered deformed region, *i.e.*, the perturbed planar strip or layer, respectively. We set $x = (x^1, \ldots, x^{n-1}) \in \mathbb{R}^{n-1}$ and $(x,u) \in \Omega_0 := \mathbb{R}^{n-1}\times(0,d)$ for the unperturbed domain. From technical reasons it is convenient to change the setting slightly, in comparison with (vii.6) and [BGRS], [EV3], and to deform the "lower" boundary of Ω_0 what we certainly can do without loss of generality. We denote therefore in this section

$$\Omega_\lambda := \{(x,u) \in \mathbb{R}^n : -\lambda dv(x) < u < d\} \tag{vii.16}$$

with $v \in \boldsymbol{C}_0^\infty(\mathbb{R}^{n-1})$. We denote by $-\Delta'$ the $(n-1)$-dimensional Laplacian, while $-\Delta$ stands for the n-dimensional one. We also use

$$\langle f\rangle := \int_{\mathbb{R}^{n-1}} f(x)\,dx\,,$$

$\|\cdot\|$ as the norm in $\boldsymbol{L}^2(\mathbb{R}^{n-1})$, and

$$\alpha(m) := \begin{cases} m \\ (\ln m)^{-1} \end{cases} \qquad \beta(t) := \begin{cases} t & \text{if} \quad n=2 \\ \ln t & \text{if} \quad n=3 \end{cases}$$

vii.3.1 The asymptotic expansion

Let us now construct the asymptotics of the eigenvalues m_λ of the following boundary value problem :

$$\begin{aligned} &(\Delta + \kappa_1^2)\Psi_\lambda = m_\lambda^2\Psi_\lambda \quad \text{in } \Omega_\lambda \\ &\Psi_\lambda\,(x, \lambda dv(x)) = \Psi_\lambda(x,d) = 0 \end{aligned}$$

as they approach zero. We will seek it in the form

$$m_\lambda = \begin{cases} \sum_{i=1}^\infty \lambda^i m_i & \text{if} \quad n=2 \\ \exp\left(-\left(\sum_{i=1}^\infty \lambda^i m_i\right)^{-1}\right) & \text{if} \quad n=3 \end{cases} \tag{vii.17}$$

where the existence of such expansions follows from [BGRS] and Theorem vii.4, respectively. Notice that this corresponds to the expansion of $E(\lambda) = \kappa_1^2 - m_\lambda^2$,

the ground-state eigenvalue of $-\Delta_D^{\Omega_\lambda}$ in the problem discussed above, because the mirror transformation of Ω_λ on (vii.16) does not affect the spectral properties.

Suppose that a function $f \in \boldsymbol{C}_0^\infty(\mathbb{R}^{n-1})$, $\operatorname{supp} f \cap \operatorname{supp} v = \emptyset$, and $\langle f \rangle \neq 0$ is given. If we manage to construct a solution $\psi_\lambda(x,u;m)$ of the boundary value problem

$$\begin{aligned} (\Delta + \kappa_1^2)\psi_\lambda = m^2\psi_\lambda + (\alpha(m) - \alpha(m_\lambda))\, f\chi_1 \quad &\text{in} \quad \Omega_\lambda \\ \psi_\lambda = 0 \quad &\text{on} \quad \partial\Omega_\lambda \end{aligned} \tag{vii.18}$$

which is bounded and non-vanishing w.r.t. m for small nonzero m, then $\Psi_\lambda(x,u) = \psi_\lambda(x,u;m_\lambda)$. We shall look for the asymptotics of ψ_λ in the following form,

$$\psi_\lambda(x,u;m) = \sum_{i=0}^{\infty} \lambda^i \psi_i(x,u;m)\,. \tag{vii.19}$$

Substituting (vii.19) and (vii.17) into (vii.18), we obtain a family of the boundary value problems :

$$\begin{aligned} (\Delta + \kappa_1^2)\psi_0 = m^2\psi_0 + \alpha(m) f\chi_1 \quad &\text{in} \quad \Omega_0 \qquad i = 0 \\ \psi_0 = 0 \quad &\text{on} \quad \partial\Omega_0 \end{aligned} \tag{vii.20}$$

$$\begin{aligned} (\Delta + \kappa_1^2)\psi_i = m^2\psi_i + (-1)^{n-1} m_i f\chi_1 \quad &\text{in} \quad \Omega_0 \qquad i \geq 1 \\ \psi_i = 0 \quad &\text{if} \quad u = d \\ \psi_i = -\sum_{j=1}^{i} \frac{d^j(-v)^j}{j!} \frac{\partial^j \psi_{i-j}}{\partial u^j} \quad &\text{if} \quad u = 0 \end{aligned} \tag{vii.21}$$

One can check easily that $\psi_0 = -\alpha(m)(-\Delta' + m^2)^{-1} f\chi_1$ solves (vii.20) and has the asymptotics

$$\begin{aligned} \psi_0(x,u;m) = \frac{(-1)^{n-1}}{2\pi^{n-2}}\, \chi_1(u) \Bigg[& \langle f \rangle \\ & + (-1)^{n-1}\alpha(m) \left(\int_{\mathbb{R}^{n-1}} \beta(|x-x'|) f(x')\, dx' + \delta_n^3(\gamma - \ln 2)\langle f \rangle \right) \\ & + \mathcal{O}\left(\alpha(m)^2\right) \Bigg] \end{aligned} \tag{vii.22}$$

as $m \to 0$, where γ is the Euler number and δ_n^j the Kronecker delta.

Lemma vii.5. *Suppose that $F \in \boldsymbol{C}^\infty(\overline{\Omega_0})$ with a bounded support and $H \in \boldsymbol{C}_0^\infty(\mathbb{R}^{n-1})$ have the expansions*

$$F(x,u;m) = \sum_{i=0}^{\infty} \alpha(m)^i F_i(x,u)\,, \qquad H(x;m) = \sum_{i=0}^{\infty} \alpha(m)^i H_i(x)$$

as $m \to 0$. Define $F_{i,k} := \int_0^d F_i(\cdot,u)\, \chi_k(u)\, du$. Let ϕ_0 be the solution of the boundary value problem

$$\begin{aligned} (\Delta + \kappa_1^2)\phi_0 = F_0 \quad &\textit{in} \quad \Omega_0\,, \\ \phi_0 = 0 \quad &\textit{if} \quad u = d\,, \\ \phi_0 = H_0 \quad &\textit{if} \quad u = 0\,; \end{aligned} \tag{vii.23}$$

then the condition

$$\langle F_{0,1}\rangle = \sqrt{\frac{2}{d}}\,\kappa_1\,\langle H_0\rangle \tag{vii.24}$$

is necessary and sufficient for existence of a solution of the boundary value problem

$$\begin{aligned}(\Delta+\kappa_1^2)\phi = m^2\phi + F \quad &in \quad \Omega_0\,,\\ \phi = 0 \quad &if \quad u = d\,,\\ \phi = H \quad &if \quad u = 0\,,\end{aligned}$$

which is bounded as $m \to 0$. *If it is satisfied, the solution has the asymptotics*

$$\begin{aligned}&\phi(x,u;m)\\ &\quad = \phi_0(x,u) + \frac{(-1)^{n-1}}{2\pi^{n-2}}\,\chi_1(u)\left(\langle F_{1,1}\rangle - \sqrt{\frac{2}{d}}\,\kappa_1\,\langle H_1\rangle\right) + \mathcal{O}\left(\alpha(m)\right)\,.\end{aligned}$$

Proof. The statement is obvious if $H = 0$. In particular, the solution ϕ is constructed by the Fourier method in the explicit form

$$\phi(x,u;m) = \sum_{i=1}^{\infty} \tilde{\phi}_i(x;m)\chi_i(u).$$

By a direct calculation it is easy to see that $\tilde{\phi}_i$ are bounded functions for $m \geq 0$ so long as $i \geq 2$. The problem arises for $i = 1$, because in general $\tilde{\phi}_1$ tends to infinity as $m \to 0$. The condition (vii.24) guarantees that the explicit solution ϕ has no such pole. This proves the sufficiency. To see that the condition is necessary at the same time, one integrates by parts in the scalar product equation

$$\left(\chi_1, (\Delta+\kappa_1^2-m^2)\phi\right) = (\chi_1, F)$$

and puts $m = 0$ afterwards. In the opposite case, $H \neq 0$, we use the replacement

$$\phi(x,u;m) = \varphi(x,u;m) + \left(1-\frac{u}{d}\right)H(x;m)$$

and expand the r.h.s. of the equation for φ in the Fourier series, which reduces the task to the previous situation. □

Corollary vii.6. $\phi \in \boldsymbol{C}^\infty(\overline{Q})$ *holds for any bounded domain* $Q \subset \Omega_0$.

It follows from Lemma vii.5 that the recursive system of the boundary value problem (vii.21) has solutions which are continuous with respect to m in the vicinity of $m = 0$ and decay as $|x| \to \infty$ for $m > 0$, provided the m_i's satisfy the following recursive relations :

$$m_i = (-1)^n\sqrt{\frac{2}{d}}\,\frac{\kappa_1}{\langle f\rangle}\sum_{j=1}^{i}\left\langle \frac{d^j(-v)^j}{j!}\frac{\partial^j\psi_{i-j}}{\partial u^j}(\cdot,0;0)\right\rangle. \tag{vii.25}$$

In particular, owing to (vii.22) and Lemma vii.5 we get

$$m_1 = \frac{\kappa_1^2}{\pi^{n-2}}\,\langle v\rangle\,, \tag{vii.26}$$

which agrees with the leading term obtained by the Birman-Schwinger method in the previous section – *cf.* Theorem vii.4 and (vii.17) – as well as with the corresponding result (vii.1) in the strip case.

vii.3.2 The next-to-leading order

Let us now calculate m_2. By virtue of (vii.21), (vii.22) and (vii.26) the boundary value problem for ψ_1 together with the boundary condition for $\psi_2(x,u;0)$ look as follows

$$\begin{aligned}(\Delta+\kappa_1^2)\psi_1 = m^2\psi_1 + (-1)^{n-1}\frac{\kappa_1^2}{\pi^{n-2}}\langle v\rangle\, f\chi_1 \quad &\text{in} \quad \Omega_0 \\ \psi_1 = 0 \quad &\text{if} \quad u=d \\ \psi_1 = dv\frac{\partial\psi_0}{\partial u} \quad &\text{if} \quad u=0 \\ \psi_2 = 0 \quad &\text{if} \quad u=d \\ \psi_2 = dv\frac{\partial\psi_1}{\partial u} \quad &\text{if} \quad u=d,\ m=0\end{aligned} \tag{vii.27}$$

with

$$\frac{\partial\psi_0}{\partial u}(x,0;m) = \frac{(-1)^{n-1}}{2\pi^{n-2}}\sqrt{\frac{2}{d}}\,\kappa_1\mathcal{B}(f)\,, \tag{vii.28}$$

where $\mathcal{B}(f)$ is the square bracket from (vii.22). Hence

$$m_2 = (-1)^{n-1}\sqrt{\frac{2}{d}}\,\frac{\kappa_1 d}{\langle f\rangle}\left\langle v\frac{\partial\psi_1}{\partial u}(\cdot,0;0)\right\rangle \tag{vii.29}$$

and it is sufficient to find ψ_1. With eq. (vii.27) and Lemma vii.5 in mind, we consider the following boundary value problem

$$\begin{aligned}(\Delta+\kappa_1^2)\phi_0 = (-1)^{n-1}\frac{\kappa_1^2}{\pi^{n-2}}\langle v\rangle\, f\chi_1 \quad &\text{in} \quad \Omega_0 \\ \phi_0 = 0 \quad &\text{if} \quad u=d \\ \phi_0 = \frac{(-1)^{n-1}}{2\pi^{n-2}}\sqrt{\frac{2}{d}}\,\kappa_1\, d\, v\,\langle f\rangle \quad &\text{if} \quad u=0\end{aligned} \tag{vii.30}$$

and seek ϕ_0 in the form

$$\phi_0(x,u) = \frac{(-1)^{n-1}}{2\pi^{n-2}}\sqrt{\frac{2}{d}}\,\kappa_1\left[\left(1-\frac{u}{d}\right)\langle f\rangle\, d\, v(x) - \varphi(x,u)\right]; \tag{vii.31}$$

substituting it into (vii.30), we arrive at the boundary value problem

$$\begin{aligned}(\Delta+\kappa_1^2)\varphi = -d\,\langle f\rangle\left(1-\frac{u}{d}\right)(\Delta'+\kappa_1^2)v + 2\kappa_1\sqrt{\frac{2}{d}}\,\langle v\rangle\, f\chi_1 \quad &\text{in} \quad \Omega_0 \\ \varphi = 0 \quad &\text{on} \quad \partial\Omega_0.\end{aligned}$$

