Thesis in collaboration submitted to

Doctoral School of Science and technology (Lebanese University)

&

Graduate School of Science and Technology (Aarhus University)

in partial fulfilment for the award of the degree of

DOCTOR OF PHILOSOPHY

Major: MATHEMATICS

By

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Subject:

Energy of surface states for 3D magnetic Schrödinger operators

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To Khalil and Asia,
my dear parents...

To my siblings,
Mohammed, Aya, Soha and Hadi...

To my country Lebanon...

Acknowledgements

"Pursuing a Ph.D. project is both a difficult and enjoyable experience". In pursuing this path, first and foremost, I would like to thank my supervisors Søren Fournais and Ayman Kachmar whose academic guidance were vital in making this dissertation a reality.

My sincere appreciation goes to my supervisor Søren Fournais for his patience, optimism and continuous help during my research at Aarhus University. His insightful comments and constructive criticisms were thought-provoking. He is certainly a great mentor who is very generous in sharing his rich and valuable knowledge in many fields of research.

I am extremely indebted to my supervisor Ayman Kachmar for introducing me to the subject of this thesis, for guiding and supporting me during these past three years. His enthusiasm for my topic and his tremendous expertise are very much appreciated.

I would like to thank Raafat Talhouk for accepting to be a formal advisor of this thesis. I am indebted to his encouragement, scientific and administrative helps.

I would like to thank Didier Robert and Konstantin Pankrashkin for their interest in my work, and for the time they devoted to review this thesis.

I would like to thank ..... for accepting to be a member of the examination committee.

My special thanks go to the Dean of the Doctoral school of Sciences and Technology Professor Zainab Saad.

I take the opportunity to acknowledge the Lebanese national council for scientific research CNRS and the Lebanese university for providing me with financial support.

During the preparation of this thesis, I had the opportunity to visit Mittag-Leffler institute in Stockholm and Henri-Poincarré institute in Paris. I would like to thank the organizers of the programs in both institutes for their hospitality.

I would like to thank Sergey Morozov for his help, friendship and fruitful Mathematical discussions we had when he was a post-doc in Aarhus. I also thank Anders Aaen for his sincere friendship and his help in practical things during my stay in Aarhus.

I would like to thank my colleagues from the Lebanese university. In particular, I thank Ayda Salman, Sari Nehme and Hanan Dbouk for their close friendship.

During my stay in Denmark, I had the opportunity to meet two wonderful friends, Sandy Mohammed and Farzaneh Safavimaneh. I thank them for the enjoyable moments we spend together in Denmark.

I am very grateful for my father. His firm and kind-hearted personality has affected me to be steadfast and never bend to difficulty.

Abstract

Energy of surface states for 3D magnetic Schrödinger operators

In this dissertation, we study the Schrödinger operator with magnetic field in a three dimensional domain with compact smooth boundary. Functions in the domain of the operator satisfy (magnetic) Neumann condition on the boundary. The operator depends on the semi-classical parameter. As this parameter becomes small, certain eigenfunctions of the operator are localized near the boundary of the domain, hence they will be called *surface states*. The main result of this dissertation is the calculation of the leading order terms of the energy and the number of surface states when the semi-classical parameter tends to zero.

Keywords. Magnetic Schrödinger operator, Neumann boundary condition, spectral theory, variational principle, semi-classical analysis, energy of the sum of eigenvalues.

Resume

Energi af overfladetilstande hørende til magnetiske Schrödinger operatorer i 3D

I denne afhandling studerer vi Schrödinger operatorer med magnetisk felt i et tredimensionelt område med kompakt, glat rand. Funktioner i domænet for operatoren opfylder (magnetiske) Neumann randbetingelser. Operatoren afhænger af en semi-klassisk parameter. Når denne parameter bliver lille, bliver nogle af egenfunktionerne for operatoren lokaliseret nær randen af området, og derfor vil de blive kaldt *overfladetilstande.* Det vigtigste resultat i denne afhandling er beregningen af det ledende ordens led i henholdsvis energi og antallet af overfladetilstande når den semi-klassiske parameter går mod nul.

Nøgleord. Magnetisk Schrödinger operator, Neumann randbetingelse, spektral teori, semi-klassisk analyse, energi af summen af egenværdier.