The Fourier method gives

$$\begin{aligned}\varphi \;=\; &-\sqrt{\frac{2}{d}}\,d\,\langle f\rangle\sum_{k=2}^{\infty}\frac{\chi_k}{\kappa_k}\,(-\Delta'+\kappa_k^2-\kappa_1^2)^{-1}(-\Delta'-\kappa_1^2)\,v \\ &-\sqrt{\frac{2}{d}}\,d\,\frac{\chi_1}{\kappa_1}\left[\langle f\rangle\, v + \kappa_1^2(-\Delta')^{-1}\left(\langle v\rangle\, f - \langle f\rangle\, v\right)\right].\end{aligned}$$

Lemma vii.5 an relations (vii.27), (vii.28), (vii.30), and (vii.31) together with the last result imply that

$$\begin{aligned}\frac{\partial\psi_1}{\partial u}(x,0;0) &= \frac{(-1)^n}{2\pi^{n-2}}\sqrt{\frac{2}{d}}\,\kappa_1 \\ &\times\Bigg\{\frac{\kappa_1^2}{\pi^{n-2}}\Bigg[\int\limits_{\mathbb{R}^{n-1}\times\mathbb{R}^{n-1}} v(x)\,\beta(|x-x'|)\,f(x')\,dx\,dx' \\ &+\langle f\rangle\int_{\mathbb{R}^{n-1}}\beta(|x-x'|)\,v(x')\,dx' - \langle v\rangle\int_{\mathbb{R}^{n-1}}\beta(|x-x'|)\,f(x')\,dx'\Bigg] \\ &+\langle f\rangle\Bigg[3\,v(x)+2\sum_{k=2}^{\infty}\left[(-\Delta'+\kappa_k^2-\kappa_1^2)^{-1}(-\Delta'-\kappa_1^2)\,v\right](x) \\ &+\delta_n^3\,\frac{\kappa_1^2}{\pi}\,(\gamma-\ln 2)\,\langle v\rangle\Bigg]\Bigg\},\end{aligned}$$

where we have employed also the implication

$$\langle F\rangle = 0 \;\Rightarrow\; (-\Delta')^{-1}F = \frac{-1}{2\pi^{n-2}}\int_{\mathbb{R}^{n-1}}\beta(|\cdot-x'|)\,F(x')\,dx'.$$

Substituting this into (vii.29) we get the sought coefficient :

$$\begin{aligned}m_2 \;=\; &-\frac{\kappa_1^2}{\pi^{n-2}}\Bigg\{3\,\langle v^2\rangle + \frac{\kappa_1^2}{\pi^{n-2}}\int\limits_{\mathbb{R}^{n-1}\times\mathbb{R}^{n-1}} v(x)\,\beta(|x-x'|)\,v(x')\,dx\,dx' \\ &+2\left\langle v\sum_{k=2}^{\infty}(-\Delta'+\kappa_k^2-\kappa_1^2)^{-1}(-\Delta'-\kappa_1^2)\,v\right\rangle \\ &+\delta_n^3\,\frac{\kappa_1^2}{\pi}\,(\gamma-\ln 2)\,\langle v\rangle^2\Bigg\}. \qquad \text{(vii.32)}\end{aligned}$$

vii.3.3 The critical case

As we have pointed out in the introduction, the above result is most interesting in the critical case, $\langle v\rangle = 0$, when the first coefficient (vii.26) equals zero and m_2 given by (vii.32) determines the leading order. In this situation we have the following result.

Theorem vii.7. *Let $V \in \boldsymbol{C}_0^\infty(\mathbb{R}^{n-1})$ be an arbitrary function such that $\langle V\rangle = 0$ and*

$$v(x) = V\left(\frac{x}{\sigma}\right), \qquad \sigma > 0\,.$$

Then the following inequalities hold,

$$\begin{aligned}-\frac{\kappa_1^2\sigma^{n-1}}{\pi^{n-2}}&\left(\frac{8}{2}\|V\|^2+\frac{3}{2\kappa_1^2\sigma^2}\|V\|\|\Delta' V\|-2\kappa_1^2\sigma^2\|\nabla'(\Delta')^{-1}V\|^2\right) \\ &\le m_2 \le -\frac{\kappa_1^2\sigma^{n-1}}{\pi^{n-2}}\left(\frac{3}{2}\|V\|^2-2\kappa_1^2\sigma^2\|\nabla'(\Delta')^{-1}V\|^2\right).\end{aligned}$$

Proof. In the first place, note that $\langle V\rangle = 0$ implies

$$-\frac{\kappa_1^2}{\pi^{n-2}} \int\limits_{\mathbb{R}^{n-1}\times\mathbb{R}^{n-1}} V(x)\,\beta(|x-x'|)\,V(x')\,dx\,dx' = \|\nabla'(\Delta')^{-1}V\|^2 > 0\,,$$

because $\Delta'\beta(|x|) = 2\pi^{n-2}\delta(x)$ holds in the sense of distribution. Under the stated assumptions, the formula (vii.32) yields therefore

$$m_2 = -\frac{\kappa_1^2\sigma^{n-1}}{\pi^{n-2}}\Big(3\|V\|^2 - 2\kappa_1^2\sigma^2\|\nabla'(\Delta')^{-1}V\|^2 + 2A(\sigma)\Big),$$

where

$$A(\sigma) := \sum_{k=2}^{\infty}\Big\langle V\left(-\Delta' + (\kappa_k^2-\kappa_1^2)\,\sigma^2\right)^{-1}(-\Delta' - \kappa_1^2\sigma^2)\,V\Big\rangle\,,$$

and it suffices to find suitable bounds on $A(\sigma)$.

Since the Fourier transformation together with the Plancherel theorem give the estimate

$$\Big\|\left(-\Delta' + (\kappa_k^2-\kappa_1^2)\,\sigma^2\right)^{-1}F\Big\| \le \frac{\|F\|}{(\kappa_k^2-\kappa_1^2)\sigma^2}\,, \tag{vii.33}$$

we obtain the upper bound

$$A(\sigma) \le \frac{3}{4}\left(\|V\|^2 + \frac{1}{\kappa_1^2\sigma^2}\|V\|\|\Delta' V\|\right),$$

where the numerical factor comes from $\sum_{k=2}^{\infty}(k^2-1)^{-1} = \frac{3}{4}$.

On the other hand, denoting

$$U_k(x;\sigma) := \Big[\left(-\Delta' + (\kappa_k^2-\kappa_1^2)\,\sigma^2\right)^{-1}V\Big](x),$$

we see that

$$\begin{aligned}&\Big\langle V\left(-\Delta' + (\kappa_k^2-\kappa_1^2)\,\sigma^2\right)^{-1}(-\Delta' - \kappa_1^2\sigma^2)\,V\Big\rangle\\ &\qquad = \Big\langle\left(-\Delta' + (\kappa_k^2-\kappa_1^2)\,\sigma^2\right)U_k(-\Delta' - \kappa_1^2\sigma^2)U_k\Big\rangle\,.\end{aligned}$$

Integrating the *r.h.s.* by parts and using (vii.33), we get the lower bound

$$\begin{aligned}A(\sigma) &= \sum_{k=2}^{\infty}\Big(\|\Delta' U_k\|^2 + \kappa_1^2(k^2-2)\sigma^2\|\nabla' U_k\|^2 - \kappa_1^4(k^2-1)\sigma^4\|U_k\|^2\Big)\\ &> -\sum_{k=2}^{\infty}\kappa_1^4(k^2-1)\sigma^4\|U_k\|^2 \ge -\|V\|^2\sum_{k=2}^{\infty}\frac{1}{k^2-1} = -\frac{3}{4}\|V\|^2,\end{aligned}$$

which concludes the proof. □

This theorem confirms the spectral picture we got from (vii.2) and (vii.3). More specifically, $m_2 > 0$ as $\sigma\to\infty$ so the critical weakly bound state exists for sufficiently smeared deformations, and vice versa. In contrast to (vii.2) and (vii.3), however, we are able now to tell from (vii.32) for any given zero-mean v the sign of m_2.

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Chapitre viii

Sur le spectre des variétés non-compactes

Résumé

Nous avons vu que les guides d'ondes bidimensionnels peuvent posséder des états liés au-dessous du spectre essentiel si la surface de référence est asymptotiquement plate. Sous cette hypothèse, nous avons trouvé une borne inférieure κ_1^2 du seuil du spectre essentiel. Nous établissons ici des conditions suffisantes pour que tout l'intervalle $[\kappa_1^2, \infty)$ appartienne à ce type du spectre. Nous récapitulons et révisons aussi les résultats analogues concernant le guide d'ondes unidimensionnel.

Nous étudions aussi le spectre du laplacien sur les variétés non-compactes qui sont complètes et possèdent au moins un pôle. Nous nous concentrons sur les variétés à symétrie radiale et les surfaces. Dans ces cas particuliers, nous établissons que le spectre est l'intervalle $[0, \infty)$ en posant certaines conditions supplémentaires sur la décroissance des courbures à l'infini.

The relationship between the geometry of a Riemannian manifold and the spectrum of the associated Laplace-Beltrami operator constitutes one area of interest for the *spectral geometry*. The subject of this thesis is to perform such a spectral analysis for the layer manifold Ω which is defined as a tubular neighbourhood constructed over a non-compact surface in $\mathbb{R}^3$. Note that $\bar{\Omega}$ is a manifold with boundary and so the layer is not geodesically complete. Section viii.1 below is dedicated to the study of the essential spectrum of $-\Delta_D^\Omega$. In Section viii.2 we make some comments on the same question in planar strips, *i.e.*, the one-dimensional analogy of quantum layers. A part of the problem in locating the essential spectrum of Ω is to answer the analogous question for the reference surface Σ. This is the reason why we add Section viii.3 where the spectrum of a complete and non-compact manifold is also touched; the results discussed here are of independent interest.

viii.1 Curved Layers

The essential spectrum of a planar quantum layer is clearly the interval $[\kappa_1^2, \infty)$ and there is no discrete spectrum. In the previous parts of the thesis we have seen that as long as one considers curved layers built over asymptotically planar surfaces $\langle \Sigma 0 \rangle$, the threshold of the essential spectrum does not descend below the lowest transverse eigenvalue κ_1^2 and the curvature may produce bound states in $[0, \kappa_1^2)$. In this section we are interested in the nature of the spectrum in the remaining interval. In particular, we seek the conditions under which all energies above κ_1^2 belong to the essential spectrum. Recall that this is trivially true if a planar layer is curved only locally – *cf.* Chapitre iv – however, the general situation of Chapitre v requires more attention.

viii.1.1 Preliminaries

From now we shall suppose that Σ is of class C^3 and possesses at least one *pole* [52], *i.e.*, the point $o \in \Sigma$ such that the exponential mapping [60, Sec. 5.2], $\exp_o : \mathrm{T}_o\Sigma \to \Sigma$, is a diffeomorphism. The latter assumption enables us to parameterize the surface by the unique chart

$$p : \Sigma_0 \to \Sigma \setminus \{o\} : \{(s, \vartheta) \mapsto \exp_o(s \cos\vartheta \; e_1 + s \sin\vartheta \; e_2)\},$$

where $\Sigma_0 := (0, \infty) \times S^1$ and $\{e_1, e_2\}$ is an orthonormal basis of $\mathrm{T}_o\Sigma$. We can now abuse the notation and identify the surface points with the vectors in $\mathbb{R}^3$ in the canonical way and consider p as the parametrized chart $p : \Sigma_0 \to \mathbb{R}^3$.

Remark. Notice that this mapping is not a coordinate system in the usual sense in the theory of surfaces where Σ_0 is considered to be an open region of $\mathbb{R}^2$ – *cf.* (ii.1). However, it would require to take, *e.g.*, $(0, 2\pi)$ instead of S^1, and removing thus an entire radius from Σ – *cf.* [60, Sec. 5.3].

The induced metric has the form $(g_{\mu\nu}) = \mathrm{diag}(1, r^2)$, where $r(s,\vartheta)$ is the Jacobian of the exponential mapping, which satisfies the classical Jacobi equation

$$\ddot{r} + K\, r = 0 \qquad \text{with} \qquad r(0,\vartheta) = 0,\ \dot{r}(0,\vartheta) = 1. \tag{viii.1}$$

We have introduced here the *dot* notation for the partial derivatives w.r.t. the radial variable $q^1 \equiv s$ which we shall use hereafter. Later we shall employ as well the *dash* notation for the derivatives w.r.t. the transverse variable $q^3 \equiv u$. For further purpose let us mention here that only the following components of the Christoffel symbols $\gamma^\sigma_{\mu\nu}$ of Σ in the geodesic polar coordinates are non-zero

$$\gamma^1_{22} = -r r_{,1}, \qquad \gamma^2_{12} = \gamma^2_{21} = \frac{r_{,1}}{r}, \qquad \gamma^2_{22} = \frac{r_{,2}}{r}. \tag{viii.2}$$

The Weingarten tensor in the geodesic polar coordinates can be written as the matrix

$$(h_\mu{}^\nu) = \begin{pmatrix} k_s & h_{12} r^{-2} \\ h_{12} & k_\vartheta \end{pmatrix}, \tag{viii.3}$$

where $k_s(s,\vartheta)$, $k_\vartheta(s,\vartheta)$ are the normal curvatures corresponding to the coordinates curves, *i.e.*, to the geodesic lines $p(s, \vartheta = \vartheta_0)$ or the geodesic circles $p(s = s_0, \vartheta)$, respectively, and $h_{12}(s,\vartheta)$ is a non-specified off-diagonal component of the second fundamental form.

The assumption $\langle \Sigma 0 \rangle$ that the surface Σ is asymptotically planar means in the geodesic polar coordinates that the fundamental invariants K and M go to zero uniformly w.r.t. ϑ as $s \to \infty$. The following statement provides an alternative definition of this property.

Proposition viii.1. *The surface Σ is asymptotically planar if and only if*

$$h_\mu{}^\nu \xrightarrow{\ \infty\ } 0$$

Then also $k_s, k_\vartheta, h_{12} r^{-1} \longrightarrow 0$ as $s \to \infty$.

By the limit of the Weingarten tensor we mean precisely the limit of the operator norm of the functional $h_\mu{}^\nu : \mathrm{T}_p\Sigma \to \mathrm{T}_p\Sigma$, *i.e.*, the limit of the expression

$$|h_\mu{}^\nu|_g := \sup_{t_\nu \in \mathrm{T}_p\Sigma} \frac{|h_\mu{}^\nu t_\nu|_g}{|t_\nu|_g}, \tag{viii.4}$$

where $|\cdot|_g$ at the right hand side of this definition means the usual vector norm induced by the metric $g_{\mu\nu}$. We notice that one could also understand the limit as the limit of the scalar function $h_\mu{}^\nu h_\nu{}^\mu$ which is sometimes called the matrix norm.

PROOF: Since the principal curvatures $k_\pm$ are the eigenvalues of the Weingarten tensor, the first claim of the proposition follows by the elementary fact $|h_\mu{}^\nu|_g = \max\{|k_+|, |k_-|\}$ and by the explicit dependence of K and M on these curvatures. At the same time, if the expression (viii.4) tends to zero as $s \to \infty$, it has to be true also for $|h_\mu{}^\nu t_\nu|_g$ with an arbitrary normalized vector t_ν in $\mathrm{T}_p\Sigma$. Taking consecutively $t_\nu = (1, 0)$ and $t_\nu = (0, r)$ which are in fact the renormalized coordinate vectors, we obtain the second statement. □

Apart of the fundamental condition $\langle\Sigma 0\rangle$ we shall suppose that also the derivatives of surface curvatures decay at infinity. In particular, we require

$$\boxed{\langle\sigma 1\rangle \quad h_{\mu\,;\rho}^{\ \ \nu} \overset{\infty}{\longrightarrow} 0} \quad :\Longleftrightarrow \quad \left|h_{\mu\,;\rho}^{\ \ \nu}\right|_g^2 := h_{\mu\,;\rho}^{\ \ \nu}\, g^{\rho\sigma} h_{\nu\,;\sigma}^{\ \ \mu} \overset{\infty}{\longrightarrow} 0$$

where the *semicolon* denotes the covariant differentiation. This is evidently a covariant condition which implies in particular the following.

Proposition viii.2. *The surface Σ fulfills the hypothesis $\langle\sigma 1\rangle$ if and only if*

$$\begin{array}{llll} (1) & k_{s,1} \longrightarrow 0 & (2) & \dfrac{k_{s,2}}{r} - 2\dfrac{r_{,1}}{r}\dfrac{h_{12}}{r} \longrightarrow 0 \\ (3) & k_{\vartheta,1} \longrightarrow 0 & (4) & \dfrac{k_{\vartheta,2}}{r} + 2\dfrac{r_{,1}}{r}\dfrac{h_{12}}{r} \longrightarrow 0 \\ (5) & \left(\dfrac{h_{12}}{r}\right)_{,1} \longrightarrow 0 & (6) & \dfrac{1}{r}\left(\dfrac{h_{12}}{r}\right)_{,2} + \dfrac{r_{,1}}{r}(k_s - k_\vartheta) \longrightarrow 0 \end{array}$$

uniformly w.r.t. ϑ as $s \to \infty$. As a consequence of $\langle\Sigma 0\rangle$ and $\langle\sigma 1\rangle$, we get also that

$$(7) \quad \nabla_g K \longrightarrow 0 \qquad\qquad (8) \quad \nabla_g M \longrightarrow 0$$

uniformly w.r.t. ϑ as $s \to \infty$.

PROOF: First of all we recall that the limit "$\overset{\infty}{\longrightarrow}$" introduced in a general way in Section ii.1.1 means in the geodesic polar coordinates just the uniform convergence w.r.t. ϑ as $s \to \infty$. Expanding $|h_{\mu\,;\rho}^{\ \ \nu}|_g$ we obtain

$$\left|h_{\mu\,;\rho}^{\ \ \nu}\right|_g^2 = \left(h_{1\,;1}^{\ \ 1}\right)^2 + \left(h_{2\,;1}^{\ \ 2}\right)^2 + \left(\frac{h_{1\,;2}^{\ \ 1}}{r}\right)^2 + \left(\frac{h_{2\,;2}^{\ \ 2}}{r}\right)^2 + 2h_{1\,;1}^{\ \ 2} h_{2\,;1}^{\ \ 1} + 2\frac{h_{1\,;2}^{\ \ 2} h_{2\,;2}^{\ \ 1}}{r^2}.$$

We use (viii.2) together with the identity which defines the covariant derivative of a tensor field [70, Sec. 3.5]

$$h_{\mu\,;\rho}^{\ \ \nu} = h_{\mu\,,\rho}^{\ \ \nu} - \gamma_{\mu\rho}^{\sigma} h_\sigma{}^\nu + \gamma_{\sigma\rho}^{\nu} h_\mu{}^\sigma$$

in order to evaluate the individual terms $h_{\mu\,;\rho}^{\ \ \nu}$. In particular, one finds

$$h_{1\,;1}^{\ \ 2} h_{2\,;1}^{\ \ 1} = \left(\frac{h_{12}}{r}\right)_{,1}^2 \qquad \text{and} \qquad h_{1\,;2}^{\ \ 2} h_{2\,;2}^{\ \ 1} = \left[\left(\frac{h_{12}}{r}\right)_{,2} + r_{,1}(k_s - k_\vartheta)\right]^2,$$

and since the other terms in the expansion of $|h_{\mu\ ;\rho}^{\ \nu}|_g$ are also positive, we have just established the limits (5) and (6). In the same way, one arrives at

$$h_{1\ ;1}^{\ 1} = k_{s,1} \qquad h_{1\ ;2}^{\ 1} = k_{s,2} - 2r_{,1}\frac{h_{12}}{r}$$
$$h_{2\ ;1}^{\ 2} = k_{\vartheta,1} \qquad h_{2\ ;2}^{\ 2} = k_{\vartheta,2} + 2r_{,1}\frac{h_{12}}{r}$$

which gives the remaining relations (1)–(4). Assume now $\langle\Sigma 0\rangle$, in particular, its consequences stated in Proposition viii.1. Since $|\nabla_g M|_g^2 = (M_{,1})^2 + (M_{,2}r^{-1})^2$ and $M = \frac{1}{2}(k_s + k_\vartheta)$, the consequence (8) of the assumption $\langle\sigma 1\rangle$ follows easily by using the properties (1)–(4). Using in addition (5)–(6) together with $K = k_s k_\vartheta - (h_{12}r^{-1})^2$, one establishes (7) as well. □

Furthermore, we suppose

$$\boxed{\langle\sigma 2\rangle \quad k_g \xrightarrow{\infty} 0}$$

where $k_g := \dot{r}r^{-1}$ is the geodesic curvature of the geodesic circles $\{p(s,\vartheta) : \vartheta \in S^1\}$. Notice that this hypothesis is not covariant. It will play an important role in Section viii.3.3 in attempts to localize the essential spectrum of surfaces. The asymptotic properties $\langle\Sigma 0\rangle$ and $\langle\sigma 1\text{–}2\rangle$ have the following consequence on the layer geometry at infinity which we shall need further on.