Contents

Chapter 1

Introduction

The computation of the number and the sum of eigenvalues of Schrödinger operators in various asymptotic regimes is a central question in mathematical physics. One motivation comes from the problem of stability of matter (see Lieb-Solovej-Yngvason [?]). The object of study in [?] is mainly the Pauli operator; this operator is also a Schrödinger operator with constant magnetic field and an electric potential; it is given as follows:

$$H(h,b,V) = \mathcal{P}_h + V(x) + \sigma\cdot\mathbf{B}\,,\quad \text{in } L^2(\mathbb{R}^3;\mathbb{C}^2)\,,$$

where

$$\begin{aligned}
&\mathcal{P}_h = (-ih\nabla + \mathbf{A})^2 = -h^2\Delta + ih[\operatorname{div}(\mathbf{A}) + 2\mathbf{A}\cdot\nabla] + |\mathbf{A}|^{\mathbf{2}}\,,\\
&\mathbf{A}(x_1,x_2,x_3) = (-bx_2/2, bx_1/2, 0)\,,\\
&\mathbf{B} = \operatorname{curl}\mathbf{A} = (0,0,b)\,,\\
&\sigma = (\sigma_1,\sigma_2,\sigma_3)\,,\quad b>0\,,\quad h>0\,.
\end{aligned}$$

Let us mention that operator $\mathcal{P}_h$ is the Schrödinger operator with magnetic field ($\mathbf{B}$ is the magnetic field); σ is the vector of Pauli matrices; $V\in L^{5/2}(\mathbb{R}^3)\cap L^{3/2}(\mathbb{R}^3)$ is the electric potential; h is the semi-classical parameter; b is the strength of the magnetic field.

The operator $H(h,b,V)$ has discrete spectrum in the interval $(-\infty,0)$ consisting of eigenvalues $\lambda_1(h,b,V)$, $\lambda_2(h,b,V)$, etc. Let us introduce the number and the sum of these eigenvalues:

$$\mathcal{N} = \sum_j \dim\Big(\operatorname{Ker}(H(h,b,V) - \lambda_j(h,b,V))\Big)\,,\quad \mathcal{E} = \sum_j \lambda_j(h,b,V)\,.$$

The sum $\mathcal{E}$ is usually called the *energy* of the eigenfunctions corresponding to the eigenvalues $\lambda_1(h,b,V)$, $\lambda_2(h,b,V)$, etc. Under specific assumptions on the magnetic field $\mathbf{B}$ and the electric potential potential V, it can be shown that the number $\mathcal{N}$ and the energy $\mathcal{E}$ are finite. The study of the finiteness of $\mathcal{N}$ and $\mathcal{E}$ has been the object of study of numerous papers, starting probably with the establishing of the Cwickle-Rozenblum-Lieb and Lieb-Thirring bounds, and followed up by many important papers `such as` [?, ?, ?, ?]. Under the assumption $V\in L^{5/2}(\mathbb{R}^3)\cap L^{3/2}(\mathbb{R}^3)$, the energy $\mathcal{E}$ is finite; this is established in [?]. A natural question is then to study the asymptotic behaviour as $h\to 0_+$ of the energy $\mathcal{E}$. This is done in [?]. The computation of $\mathcal{E}$ is used to compute the ground state energy of large atoms in strong magnetic fields, and then later is used to establish *stability of matter* in many important regimes. We refer the reader to [?] for details. Another important application of the computation of the energy $\mathcal{E}$ is the calculation of the quantum current. The paper [?] is about this topic.

The analysis in [?] is generalized for various settings. Among many other papers, we mention that such extensions hold for the case of variable magnetic fields [?] and for fractional powers of the Laplacian [?].

This work aims at answering the same question in [?] and presented previously but for the Schrödinger operator with magnetic field. The electric potential is removed but the operator is defined in a domain with boundary. This leads to a similar situation as in [?], but the geometry of the boundary will have a significant influence in the expression of the leading order terms. Details will be discussed at a later point of this introduction.

An important problem in mathematical physics is the computation of the ground state energy and the analysis of the tunnelling effect for various Schrödinger operators while the semi-classical parameter h tends to 0, see Helffer [?]. In [?], while estimating the ground state energy of a Schrödinger operator in a domain with boundary, Helffer-Mohamed observed an analogy between the semi-classical analysis of Schrödinger operators with electric potentials and that of Schrödinger operators in domains with boundaries. Loosely speaking, this analogy can be summarized by saying that 'boundaries' play a similar role to 'electric potentials'. More precisely, this analogy is established in [?] for the question of computing the ground state energy for an operator in a domain with boundary. Guided by this analogy, several important applications to the analysis of the Ginzburg-landau model of superconductivity are given. We refer the reader to the monograph [?] and references therein.