Lemma viii.3. *Define* $\Gamma^\mu := G^{\mu\nu}_{\ \ ,\nu} + 2G^{\mu\nu}F_{,\nu}$ *with* $F := \ln G^{\frac{1}{4}}$ *and assume* $\langle\Sigma 0\rangle$ *and* $\langle\sigma 1\text{–}2\rangle$. *Then*

$$G^{11} \longrightarrow 1 \qquad \textit{and} \qquad \Gamma^1 \longrightarrow 0$$

uniformly w.r.t. ϑ *as* $s \to \infty$.

Proof: Using (ii.4), (viii.3) and the common rule for inverting a 2×2 matrix, we get

$$G^{\mu\nu} = e^{4J}\begin{pmatrix} (1-uk_\vartheta)^2 + u^2\left(h_{12}r^{-1}\right)^2 & 2\,r^{-1}\,u\,h_{12}r^{-1}\,(1-uM) \\ 2\,r^{-1}\,u\,h_{12}r^{-1}\,(1-uM) & r^{-2}\left[(1-uk_s)^2 + u^2\left(h_{12}r^{-1}\right)^2\right] \end{pmatrix}$$

with the notation J introduced at the formula (ii.9). The first claim of the above lemma follows by Proposition viii.1. Since $F = \frac{1}{2}\ln r + J$, one checks easily that

$$\begin{aligned} 2G^{11}F_{,1} &= e^{4J}\left(r_{,1}r^{-1} + 2J_{,1}\right)\left[(1-uk_\vartheta)^2 + u^2\left(h_{12}r^{-1}\right)^2\right] \\ 2G^{12}F_{,2} &= 2\,e^{4J}\left(r_{,2}r^{-2} + 2J_{,2}r^{-1}\right)u\,h_{12}r^{-1}\,(1-uM)\,, \end{aligned}$$

while the calculation of $G^{1\nu}_{,\nu}$ yields

$$\begin{aligned} G^{11}_{,1} &= 4\,e^{4J}J_{,1}\left[(1-uk_\vartheta)^2+u^2\left(h_{12}r^{-1}\right)^2\right] \\ &\quad +2\,e^{4J}\left[-u\,k_{\vartheta,1}\,(1-uk_\vartheta)+u^2\,h_{12}r^{-1}\left(h_{12}r^{-1}\right)_{,1}\right] \\ G^{12}_{,2} &= 8\,e^{4J}J_{,2}r^{-1}\,u\,h_{12}r^{-1}\,(1-uM)+2\,u\,e^{4J}\Big[-r_{,2}r^{-2}\,h_{12}r^{-1}\,(1-uM) \\ &\quad +r^{-1}\left(h_{12}r^{-1}\right)_{,2}(1-uM)-u\,h_{12}r^{-1}\,M_{,2}r^{-1}\Big]. \end{aligned}$$

Using Proposition viii.1, viii.2, the hypothesis $\langle\sigma 2\rangle$ and the explicit expression for J, we obtain immediately that $G^{11}_{,1}$ and $2G^{11}F_{,1}$ tend to zero as $s\to\infty$. A similar analysis of the remaining term in Γ^1 is a slightly more complicated

$$\begin{aligned} &\lim_{s\to\infty}\left(G^{12}_{,2}+2G^{12}F_{,2}\right) \\ &\quad=\lim_{s\to\infty}\left\{2\,u\left[-r_{,2}r^{-2}\,h_{12}r^{-1}+r^{-1}\left(h_{12}r^{-1}\right)_{,2}\right]+2\,u\,r_{,2}r^{-2}\,h_{12}r^{-1}\right\} \\ &\quad=\lim_{s\to\infty}2\,u\,r^{-1}\left(h_{12}r^{-1}\right)_{,2}=-\lim_{s\to\infty}2\,u\,r_{,1}r^{-1}\,(k_s-k_\vartheta)=0. \end{aligned}$$

Summing up the results we obtain the second claim of Lemma viii.3. □

To finish these preliminaries, we find useful to execute the proof of the property (v.4) which estimates the perimeter

$$\langle r\rangle := \int_0^{2\pi} r(\cdot,\vartheta)\,d\vartheta \tag{viii.5}$$

of geodesic circles $p(\cdot,\vartheta)$ by means of its distance to the pole.

Lemma viii.4. *Assume* $\langle\Sigma 1\rangle$. *Then*

$$\forall s\in\mathbb{R}^+:\quad \langle r\rangle(s)\le C_\Sigma\,s\,,\qquad \textit{where}\qquad C_\Sigma:=2\pi+\|K\|_{g,1}$$

and $\|\cdot\|_{g,1}$ *denotes the norm in* $L^1(\Sigma_0,d\Sigma)$.

Proof: An integration of the Jacobi equation (viii.1) yields the estimate

$$\dot r(s,\vartheta)=\dot r(0,\vartheta)-\int_0^s K(\xi,\vartheta)\,r(\xi,\vartheta)\,d\xi\le 1+\int_0^\infty |K(\xi,\vartheta)|\,r(\xi,\vartheta)\,d\xi.$$

Therefore, $\int_0^{2\pi}\dot r(s,\vartheta)\,d\vartheta\le 2\pi+\|K\|_{g,1}$ and integrating this inequality w.r.t. s once more, we obtain the desired estimate

$$\int_0^{2\pi}\left(r(s,\vartheta)-r(0,\vartheta)\right)\,d\vartheta=\int_0^{2\pi}r(s,\vartheta)\,d\vartheta\le(2\pi+\|K\|_{g,1})\,s\,.$$

□

Remark. It is not needed to assume $\langle\Sigma 1\rangle$ in order to get an estimate on $\langle r\rangle(s)$ via the geodesic distance s. The inequality of the Lemma will hold with an unspecified constant C_Σ as well provided we suppose only that the total Gauss curvature *exists* and is *finite*. If $\langle\Sigma 1\rangle$ is not satisfied we mean by the integral of the Gauss curvature the principal value defined through the area restricted by the geodesic circle $p(s,\cdot)$ as $s\to\infty$. It can be seen by the following considerations. Integrating the Jacobi equation (viii.1) we obtain

$$f(s) := \int_0^{2\pi} \dot{r}(s,\vartheta)\,d\vartheta = 2\pi - \int_0^s d\xi \int_0^{2\pi} K(\xi,\vartheta)\,r(\xi,\vartheta)\,d\vartheta,$$

where the function $s\mapsto f(s)$ is certainly continuous since the surface is supposed to be C^2-smooth. This together with $f(0)=0$ and the fact that $\lim_{s\to\infty} f(s)$ is finite by assumption yields that f is uniformly bounded on $\mathbb{R}^+$ by some C_Σ and its primitive is therefore estimated by $C_\Sigma s$.

viii.1.2 Essential Spectrum

It is seen for instance from Theorem v.2 that the condition $\langle\Sigma 0\rangle$ is sufficient to ensure that $\inf\sigma_{\mathrm{ess}}(-\Delta_D^\Omega)\geq\kappa_1^2$. We shall now prove that the opposite inclusion, $\sigma_{\mathrm{ess}}(-\Delta_D^\Omega)\supset[\kappa_1^2,\infty)$, holds. The proof is based on the construction of an appropriate Weyl's sequence for H.

Theorem viii.5. *Assume* $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$, $\langle\Sigma 1\rangle$, *and suppose that* Σ *is* C^3*-smooth, possesses at least one pole and obeys* $\langle\Sigma 0\rangle$, $\langle\sigma 1\text{–}2\rangle$. *Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = [\kappa_1^2,\infty).$$

Proof: According to the Weyl criterion [55, Thm. 7.2], $\eta\in\sigma_{\mathrm{ess}}(H)$ if and only if there exists a Weyl sequence for H and η, *i.e.*, $\exists\{\psi_n\}\subset\mathrm{Dom}\,H$, such that $\|\psi_n\|_G=1$, $\psi_n\overset{w}{\longrightarrow}0$ and $(H-\eta)\psi_n\overset{s}{\longrightarrow}0$. In our case, we have to construct the sequence for $\eta=\lambda^2+\kappa_1^2$ with $\lambda\in\mathbb{R}$. We take the following radially symmetric family of functions

$$\left\{\hat{\psi}_n(s,u) := \varphi_n(s)\chi_1(u)\,e^{i\lambda s}\right\}_{n=1}^\infty,$$

where χ_1 is the lowest transverse-mode function (ii.8) and $\{\varphi_n\}$ is a sequnce of twice differentiable functions of compact supports which is localized at infinity for large n. It will be specified later. It is easy to verify that each of the functions belongs to the domain of H since it is C^2-differentiable and of a compact support. The sequence $\hat{\psi}_n$ is not normalized in $L^2(\Omega_0,d\Omega)$, so we introduce $\psi_n := \hat{\psi}_n/\|\hat{\psi}_n\|_G$ and we will show that this is a good Weyl sequence for our case. Taking into account (ii.4) together with $\langle\Omega 1\rangle$ and the normalization of χ_1, one has

$$C_-\|\varphi_n\|_g \leq \|\hat{\psi}_n\|_G \leq C_+\|\varphi_n\|_g \qquad \text{with} \qquad C_\pm := (1\pm a\rho_m^{-1})^2. \quad \text{(viii.6)}$$

The weak convergence $\psi_n \xrightarrow{w} 0$ means that $(\psi_n, \phi)_G \to 0$ for all $\phi \in \mathrm{Dom}\, H$. However, we do not need to check this property because if we show the strong convergence of our Weyl sequence ψ_n for all $\lambda \in \mathbb{R}$, we get that $[\kappa_1^2, \infty)$ belongs to the spectrum of H and then it follows immediately that $[\kappa_1^2, \infty) \subset \sigma_{\mathrm{ess}}(H)$ because intervals have no isolated points.

It remains to check the strong convergence now, *i.e.*, the limit $\|(H - (\lambda^2 + \kappa_1^2))\psi_n\|_G \to 0$ as $n \to \infty$. Employing the block form (ii.4) of G_{ij}, we can split H into a sum of two parts, $H = H_1 + H_2$, given by

$$H_1 := -G^{-\frac{1}{2}}\partial_\mu G^{\frac{1}{2}} G^{\mu\nu}\partial_\nu = -\partial_\mu G^{\mu\nu}\partial_\nu - 2F_{,\mu}G^{\mu\nu}\partial_\nu \qquad \text{(viii.7)}$$

$$H_2 := -G^{-\frac{1}{2}}\partial_3 G^{\frac{1}{2}}\partial_3 = -\partial_3^2 - 2\,\frac{Ku - M}{1 - 2Mu + Ku^2}\,\partial_3\,, \qquad \text{(viii.8)}$$

where we have used F introduced in Lemma viii.3 and expressed it explicitly for H_2. This decomposition leads to the bound

$$\left\|(H - (\lambda^2 + \kappa_1^2))\hat{\psi}_n\right\|_G \le \left\|(H_1 - \lambda^2)\hat{\psi}_n\right\|_G + \left\|(H_2 - \kappa_1^2)\hat{\psi}_n\right\|_G. \qquad \text{(viii.9)}$$

Denote $\|A\|_{\infty,n} := \sup\left\{A(s,\vartheta,u)\,\middle|\,(s,\vartheta,u) \in \mathrm{supp}\,\varphi_n \times S^1 \times I\right\}$. By virtue of (viii.8), (viii.6) and the Schwarz inequality together with $\|\chi_1'\|_{L^2(I)} = \kappa_1$, we have

$$\left\|(H_2 - \kappa_1^2)\hat{\psi}_n\right\|_G = \left\|2F_{,3}\varphi_n\chi_1'\right\|_G \le 2C_+\kappa_1\,\|F_{,3}\|_{\infty,n}\|\varphi_n\|_g.$$

Using (viii.6) once more, we obtain $\|(H_2 - \kappa_1^2)\psi_n\|_G \le 2C_+C_-^{-1}\kappa_1\|F_{,3}\|_{\infty,n}$, which goes to zero as $n \to \infty$ because of $\langle\Sigma 0\rangle$ as one can see from the explicit expression for $F_{,3}$ – see (viii.8).

Calculation of the first term of the right hand side of (viii.9) is a little more toilsome matter

$$\begin{aligned}\left\|(H_1 - \lambda^2)\hat{\psi}_n\right\|_G^2 &= \left\|\left(\lambda^2(1 - G^{11})\varphi_n + \Gamma^1\dot{\varphi}_n + G^{11}\ddot{\varphi}_n\right)\chi_1\right\|_G^2 \\ &\quad + \lambda^2\left\|\left(\Gamma^1\varphi_n + 2G^{11}\dot{\varphi}_n\right)\chi_1\right\|_G^2 \qquad \text{(viii.10)}\end{aligned}$$

with Γ^μ which was introduced in Lemma viii.3. Since

$$\|(1 - G^{11})\varphi_n\chi_1\|_G \le C_+\|1 - G^{11}\|_{\infty,n}\|\varphi_n\|_g,$$

and similarly for all the terms of the right hand side of (viii.10), it is enough to check the zero limit as $n \to \infty$ of the following expressions :

$$\left\|1 - G^{11}\right\|_{\infty,n}, \quad \left\|\Gamma^1\right\|_{\infty,n}, \quad \frac{\|\dot{\varphi}_n\|_g}{\|\varphi_n\|_g}, \quad \frac{\|\ddot{\varphi}_n\|_g}{\|\varphi_n\|_g}. \qquad \text{(viii.11)}$$

This is evident for the first two terms by virtue of Lemma viii.3 and the stated assumptions.

In order to treat the last two terms of (viii.11) we will specify the radial function φ_n. Employing the notation (viii.5) we can write

$\|\varphi_n\|_g = \|\varphi_n\langle r\rangle^{\frac{1}{2}}\|_+$, where $\|\cdot\|_+$ denotes the norm in $L^2(\mathbb{R}^+)$. Our aim is to eliminate the metric term in the integrals of this type since we do not suppose anything about its behaviour at infinity. This can be achieved by putting $\varphi_n := \langle r\rangle^{-\frac{1}{2}}\jmath_n$ which gives $\|\varphi_n\|_g = \|\jmath_n\|_+$. The family $\{\jmath_n\}$ is defined by $\jmath_n(s) := \jmath(n^{-1}s - n)$ where $\jmath$ is a C^∞-smooth function with a compact support in $(-1, 1)$. Notice that the definition of φ_n is meaningful because r^2 is the determinant of the surface metric tensor which is a positive definite matrix and so $\langle r\rangle \neq 0$ in all the interval $(0, \infty)$. Using now the triangle inequality together with the explicit formulae

$$\begin{aligned}
\dot\varphi_n\langle r\rangle^{\frac{1}{2}} &= \dot\jmath_n - \frac{1}{2}\frac{\langle r\rangle^{\cdot}}{\langle r\rangle}\jmath_n \\
\ddot\varphi_n\langle r\rangle^{\frac{1}{2}} &= \ddot\jmath_n - \frac{\langle r\rangle^{\cdot}}{\langle r\rangle}\dot\jmath_n + \left[-\frac{1}{2}\frac{\langle r\rangle^{\cdot\cdot}}{\langle r\rangle} + \frac{3}{4}\left(\frac{\langle r\rangle^{\cdot}}{\langle r\rangle}\right)^2\right]\jmath_n,
\end{aligned}$$

we get that the zero limit as $n \to \infty$ of the two last fractions of (viii.11) is achieved provided it is true for the following expressions

$$\left\|\frac{\langle r\rangle^{\cdot}}{\langle r\rangle}\right\|_{\infty,n}, \quad \left\|\frac{\langle r\rangle^{\cdot\cdot}}{\langle r\rangle}\right\|_{\infty,n}, \quad \frac{\|\dot\jmath_n\|_+}{\|\jmath_n\|_+}, \quad \frac{\|\ddot\jmath_n\|_+}{\|\jmath_n\|_+}. \tag{viii.12}$$

It is evident for the two last fractions because

$$\frac{\|\dot\jmath_n\|_+}{\|\jmath_n\|_+} = \frac{1}{n}\frac{\|\dot\jmath\|_{L^2(-1,1)}}{\|\jmath\|_{L^2(-1,1)}} \to 0, \qquad \frac{\|\ddot\jmath_n\|_+}{\|\jmath_n\|_+} = \frac{1}{n^2}\frac{\|\ddot\jmath\|_{L^2(-1,1)}}{\|\jmath\|_{L^2(-1,1)}} \to 0$$

as $n \to \infty$. At the same time, for all $s \in \operatorname{supp}\jmath_n$ on has

$$\left|\frac{\langle r\rangle^{\cdot}}{\langle r\rangle}\right| = \left|\frac{1}{\langle r\rangle}\left\langle\frac{\dot r}{r}\, r\right\rangle\right| \leq \left\|\frac{\dot r}{r}\right\|_{\infty,n}, \qquad \left|\frac{\langle r\rangle^{\cdot\cdot}}{\langle r\rangle}\right| = \left|\frac{1}{\langle r\rangle}\langle Kr\rangle\right| \leq \|K\|_{\infty,n},$$

where the right hand sides of the inequalities go to zero by the assumptions $\langle\sigma 2\rangle$ and $\langle\Sigma 0\rangle$. We have employed there $\langle r\rangle^{\cdot} = \langle\dot r\rangle$ and $\langle r\rangle^{\cdot\cdot} = \langle\ddot r\rangle$, which follow by the dominated convergence theorem whose assumptions are fulfilled due to $\langle\Sigma 1\rangle$ – *cf.* proof of Lemma viii.4. In the second term we have in addition expressed $\ddot r$ by means of K which follows from the Jacobi equation (viii.1). The theorem is proven. □

One could naturally ask whether one may get rid of the non-covariant condition $\langle\sigma 2\rangle$. Recall that while $\langle\sigma 1\rangle$ can be checked in any other parameterization of Σ, the condition $\langle\sigma 2\rangle$ requires the geodesic polar coordinates. In Section viii.3 we will see that $\langle\sigma 2\rangle$ is exactly the property which plays an important role in the study of the essential spectrum of complete and non-compact surfaces.

viii.1.3 Cylindrically Symmetric Layers

As an example of the situation when the non-covariant condition $\langle\sigma 1\rangle$ can be eliminated, let us now consider quantum layers which are endowed with a rotational symmetry w.r.t. a given axis in $\mathbb{R}^3$. In this case we profit from the fact that Σ is a surface of revolution parametrized by means of a chart which we know explicitly – *cf.* Section v.6. Using (v.17), one finds

$$|k_\vartheta| = \frac{\sqrt{1-\dot{r}^2}}{r}, \tag{viii.13}$$

where $s \mapsto \dot{r}(s)$ is a bounded function whose limit as $s \to \infty$ exists and it is contained in the interval $[0,1]$ – *cf.* (v.19). Denote the limit by $\dot{r}(\infty)$. Since the left hand side of the relation (viii.13) must tend to zero as $s \to \infty$ due to $\langle\Sigma 0\rangle$, we arrive at the two possible situations. If $\dot{r}(\infty) \neq 1$, then the function r tends necessarily to infinity and therefore $k_g = \dot{r}r^{-1} \to 0$ as $s \to \infty$. On the other hand, the case $\dot{r}(\infty) = 1$ corresponds to $\mathcal{K} = 0$ when the fact $r \to \infty$ as $s \to \infty$ follows by the general Lemma viii.11. Summing up these considerations we obtain as a corollary of Theorem viii.5 the following result.

Theorem viii.6. *Assume* $\langle\Omega 0\rangle$, $\langle\Omega 1\rangle$, $\langle\Sigma 1\rangle$, *and suppose that* Σ *is a* C^3*-smooth asymptotically planar surface of revolution which obeys in addition* $\langle\sigma 1\rangle$. *Then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = [\kappa_1^2, \infty).$$

viii.1.4 Addendum. Partial Wave Decomposition

If the layer Ω is cylindrically symmetric one can decompose the Hamiltonian $-\Delta_D^\Omega$ with respect to angular momentum subspaces. We describe the decomposition even if does not seem to bring onto the problems. There are two possible approaches.

Reconstruction of the Layer via the Profile Curve

It is more efficient to go back to the initial operator $-\Delta_D^\Omega$ and start with Cartesian coordinates of the ambient space $\mathbb{R}^3$ rather than treat the Hamiltonian H expressed in the intrinsic coordinates (q,u). Suppose that the layer Ω is invariant under rotations in $\mathbb{R}^3$ around the axis x^3. Let Ω^+ be its axial half-section, $\Omega^+ := \{(x^1,x^2,x^3) \in \Omega \,|\, x^1 \geq 0 \;\&\; x^2 = 0\}$, and $\mathcal{B} := \partial\Omega \cap \Omega^+$ its boundary without the x^3-axis segment. Introducing cylindrical coordinates, $(x^1,x^2) =: (\rho\cos\vartheta, \rho\sin\vartheta)$, we decompose the Hilbert space $L^2(\Omega)$ into $L^2(\Omega^+, \rho\,d\rho\,dx^3) \otimes L^2(S^1)$, and using in addition the unitary transformation from $L^2(\Omega^+, \rho\,d\rho\,dx^3)$ to $L^2(\Omega^+)$ acting as $\psi \mapsto \rho^{\frac{1}{2}}\psi$, we obtain

that $-\Delta_D^\Omega$ is unitarily equivalent to the direct sum

$$\bigoplus_{m\in\mathbb{Z}} H_m \qquad \text{with} \qquad H_m := -\partial_\rho^2 - \partial_{x^3}^2 + \frac{m^2-1/4}{\rho^2} \qquad \text{on} \quad L^2(\Omega^+).$$

Define $\mathcal{H}_m := \big\{\psi \in W^{2,2}(\Omega^+) \,|\, H_m\psi \in L^2(\Omega^+) \;\&\; \psi \restriction \mathcal{B} = 0\big\}$ for $m \in \mathbb{Z}$. All the H_m, $m \in \mathbb{Z}\setminus\{0\}$, are self-adjoint with $\mathrm{Dom}\, H_m := \mathcal{H}_m$ – *cf.* [76, Chap. X] – whereas for H_0 we choose the self-adjoint extension – *cf.* [1, App.D] – arising naturally due to the regularity conditions assumed at $\rho=0$:

$$\mathrm{Dom}\, H_0 := \mathcal{H}_0 \cap \Big\{\psi \in L^2(\Omega^+) \,\Big|\, \lim_{\rho\to 0} \psi(\rho,\cdot)/(\rho^{\frac12}\ln\rho) = 0\Big\}.$$