It is natural to wonder whether the same type of analogy between 'boundaries' and 'electric potentials' still exists for the question of computing the energy, as done in [?]. The paper of Fournais-Kachmar [?] shows that the analogy between boundaries and electric potentials exists for two dimensional domains. The goal in this dissertation is to generalize the results of [?] to the case of three dimensional domains.

1.1 The magnetic Schrödinger operator in 2D

We present the Schrödinger operator with magnetic field in a two dimensional domain. Suppose that Ω is an open subset of $\mathbb{R}^2$ with smooth boundary and $A=(A_1,A_2)\in C^2(\overline{\Omega};\mathbb{R}^2)$ a given vector field. In two dimensions, the magnetic field is the function,

$$B=\operatorname{curl} A=\frac{\partial A_2}{\partial x}-\frac{\partial A_1}{\partial y}\,,\qquad (x,y)\in\overline{\Omega}. \tag{1.1.1}$$

We suppose that the magnetic field is positive. More specifically, we work under the hypothesis that

$$b=\inf_{x\in\overline{\Omega}} B(x)\;>0\,. \tag{1.1.2}$$

The quadratic form

$$\mathcal{Q}_h(u)=\int_\Omega |(-ih\nabla+\mathbf{A})u|^2\,dx$$

is closed and semi-bounded. Consequently, it defines a self-adjoint operator in $L^2(\Omega)$ by Friedrich's Theorem. This operator is the Schrödinger operator with magnetic field B given as follows:

$$\mathcal{P}_h=(-ih\nabla+\mathbf{A})^2\,. \tag{1.1.3}$$

The domain of $\mathcal{P}_h$ is

$$\mathcal{D}(\mathcal{P}_h)=\big\{u\in L^2(\Omega)\;:\;(-ih\nabla+\mathbf{A})^j u\in L^2(\Omega),\quad j=1,2,\quad \nu\,.\,(-ih\nabla+\mathbf{A})u=0\quad \text{on }\partial\Omega\big\}\,, \tag{1.1.4}$$

where ν is the unit exterior normal of the boundary $\partial\Omega$. When Ω is bounded, it results from the compact embedding of $H^1(\Omega)$ into $L^2(\Omega)$ that $\mathcal{P}_h$ has compact resolvent. In this case, the spectrum of P_h is purely discrete and consists of eigenvalues of finite multiplicity. This situation is studied in several papers in the context of the Ginzburg-Landau model of superconductivity (see [?, ?, ?, ?]). The interest in superconductivity is the calculation of the lowest eigenvalue (ground state energy) of $\mathcal{P}_h$ as the semi-classical parameter h tends to 0. Extensions to non-smooth domains are given in [?, ?].

If Ω is not bounded and the boundary of Ω is bounded, then the essential spectrum of $\mathcal{P}_h$ is known (see e.g. [?]). We describe how we locate the bottom of the essential spectrum. Indeed, we have the inequality (see [?]),

$$\forall\varphi\in C_0^\infty(\Omega)\,,\qquad \int_\Omega |(-i\nabla+\mathbf{A})\varphi|^2\geq\int_\Omega hB(x)|\varphi|^2dx\,.$$

Using this inequality and a'magnetic' version of Persson's Lemma proved in [?], we deduce that,

$$\inf \mathrm{Spec}_{\mathrm{ess}}(\mathcal{P}_h)\geq bh.$$

Here $b>0$ is the quantity introduced in (??).

Consequently, in any case whether Ω is bounded or not, the spectrum of the operator $\mathcal{P}_h$ below bh is purely discrete. This spectrum is non-empty if the magnetic field is not too large on the boundary of Ω. More precisely, in [?], it was proved that there is a universal constant $\Theta_0\in]0,1[$ such that the bottom of the spectrum of $\mathcal{P}_h$ satisfies,

$$\lambda_1(h,b)=\min(\Theta_0 b'\,,\,b)\,h+o(h)\qquad(h\to 0)\,,$$

where $b'=\min\limits_{x\in\partial\Omega}B(x)$ and b is introduced in (??). Clearly, if $\Theta_0 b'<b$ and h is sufficiently small, then $\lambda_1(h)<bh$ is in the discrete spectrum.