In the next step we introduce the curvilinear coordinates (s,u) by means of the equations

$$\rho = r(s) - u\,\dot z(s), \qquad\qquad x^3 = z(s) + u\,\dot r(s),$$

where r, z are C^2-smooth functions that characterize the profile curve of the surface Σ – *cf.* the notation introduced in the beginning of Section v.6. We assume $\dot r^2 + \dot z^2 = 1$ which means that s is the arc length of the curve, while u measure the distance to the point (ρ, x^3). We put $k_s := \dot r\ddot z - \ddot r\dot z$ which is the meridian curvature of Σ or (up to sign) the signed curvature used in [40, 22]. In fact, it is sufficient to know the function $s \mapsto k_s(s)$ only, since r, z can be constructed from the relations (v.18). Denote $\Omega_0^+ := \mathbb{R}^+ \times I$, $\tilde g := (1-uk_s)^2$ and $d\tilde g := \tilde g^{\frac12} ds du$. Translating the action of H_m into the curvilinear coordinates (s,u) we can write the partial-wave operators on the straightened half-strip Ω^+

$$\tilde H_m := -\tilde g^{-\frac12}\partial_s \tilde g^{-\frac12}\partial_s - \tilde g^{-\frac12}\partial_u \tilde g^{\frac12}\partial_u + \frac{m^2-1/4}{\rho(s,u)^2} \qquad \text{on} \quad L^2(\Omega_0^+, d\tilde g).$$

Define $\tilde{\mathcal{H}}_m := \big\{\psi \in W^{2,2}(\Omega_0^+, d\tilde g) \,|\, H_m\psi \in L^2(\Omega_0^+, d\tilde g) \;\&\; \psi(\cdot,\pm a) = 0\big\}$. We thus have $\mathrm{Dom}\, \tilde H_m = \tilde{\mathcal{H}}_m$ if $m \in \mathbb{Z}\setminus\{0\}$ and

$$\mathrm{Dom}\, \tilde H_0 = \tilde{\mathcal{H}}_0 \cap \Big\{\psi \in L^2(\Omega_0^+, d\tilde g) \,\Big|\, \lim_{s\to 0} \psi(s,\cdot)/(s^{\frac12}\ln s) = 0\Big\}.$$

The boundary condition on the x^3-axis segment follows by $\langle\Omega 1\rangle$ and the observation that $\rho = r(1-uk_\vartheta)$, where k_ϑ is the normal curvature of parallels. One uses at the same time the small value behaviour, $r(s) \sim s$, which holds true due to the integral representation (v.18) or the Jacobi equation (viii.1).

The obtained series of Hamiltonians $\{H_m\}_{m\in\mathbb{Z}}$ have similar form as the pure strip Hamiltonian – *cf.* [40, 22] – except the additional centrifugal term and the boundary condition for $m = 0$. This, however, make the spectral analysis of layers more complicated than a direct use of the non-decomposed Hamiltonian H. For instance, we cannot take the function $\varphi(s)\chi_1(u)$ with $\varphi \equiv 1$

for the generalized annulator of the quadratic form corresponding to $\tilde{H}_0$ as one does in [22, Thm. 2.1] in order to demonstrate the existence of bound states because this function does not fulfils the boundary condition at $s = 0$. On the other hand, if we modified φ at the origin we would get a nontrivial contribution to the value of the quadratic form coming from the derivatives w.r.t. s.

Unitary Transformation of H

Let us now show how to obtain the precedent result directly within the concept of the operator H. We refer to Section v.6 for the notation employing here. At the same time, we use $\tilde{g} \equiv (1 - uk_s)^2$ and $\rho \equiv r(1 - uk_\vartheta)$ as introduced a few lines above. Employing the fact that the surface geometrical quantities do not depend on ϑ and that $(G_{ij}) = \mathrm{diag}(\tilde{g}, \rho^2, 1)$, the formula (ii.6) for H yields

$$H = -\rho^{-1}\tilde{g}^{-\frac{1}{2}}\partial_s\rho\,\tilde{g}^{-\frac{1}{2}}\partial_s - \rho^{-1}\tilde{g}^{-\frac{1}{2}}\partial_u\rho\,\tilde{g}^{\frac{1}{2}}\partial_u - \rho^{-2}\partial_\vartheta^2\,.$$

Introducing the unitary transformation

$$\tilde{U} : L^2(\Omega_0, G^{\frac{1}{2}}d^2qdu) \to L^2(\Omega_0, \tilde{g}^{\frac{1}{2}}d^2qdu) : \left\{\psi \mapsto \rho^{\frac{1}{2}}\psi\right\},$$

it is seen immediately that the corresponding unitarily equivalent operator $\tilde{H} := \tilde{U}H\tilde{U}^{-1}$ is given by

$$\tilde{H} = -\tilde{g}^{-\frac{1}{2}}\partial_s\tilde{g}^{-\frac{1}{2}}\partial_s - \tilde{g}^{-\frac{1}{2}}\partial_u\tilde{g}^{\frac{1}{2}}\partial_u + v_s + v_u - \rho^{-2}\partial_\vartheta^2\,,$$

where the potentials v_s and v_u are obtained by commuting $\rho^{-\frac{1}{2}}$ with the corresponding partial derivative operators. One has

$$\begin{aligned} v_s &:= \frac{1}{2\tilde{g}^2}\left[\frac{\rho_{,ss}}{\rho} - \frac{\rho_{,s}\tilde{g}_{,s}}{\rho\tilde{g}} - \frac{1}{2}\left(\frac{\rho_{,s}}{\rho}\right)^2\right] \\ v_u &:= \frac{1}{2}\left[\frac{\rho_{,uu}}{\rho} + \frac{\rho_{,u}\tilde{g}_{,u}}{\rho\tilde{g}} - \frac{1}{2}\left(\frac{\rho_{,u}}{\rho}\right)^2\right] \end{aligned}, \qquad v_s + v_u = -\frac{1}{4\rho^2}\,,$$

where the last relation is established by an explicit and tedious computation. Since $\sigma(-\partial_\vartheta^2) = \mathbb{Z}^2$, the Hamiltonian H_m admits the direct sum decomposition given by the operators $\tilde{H}_m$ introduced in the precedent approach.

viii.2 Curved Strips

Let us make a few remarks upon quantum strips in the plane which represent the one-dimensional analogy of our layers. Although these systems are already well studied in many papers in order to establish the existence

of bound states – *cf.* Section i.3.1 – in context of this chapter we find useful to review the question of their essential spectrum.

Let Σ be now a C^3-smooth curve in $\mathbb{R}^2$ which is complete, non-compact and simple. Without loss of generality we may assume that it is parametrized by its arc length s via a mapping $p : \mathbb{R} \to \mathbb{R}^2$. Let n be the unique normal vector field along Σ such that $\{\dot{p}, n\}$ forms the Frenet frame. We define the strip Ω as the usual tubular neighbourhood [50] of Σ

$$\mathcal{L} : \Omega_0 \to \mathbb{R}^2 : \{(s,u) \mapsto p(s) + un(s)\}, \qquad \mathcal{L}(\Omega_0) =: \Omega, \tag{viii.14}$$

where $\Omega_0 := \mathbb{R} \times I$. Notice that $s \mapsto \mathcal{L}(s,u)$ traces a parallel curve at a distance $|u|$ from Σ. Using the Frenet equations one finds easily the metric tensor of the strip

$$(G_{ij}) := (\mathcal{L}_{,i} \,.\, \mathcal{L}_{,j}) = \begin{pmatrix} (1-u\kappa)^2 & 0 \\ 0 & 1 \end{pmatrix}, \tag{viii.15}$$

where $s \mapsto \kappa(s)$ is the curvature function which up to the embedding fully determines the curve Σ. We assume here the range of Latin indices being $1, 2$ and use the association $(1,2) \leftrightarrow (s,u)$.

We could now perform the same analysis as for layers, however, it is worth to realize that we can obtain the results in the strip case immediately by a simple suppression of one dimension of the surface as the reference manifold. This can be achieved formally by putting one of their principal curvatures equals identically zero. The second one will then coincide with the curvature κ which actually represents in this way the lower dimensional analogy of the Weingarten tensor. Following this analogy, one get that the mapping $\mathcal{L} : \Omega_0 \to \Omega$ will be a diffeomorphism provided

$\boxed{\langle \Omega 0 \rangle \quad \Omega \text{ is not self-intersecting}}$ and $\boxed{\langle \Omega 1 \rangle \quad a < \|\kappa\|_\infty^{-1}}$

The condition $\langle \Sigma 1 \rangle$ does not enter in this concept because the Gauss curvature, $K = k_+ k_-$, is identically equal to zero; from (viii.1) it follows also that $r = 1$. The decay hypotheses $\langle \Sigma 0 \rangle$ and $\langle \sigma 1\text{–}2 \rangle$ reduce to

$\boxed{\langle \Sigma 0 \rangle \quad \kappa \to 0}$ and $\boxed{\langle \sigma 1 \rangle \quad \dot{\kappa} \to 0}$ as $|s| \to \infty$.

Notice that the condition on existence of at least one pole on the surface is for curves automatically fulfilled because they can be always parametrized by arc length. Using Theorem v.2, v.3 and viii.5, we may summarize the analogous results concerning quantum strips in the following.

Theorem viii.7 (Quantum Strips, revisited).
Assume $\langle \Omega 0 \rangle$ and $\langle \Omega 1 \rangle$, and suppose that the curve Σ is C^2-smooth and it is not straight. Then

$$\inf \sigma(-\Delta_D^\Omega) < \kappa_1^2. \tag{viii.16}$$

If the curve is asymptotically straight $\langle \Sigma 0 \rangle$*, then*

$$\inf \sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) \geq \kappa_1^2 \tag{viii.17}$$

and the first result implies that the discrete spectrum of $-\Delta_D^{\Omega}$ *below* κ_1^2 *is not empty. Moreover, if* Σ *is* C^3*-smooth and obeys in addition* $\langle \sigma 1 \rangle$*, then*

$$\sigma_{\mathrm{ess}}(-\Delta_D^{\Omega}) = [\kappa_1^2, \infty). \tag{viii.18}$$

Let us compare this theorem with results of the papers [22, 78]. We suppose in fact that the curvature κ is a C^0-function in order to obtain the first inequality (viii.16), however, it would be enough to assume only that it is piecewise continuous, *i.e.*, that the curve Σ is piecewise C^2-smooth. The reason is that the latter hypothesis is sufficient for a proper definition of the quadratic form (ii.7). The authors of [78] assume that κ is twice continuously differentiable but just outside a bounded interval, while the proof of [22, Thm. 2.1] requires to assume that κ and $\dot{\kappa}$ are locally integrable. On the other hand, we obtain the estimate (viii.17) on the threshold of the essential spectrum only under the assumption $\langle \Sigma 0 \rangle$ and this is a remarkable simplification because, contrary to [22, 78], no decay conditions for the derivatives of κ are required. Our third claim (viii.18) is a new result. Recall finally how the assumption $\langle \Omega 1 \rangle$ is weakened in the concept of [78]. We restrict the width of the strip in such a way that $1 - a\|\kappa\|_\infty > 0$ holds, while they require this strict inequality only with the norm where the supremum is taken over the complement of a bounded interval in the real axis and admit the equality $1 - a|\kappa(s)| = 0$ inside of this interval. Their generalization is justified by the fact that the transverse region I is an open interval and therefore the assumption $1 - a|\kappa(s)| \geq 0$ is sufficient for the strict inequality $1 - u|\kappa(s)| > 0$ which we need actually to ensure that $\mathcal{L} : \Omega_0 \to \Omega$ is an immersion.

viii.3 Complete Manifolds

Let us mention briefly some of the characteristic results which are known in the spectral theory of complete manifolds and which seem to us to be interesting in the context of this thesis. For a general exposition of spectral geometry we refer to [16] which provides instructional lectures together with an extensive bibliography to the subject.

Much of the efforts concern compact manifolds for which the spectrum is purely discrete [12]. In the non-compact case the work has centered on manifolds with a prescribed sign of the curvature. For instance, a self-contained discussion of the spectra of hyperbolic manifolds which have constant negative curvature is performed in [54]. We are rather interested in cases when the curvature varies. Escobar [25] has proven that if the manifold has a rotationally invariant metric of non-negative radial sectional curvature, then

the spectrum is $[0, \infty)$ and it does not have eigenvalues. The absence of eigenvalues was established in [20] also for non-positive curvature. Escobar's result holds as well if the radial symmetry condition is replaced by the hypothesis on the existence of a pole on the manifold, the sectional curvatures are non-negative and an additional condition on integrability of the Ricci curvature is assumed [26]. The first part of the result is true just under the assumption that the manifold possesses a pole and the Ricci curvature is non-negative [67]. The paper by Donnelly [19] establishes these facts by means of some asymptotic geometric hypotheses imposed on the exhaustion function of the manifold. In particular, one concludes that also the manifolds with a pole, non-positive sectional curvature and slow volume growth has the interval $[0, \infty)$ as the spectrum.

To the best of our knowledge, if the curvature has variable sign there does not exist a simple geometric hypothesis to ensure that all the positive real axis belongs to the spectrum. In Section viii.3.2 we contribute to this problem by proving this result under the assumption that the manifold is rotationally symmetric and the radial sectional curvature tends to zero at infinity. In Section viii.3.3 we focus on the particular case of dimension two, *i.e.*, on surfaces. We show that if the surface possesses a pole, than the decay of the Gauss curvature together with the condition $\langle \sigma 2 \rangle$ are sufficient to guarantee that $[0, \infty)$ forms the spectrum of the Laplace-Beltrami operator.

viii.3.1 The Laplacian

Let Σ be a C^2-smooth complete Riemannian manifold of dimension n. Denote by $-\Delta_g$ the Laplace-Beltrami operator on Σ associated to a metric g_{ij}. Since it follows for instance by [13] that this operator is essentially self-adjoint on $C_0^\infty(\Sigma)$, the Friedrichs extension defines a unique self-adjoint extension, also denoted $-\Delta_g$, to an unbounded operator on $L^2(\Sigma)$. Moreover, domain of the latter consists of those $\psi \in L^2(\Sigma)$ such that $-\Delta_g \psi \in L^2(\Sigma)$ in the sense of distributions – *cf.* [48].

Assume for simplicity that Σ is diffeomorphic to $\mathbb{R}^n$ and one thus disposes of global coordinates $(q^1, \ldots, q^n) \in \mathbb{R}^n$ defined by a unique chart $p : \mathbb{R}^n \to \Sigma$. Denote by g_{ij} and g the corresponding Riemannian metric and its determinant, respectively, which are supposed to be functions of q^i. Using these coordinates, the Laplacian $-\Delta_g$ can be identified with the operator

$$H := -g^{-\frac{1}{2}} \partial_i g^{\frac{1}{2}} g^{ij} \partial_j \qquad \text{on} \qquad L^2(\mathbb{R}^n, d\Sigma) \tag{viii.19}$$

where as usual $\partial_i \equiv \partial / \partial q^i$ and $d\Sigma = g^{\frac{1}{2}} d^n q$ denotes the volume element of the manifold.

Hereafter we shall always assume that Σ possesses at least one pole. Note that such a manifold is necessarily complete and diffeomorphic to $\mathbb{R}^n$ and as such it is simply connected and non-compact. In the geodesic polar

coordinates $(s, \vartheta) \in \mathbb{R}^+ \times S^{n-1}$ the metric tensor can be written as [57, Thm. 1.4.5]

$$(g_{ij}) = \begin{pmatrix} 1 & 0 \\ 0 & (\Omega_{\mu\nu}) \end{pmatrix}, \tag{viii.20}$$

where $\Omega_{\mu\nu}(s, \vartheta)$ are components of an $(n-1) \times (n-1)$ matrix which correspond to angular variables $\vartheta := (\vartheta^1, \ldots, \vartheta^{n-1})$.

viii.3.2 Radially Symmetric Case

Let Σ be a C^3-smooth complete simply connected non-compact manifold which is rotationally symmetric. This means that one can write

$$\Omega_{\mu\nu}(s, \vartheta) = r(s)^2 \, \omega_{\mu\nu}(\vartheta), \tag{viii.21}$$

where $\omega_{\mu\nu}$ is the metric of the $(n-1)$-dimensional unit sphere S^{n-1}. The function r satisfies the Jacobi equation (viii.1) where $s \mapsto K(s)$ is the radial curvature which has to be understood as the sectional curvature of the geodesic surface which contains the radial geodesic line and is tangent to the Jacobi field along the line – *cf.* proof of Corollary 2.13 in [51].

Partial Wave Decomposition

The Laplace-Beltrami operator (viii.19) in the coordinates (s, ϑ) acquires the form

$$H = -\partial_1^2 - 2f_{,1}\partial_1 - \frac{1}{r^2}\,\Delta^{S^{n-1}}, \tag{viii.22}$$

where $f := \ln g^{\frac{1}{4}} = \ln r^{\frac{n-1}{2}} + \ln \omega^{\frac{1}{4}}$ with $\omega := \det(\omega_{\mu\nu})$, and $\Delta^{S^{n-1}}$ denotes the Laplacian for the ordinary unit sphere S^{n-1}. The operator (viii.22) acts on

$$\mathcal{H} := L^2(\mathbb{R}^+ \times S^{n-1}, d\Sigma) \qquad \text{with} \qquad d\Sigma = r^{n-1}\omega \, ds \, d^{n-1}\vartheta.$$

Since $\sigma(-\Delta^{S^{n-1}}) = \{\ell(\ell+n-2) | \, \ell \in \mathbb{N}\}$, the Hilbert space $\mathcal{H}$ admits a direct sum decomposition $\mathcal{H} = \oplus_\ell \mathcal{H}_\ell$, where $\mathcal{H}_\ell := L^2(\mathbb{R}^+, r^{n-1}ds) \otimes \mathcal{V}_\ell$ is an $\mathrm{SO}(n)$-invariant subspace and, for each ℓ, $\mathcal{V}_\ell$ is a finite-dimensional carrier space for the appropriate representation of $\mathrm{SO}(n)$. Consequently, H is unitarily equivalent to

$$\bigoplus_{\ell=0}^{\infty} H_\ell \qquad \text{with} \qquad H_\ell := -\partial_1^2 - 2f_{,1}\partial_1 + \frac{\ell(\ell+n-2)}{r^2} \qquad \text{on} \quad \mathcal{H}_\ell.$$

Each H_ℓ is unitarily equivalent to the operator

$$\hat{H}_\ell := r^{\frac{n-1}{2}} \, H_\ell \, r^{-\frac{n-1}{2}} = -\partial_1^2 + V + \frac{\ell(\ell+n-2)}{r^2} \qquad \text{on} \qquad L^2(\mathbb{R}^+, ds)$$

with the potential

$$V := f_{,11} + {f_{,1}}^2 = -\frac{n-1}{2}\,K + \frac{(n-1)(n-3)}{4}\left(\frac{\dot r}{r}\right)^2. \qquad \text{(viii.23)}$$

We have employed here the relation $K = -\ddot r r^{-1}$ which follows by (viii.1).

First of all we note that H has positive spectrum because it is a positive operator. We want to show that, under some condition, the spectrum is the whole interval $[0,\infty)$. Since the spectrum of a direct sum of self-adjoint operators is given by the sum of the individual spectra – *cf.* Corollary of Theorem VIII.33 in [75] – it is sufficient to show that $\sigma(H_\ell) = [0,\infty)$ for some ℓ. We will do it for $\ell = 0$.

Remarks on Schrödinger Operators on the Half Line

We will need the following result of the theory of Schrödinger operators.

Proposition viii.8. *Let $H = -\partial_s^2 + V(s)$ on the Hilbert space $L^2(\mathbb{R}^+, ds)$ be self-adjoint and such that $C_0^\infty((0,\infty)) \subset \operatorname{Dom} H$. Suppose that there exist positive sequences $\{s_n\}_{n=1}^\infty$ and $\{b_n\}_{n=1}^\infty$ where the latter is strictly increasing such that*

$$\exists c \geq 0: \qquad \sup_{s\in(s_n, s_n+b_n)} |V(s)| < \frac{c}{n}.$$

Then $[0,\infty) \subset \sigma_{\mathrm{ess}}(H)$.

Proof: Let $\jmath \in C_0^\infty((-1,1))$ be normalize in $L^2(\mathbb{R})$. We define

$$\jmath_n(s) := \sqrt{\frac{2}{b_n}}\,\jmath\left(\frac{s-(s_n+b_n/2)}{b_n/2}\right),$$

which has then unit norm in $L^2(\mathbb{R}^+)$ and is infinitely smooth with a compact support localized in $(s_n, s_n+b_n) \subset \mathbb{R}^+$. Consequently, $\psi_n(s) := \jmath_n(s)\, e^{i\lambda s}$ with $\lambda \in \mathbb{R}$ belongs to $\operatorname{Dom} H$ and $\|\psi_n\| = 1$. We will show that $\{\psi_n\}$ is a Weyl sequence for H and λ^2 which establishes the inclusion $[0,\infty) \subset \sigma_{\mathrm{ess}}(H)$. Actually, it is sufficient to show that $(H-\lambda^2)\psi_n$ converges strongly to 0 as $n\to\infty$ for an arbitrary λ, because then $[0,\infty)$ is contained in the spectrum. However, the interval has no isolated points, so it must be from the essential spectrum. Since

$$\|(H-\lambda^2)\psi_n\| \leq \|\ddot\jmath_n + 2i\lambda\dot\jmath_n\| + \|V\jmath_n\| \leq \|\ddot\jmath_n\| + 2|\lambda|\,\|\dot\jmath_n\| + \frac{c}{n}$$

and the derivatives of $\jmath_n$ are decreasing sequences with

$$\|\dot\jmath_n\| = \frac{2}{b_n}\,\|\dot\jmath\| \qquad \text{and} \qquad \|\ddot\jmath_n\| = \left(\frac{2}{b_n}\right)^2 \|\ddot\jmath\|,$$

we get $\|(H-\lambda^2)\psi_n\| \to 0$ as $n\to\infty$ by assumption. □

Corollary viii.9. *If $V \to 0$ as $s \to \infty$, then $[0, \infty) \subset \sigma_{\mathrm{ess}}(H)$.*

PROOF: The zero limit of V means that for all $n \in \mathbb{N}\backslash\{0\}$ there exists $s_n > 0$ such that $|V| < n^{-1}$ provided $s > s_n$ and it is sufficient to choose, for example, $b_n := n$. □