We will work under the assumption that the set $\mathrm{Spec}(\mathcal{P}_h)\cap(-\infty\,,\,bh)$ is non-empty. Denote the elements of this set as an increasing sequence,

$$\mathrm{Spec}(\mathcal{P}_h)\,\cap\,(-\infty\,,\,bh)=\{\lambda_1(h,b)\,,\lambda_2(h,b)\,,\cdots\}\,.$$

The sequence $\{\lambda_1(h,b)\,,\lambda_2(h,b)\,,\cdots\}$ can consist of infinite values accumulating to the bottom of the essential spectrum. This happens when the magnetic field is constant (see [?, ?]).

Let $b_0\in(0,1)$. Since $b_0h<bh$, then the value bh is strictly below the bottom of the essential spectrum of $\mathcal{P}_h$. Consequently, the following number

$$\mathcal{N}(b_0h;\mathcal{P}_h,\Omega)=\sum_{\lambda_j(h)\leq b_0h}\dim\big(\ker\big(\mathcal{P}_h-b_0h\big)\big)$$

is finite. When counting multiplicities, $\mathcal{N}(b_0h;\mathcal{P}_h,\Omega)$ is the number of the eigenvalues of $\mathcal{P}_h$ that are below b_0h. As $h\to 0_+$, this number is approximated in [?]. This is described in the next theorem.

Theorem 1.1.1. *Suppose that Ω is has smooth and compact boundary and $b_0<b$. There holds,*

$$\lim_{h\to 0}h^{1/2}\mathcal{N}(b_0h;\mathcal{P}_h,\Omega)=\frac{1}{2\pi}\iint_{\{(x;\xi)\in\partial\Omega\times\mathbb{R}\;:\;B(x)\mu_1(\xi)<b_0\}}B(x)^{1/2}dxd\xi\,.\tag{1.1.5}$$

Here, if $\xi\in\mathbb{R}$, the number $\mu_1(\xi)$ is the lowest eigenvalue of the harmonic oscillator

$$-\partial_t^2+(t-\xi)^2,\qquad\text{in}\quad L^2(\mathbb{R}_+),$$

and Θ_0 *is the universal constant given as follows*

$$\Theta_0 = \inf_{\xi\in\mathbb{R}} \mu_1(\xi)\,.$$

Remark 1.1.2. Generalisations of Theorem **??** showing the influence of Robin boundary conditions has been obtained in [?].

Let $(x)_- = \max(-x,0)$ denotes the negative part of a number $x\in\mathbb{R}$. The energy

$$\mathcal{E}(b,h,\Omega)=\sum_j(\lambda_j(h,b)-bh)_-$$

is studied in [?]. Notice that the energy is defined for all eigenvalues below bh and not only for those below b_0h ($b_0<1$). The energy is finite thanks to the Lieb-Thirring inequality. The result obtained in [?] is recalled in the next theorem.

Theorem 1.1.3. *Suppose that the domain* Ω *has a smooth and compact boundary. There holds,*

$$\lim_{h\to 0} h^{-1/2}\sum_j(\lambda_j(h,b)-bh)_- = \frac{1}{2\pi}\iint_{\partial\Omega\times\mathbb{R}} B(x)^{3/2}\left(-\frac{b}{B(x)}+\mu_1(\xi)\right)_- dxd\xi. \tag{1.1.6}$$

Note that Theorem **??** can be obtained as a corollary of Theorem **??** (cf. [?, Remark 1.3]). Further details about the technique which allows to pass from the *energy* to the *number* of eigenvalues will be discussed later (see Corollary **??** and its proof in Subsection **??**).

Theorems **??** and **??** remain true when the domain Ω has corners. This is established in [?].

1.2 The magnetic Schrödinger operator in 3D

In this section we define the Schrödinger operator with magnetic field in a three dimensional domain. Let $\mathcal{O}\subset\mathbb{R}^3$ be a bounded domain with smooth compact boundary $\partial\mathcal{O}$. We will consider both the case of interior domains $\Omega=\mathcal{O}$ and exterior domains $\Omega=\mathbb{R}^3\setminus\overline{\mathcal{O}}$.

We consider a magnetic vector potential $\mathbf{A}\in C^\infty(\overline{\Omega};\mathbb{R}^3)$. We write $\mathbf{A}=(A_1,A_2,A_3)$. In three dimensions, the magnetic field is a vector given by

$$\mathbf{B}(x) := \text{curl }\mathbf{A}(x) = (\beta_{23},-\beta_{13},\beta_{13}),\qquad \beta_{ij}(x)=\frac{\partial A_j}{\partial x_i}(x)-\frac{\partial A_i}{\partial x_j}(x),\quad i,j=1,2,3.$$

With the magnetic field we associate the quantities

$$b:=\inf_{x\in\overline{\Omega}}|\mathbf{B}(x)|,\quad b'=\inf_{x\in\partial\Omega}|\mathbf{B}(x)|, \tag{1.2.1}$$

where $|\mathbf{B}(x)|=\sqrt{\beta_{12}^2(x)+\beta_{13}^2(x)+\beta_{23}^2(x)}$ is the strength of the magnetic field.