Remarks on the Jacobi Equation

For a further use, we define an analogy of the total Gauss curvature of surfaces

$$\mathcal{K} := |S^{n-1}| \int_{\mathbb{R}^+} K(s)\, r(s)\, ds, \tag{viii.24}$$

where $|S^{n-1}|$ denotes the volume of the $(n-1)$-sphere. If Kr does not belong to $L^1(\mathbb{R}^+)$ we mean by (viii.24) the limit as $N \to \infty$ from the corresponding integral over $[0, N]$. If the limit makes sense we then say "$\mathcal{K}$ exists". Integrating the Jacobi equation (viii.1), we get

$$\mathcal{K} + |S^{n-1}|\, \dot{r}(\infty) = |S^{n-1}|. \tag{viii.25}$$

Here $\dot{r}(\infty)$ denotes the limit of $\dot{r}$ as $s \to \infty$ which necessarily exists because we assume existence of the total curvature. Moreover, we have

Lemma viii.10. *Suppose that the total curvature $\mathcal{K}$ exists. Then $\dot{r}(\infty) \geq 0$.*

PROOF: Let $\dot{r}(\infty) < 0$. By the definition of the limit

$$\forall \varepsilon > 0\ \exists s_0 > 0 :\ s > s_0 \Rightarrow |\dot{r}(s) - \dot{r}(\infty)| < \varepsilon \tag{viii.26}$$

we get also $\dot{r}(s) < \dot{r}(\infty) + \varepsilon$ for $s > s_0$, and one can estimate

$$r(s) = r(s_0) + \int_{s_0}^{s} \dot{r}(\xi)\, d\xi < r(s_0) + (\dot{r}(\infty) + \varepsilon)\,(s - s_0).$$

We choose ε so small that $\dot{r}(\infty) + \varepsilon < 0$ and fix s_0. Clearly, $r(s)$ becomes negative as $s \to \infty$ contradicting the non-negativity of r. □

As an interesting consequence of this lemma and (viii.25) we obtain

$$\mathcal{K} \leq |S^{n-1}|.$$

If the inequality holds strictly, we may deduce the following asymptotic behaviour of r as $s \to \infty$.

Lemma viii.11. $\mathcal{K} < |S^{n-1}| \Rightarrow r(\infty) = \infty$.

PROOF: It follows from (viii.25) that the hypothesis $\mathcal{K} < |S^{n-1}|$ is equivalent to the statement that $\dot{r}(\infty)$ is strictly positive. By virtue of (viii.26) we have $\dot{r}(s) > \dot{r}(\infty) - \varepsilon$ for $s > s_0$, and by the same trick as in the proof of the precedent lemma, $r(s) > r(s_0) + (\dot{r}(\infty) - \varepsilon)\,(s - s_0)$. Now, if we choose ε so small that $\dot{r}(\infty) - \varepsilon$ is positive and fix s_0, we get $r(s) \to \infty$ as $s \to \infty$. □

The Spectrum

We are now ready to prove the following result.

Theorem viii.12. *Let Σ be a complete simply connected non-compact and rotationally symmetric manifold of class C^3. Suppose that its total curvature $\mathcal{K}$ exists. If $K \to 0$ as $s \to \infty$, then*

$$\sigma(-\Delta_g) = \sigma_{\mathrm{ess}}(-\Delta_g) = [0, \infty).$$

PROOF: It is sufficient to show that $\sigma_{\mathrm{ess}}(H_0) = [0, \infty)$. Since the Laplace-Beltrami operator is positive, the claim will follow by Proposition viii.8. The first term in the manifold potential (viii.23) decays to zero at infinity by assumption, so it is enough to investigate the function $\dot{r}r^{-1}$. We will consider all the possibilities step by step.

A : $\underline{-\infty < \mathcal{K} < |S^{n-1}|}$. By virtue of (viii.25) this assumption is equivalent to $0 < \dot{r}(\infty) < \infty$. Lemma viii.11 yields that $\dot{r}r^{-1} \to 0$ as $s \to \infty$ and the claim follows by Corollary viii.9.

B : $\underline{\mathcal{K} = -\infty}$. Now $\dot{r}(\infty) = \infty$ and since also $r(\infty) = \infty$ by Lemma viii.11, we employ the l'Hospital rule to control the asymptotic behaviour of $\dot{r}r^{-1}$:

$$\lim_{s\to\infty} \frac{\dot{r}(s)^2}{r(s)^2} = \lim_{s\to\infty} \frac{\ddot{r}(s)}{r(s)} = -\lim_{s\to\infty} K(s) = 0.$$

In the second equality we have used the relation between K and r given by the Jacobi equation (viii.1). Since again $V \to 0$ as $s \to \infty$ we use Corollary viii.9.

C : $\underline{\mathcal{K} = |S^{n-1}|}$. This case corresponds to $\dot{r}(\infty) = 0$. There are three particular situations which can occur. The first two when $0 < r(\infty) \leq \infty$ or $r(\infty) = 0$ can be treated in the same way as in the cases A or B, respectively. The remaining situation when $r(\infty)$ may not exist requires a special attention. Actually, only the situation

$$r(\underline{\infty}) := \liminf_{s\to\infty} r(s) = 0 \tag{viii.27}$$

may cause problems because otherwise $\dot{r}r^{-1} \to 0$ as $s \to \infty$. If (viii.27) occurs we choose a number $\tilde{r}$ which is squeezed between the extremal limit points in the following way : $0 = r(\underline{\infty}) < \tilde{r} < r(\overline{\infty}) \leq \infty$. There exists necessarily an increasing sequence of positive numbers $\{s_n\}_{n=1}^{\infty}$ such that $r(s_n) = \tilde{r}$. At the same time, as a consequence of (viii.26), we have

$$\forall n \in \mathbb{N}\setminus\{0\}\ \exists s_0 > 0 :\ s > s_0 \Rightarrow |\dot{r}(s)| < \frac{1}{n}.$$

We choose n_0 large enough to have $s_n > s_0$ for $n > n_0$. Then putting $b_n := \tilde{r}n/2$ for $n > n_0$ we get

$$\forall s \in (s_n, s_n + b_n) : \quad |\dot{r}(s)| < \frac{1}{n} \qquad \text{and} \qquad \frac{\tilde{r}}{2} < r(s) < \frac{3\tilde{r}}{2}$$

where the stated estimates can be seen from

$$r(s) = r(s_n) + \int_{s_n}^{s} \dot{r}(\xi)\, d\xi \lesseqgtr \tilde{r} \pm \frac{s - s_n}{n} \lesseqgtr \tilde{r} \pm \frac{\tilde{r}}{2}.$$

Now one uses Proposition viii.8. □

viii.3.3 Surfaces

Suppose now that $n = 2$, *i.e.*, Σ is a surface. We need not to assume here a rotationally symmetric case, however, we still require the existence of at least one pole on Σ. The expression (viii.22) for H holds again in this situation, just one cannot proceed with the partial wave decomposition. We can now construct a Weyl sequence $\{\psi_n := \hat{\psi}_n / \|\hat{\psi}_n\|_g\}$ for H and all λ^2 from $[0, \infty)$ by using the family of radially symmetric functions $\hat{\psi}_n(s) := \varphi_n(s)\, e^{i\lambda s}$, where the localized function φ_n is defined in the same way as in the proof of Theorem viii.5. Since

$$\left\| (H - \lambda^2)\hat{\psi}_n \right\|_g^2 = \int_\Sigma \left[4\lambda^2 \left(f_{,1}\, \varphi_n + \dot{\varphi}_n \right)^2 + \left(2 f_{,1}\, \dot{\varphi}_n + \ddot{\varphi}_n \right)^2 \right] d\Sigma$$

and $2 f_{,1} = \dot{r} r^{-1} \equiv k_g$, we obtain the following result by mimicking the proof of Theorem viii.5.

Theorem viii.13. *Let Σ be a C^3-smooth surface which possesses a pole. Assume $\langle \Sigma 1 \rangle$. If k_g and K tend to zero as $s \to \infty$, then*

$$\sigma(-\Delta_g) = \sigma_{\mathrm{ess}}(-\Delta_g) = [0, \infty).$$

The condition $K \to 0$ as $s \to \infty$ means that the surface is *asymptotically flat*. It is natural to assume this because the model case is the flat space $\mathbb{R}^2$ for which the spectrum is the half line $[0, \infty)$ and there are no eigenvalues. We have seen in Section viii.3.2 that it is possible to get rid of the non-covariant hypothesis $\langle \sigma 2 \rangle$ if the surface is endowed with the radial symmetry.

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Résumé

Nous étudions les propriétés spectrales des *guides d'ondes quantiques bidimensionnels* qui constituent un modèle raisonnable pour la dynamique quantique non-relativiste d'une particule dans les films conducteurs déposés sur une surface isolante. Mathématiquement, il s'agit du laplacien Dirichlet dans un voisinage tubulaire d'épaisseur constante construit autour d'une surface non-compacte plongée dans $\mathbb{R}^3$. Sous des hypothèses appropriées sur la décroissance des courbures de la surface à l'infini, nous localisons le spectre essentiel et fournissons des conditions suffisantes variées garantissant l'existence des états liés quantiques dûs à la géométrie. De plus, si la surface de référence est un plan courbé faiblement, nous trouvons le développement asymptotique de l'unique valeur propre correspondante par rapport au paramètre décrivant ce couplage faible. Nous établissons un développement limité d'une valeur propre aussi dans les guides d'ondes bidimensionnels droits mais avec une frontière déformée localement par des bosses et des creux. Cette thèse contient à la fin une étude du spectre d'une variété non-compacte générale qui possède au moins un pôle. Nous nous concentrons sur les variétés à symétrie radiale et les surfaces. Dans ces cas particuliers, nous montrons que le spectre est tout l'axe réel positif en posant certaines conditions supplémentaires sur la décroissance des courbures à l'infini.

Mots-Clés : Guides d'ondes quantiques, Laplacien Dirichlet, États liés, Tubes, Géométrie des surfaces, Courbure, Spectre des variétés, Coordonnées géodésiques polaires

Abstract

We study spectral properties of *quantum layers* which represent a reasonable model for the non-relativistic quantum dynamics of a particle in conductive films produced on an insulting surface. Mathematically, one considers the Dirichlet Laplacian in a tubular neighbourhood of constant width built over a non-compact surface embedded in $\mathbb{R}^3$. Under appropriate hypotheses on the decay of surface curvatures at infinity, we localize the essential spectrum and provide miscellaneous sufficient conditions which guarantee the existence of geometrically induced quantum bound states. Furthermore, if the reference surface is a mildly curved plane, we find the asymptotic expansion of the corresponding unique eigenvalue evaluated with respect to a parameter describing this weak coupling. We establish an asymptotic expansion of an eigenvalue also in layers which are straight but one of its boundaries is deformed locally by dents and bulges. This thesis contains eventually an investigation of the spectrum of a general non-compact manifold which possesses at least one pole. We restrict our attention to the manifolds with radial symmetry and surfaces. In these particular cases, we show that the spectrum is all the positive real axis provided we put some additional conditions on the decay of curvatures at infinity.

Key-Words : Quantum waveguides, Dirichlet Laplacian, Bound states, Tubes, Geometry of surfaces, Curvature, Spectrum of manifolds, Geodesic polar coordinates