We shall work under the assumption that

$$b:=\inf_{x\in\overline{\Omega}}|\mathbf{B}(x)|>0. \tag{1.2.2}$$

Let $h>0$ be a small parameter (the so called semi-classical parameter). Consider the quadratic form

$$\mathcal{Q}_h(u)=\int_\Omega|(-ih\nabla+\mathbf{A})u|^2dx, \tag{1.2.3}$$

with domain,

$$\mathcal{D}(\mathcal{Q}_h) = \{u \in L^2(\Omega) \,:\, (-ih\nabla + \mathbf{A})u \in L^2(\Omega)\}. \tag{1.2.4}$$

This is clearly a semi-bounded closed quadratic form. We associate by Friedrich's theorem a self-adjoint operator, $\mathcal{P}_h$, whose domain is

$$\mathcal{D}(\mathcal{P}_h) = \big\{u \in L^2(\Omega) \,:\, (-ih\nabla+\mathbf{A})^j u \in L^2(\Omega), \quad j = 1, 2, \quad \nu\,.\,(-ih\nabla+\mathbf{A})u = 0 \quad \text{on } \partial\Omega\big\}\,, \tag{1.2.5}$$

and for all $u \in \mathcal{D}(\mathcal{P}_h)$, we have

$$\mathcal{P}_h u = (-ih\nabla + \mathbf{A})^2 u\,. \tag{1.2.6}$$

Here, for $x \in \partial\Omega$, $\nu(x)$ denotes the unit interior normal vector to $\partial\Omega$ at x.

If the domain Ω is bounded (interior case), it results from the compact embedding of $\mathcal{D}(\mathcal{Q}_h)$ into $L^2(\Omega)$ that $\mathcal{P}_h$ has compact resolvent. Hence the spectrum is purely discrete consisting of a sequence of positive eigenvalues accumulating at infinity.

In the case of exterior domains, the operator $\mathcal{P}_h$ can have essential spectrum. In Chapter 2, we will see that if $\Lambda < b$ (b from (**??**)) and h is sufficiently small, then the spectrum of $\mathcal{P}_h$ in the interval $[0, \Lambda h]$ is purely discrete.

The operator $\mathcal{P}_h$ is studied in several papers, mainly in the context of the Ginzburg-Landau model of superconductivity (see [**?**, **?**, **?**, **?**]). The objective was mainly the estimation of the ground state energy as $h \to 0_+$. Compared to the situation for two dimensional domains, the analysis of the problem in three dimensional domains is considerably more complicated. The reason is that the boundary in 3D is a surface and has richer geometry than that in 2D.

If the magnetic field is constant and the domain Ω has a smooth boundary, it is established that (see [**?**, **?**]):

$$\inf \operatorname{Spec} \mathcal{P}_h = h\Theta_0 b + o(h)\,, \quad (h \to 0_+)\,, \tag{1.2.7}$$

where $\Theta_0 \in (0,1)$ is the universal constant introduced in (**??**). In such a situation, we see that the set

$$\operatorname{Spec} \mathcal{P}_h \,\cap\, [0, \Lambda h] \neq \emptyset\,.$$

In general, we will work under the assumption that $\operatorname{Spec} \mathcal{P}_h \,\cap\, [0, \Lambda h] \neq \emptyset$ and denote the elements of this set as an increasing sequence of eigenvalues counting multiplicities,

$$\operatorname{Spec}(\mathcal{P}_h) \,\cap\, (-\infty\,, \Lambda h) = \{e_1(h)\,, e_2(h)\,, \cdots\}\,.$$

In this dissertation, we are interested in studying the asymptotic behaviour of the energy

$$\mathcal{E}(h, \mathbf{B}, \Lambda) = \operatorname{Tr}\big(\mathcal{P}_h - \Lambda h\big)_- = \sum_j (e_j(h) - \Lambda h)_- \tag{1.2.8}$$

in the semi-classical limit $h \to 0$. The leading order asymptotics of $\mathcal{E}(h, \mathbf{B}, \Lambda)$ is given in Theorem **??** below.

1.2.1 Notation

To introduce the main result, we shall need the following notation

- If x is a point on the boundary of Ω, then $\theta(x)$ denotes the angle in $[0, \pi/2]$ between the magnetic field $\mathbf{B} = \operatorname{curl} \mathbf{A}$ and the tangent plane to $\partial\Omega$ at the point x. More precisely,

$$\partial\Omega \ni x \mapsto \theta(x) = \arcsin\left(\frac{|\mathbf{B}(x) \cdot \nu(x)|}{|\mathbf{B}(x)|}\right) \in [0, \pi/2]. \tag{1.2.9}$$

- We let $\mathbb{R}_+ = (0, \infty)$, $\mathbb{R}^2_+ = \mathbb{R} \times (0, \infty)$ and $\mathbb{R}^3_+ = \mathbb{R}^2 \times (0, \infty)$.
- For $\xi \in \mathbb{R}$, we denote by $\mu_1(\xi)$ the lowest eigenvalue of the harmonic oscillator
$$-\partial_t^2 + (t - \xi)^2 \qquad \text{in} \quad L^2(\mathbb{R}_+)$$
with Neumann boundary conditions at $t = 0$.
- For $\theta \in (0, \pi/2]$, we introduce the two-dimensional operator
$$\mathcal{L}(\theta) := -\partial_t^2 - \partial_s^2 + (t\cos(\theta) - s\sin(\theta))^2 \quad \text{in} \quad L^2(\mathbb{R}^2_+). \tag{1.2.10}$$
It is well known (see [?]) that the essential spectrum of $\mathcal{L}(\theta)$ is the interval $[1, \infty)$, and we shall denote by $\{\zeta_j(\theta)\}_j$ the countable set of eigenvalues of $\mathcal{L}(\theta)$ in the interval $[\zeta_1(\theta), 1)$.
- We define the positive and negative parts of a real number x by $(x)_\pm = \max(\pm x, 0)$.
- If $a(h)$ and $b(h)$ are positive functions of h, then $a(h) \ll b(h)$ means that $a(h)/b(h) \to 0$ as $h \to 0_+$. Similarly, the notation $a(h) \gg b(h)$ means that $a(h)/b(h) \to \infty$ as $h \to 0_+$.

1.2.2 Main results

The main result in this thesis is :

Theorem 1.2.1. *Suppose Ω is either an interior or an exterior domain with compact smooth boundary $\partial\Omega$. Given $\Lambda \in [0, b)$, the following asymptotic formula holds,*
$$\sum_j (e_j(h) - \Lambda h)_- = \int_{\partial\Omega} |\mathbf{B}(x)|^2 E(\theta(x), \Lambda|\mathbf{B}(x)|^{-1}) d\sigma(x) + o(1), \qquad \text{as} \quad h \to 0. \tag{1.2.11}$$
Here, the function $E(\theta, \lambda)$ is defined for $(\theta, \lambda) \in [0, \pi/2] \times [0, 1)$ as follows,
$$E(\theta, \lambda) = \begin{cases} \dfrac{1}{3\pi^2} \displaystyle\int_0^\infty (\mu_1(\xi) - \lambda)_-^{3/2} d\xi & \text{if} \quad \theta = 0, \\ \dfrac{\sin(\theta)}{2\pi} \displaystyle\sum_j (\zeta_j(\theta) - \lambda)_- & \text{if} \quad \theta \in (0, \pi/2], \end{cases}$$
and $d\sigma(x)$ denotes the two dimensional surface measure on the boundary $\partial\Omega$.

Remark 1.2.2. In the case $\theta = \frac{\pi}{2}$, it is well known (see [?]) that the first eigenvalue $\zeta_1(\frac{\pi}{2}) = 1$ which implies that $E(\frac{\pi}{2}, \lambda) = 0$ for any $\lambda \in [0, 1)$.

Remark 1.2.3. In the case of $\theta \in (0, \pi/2)$, we emphasize that the sum appearing in the formula of $E(\theta, \lambda)$ above, is a finite sum. Indeed, in view of Lemma **??** below, we learn that the number of eigenvalues of $\mathcal{L}(\theta)$, below a fixed $\lambda \in [0, 1)$, is finite.

Remark 1.2.4. Theorem **??** is an extension to three-dimensional domains of the analogous Theorem 1.1 in [?] established for two-dimensional domains.

Remark 1.2.5. In Lemma **??** below, we show that the function
$$(\theta, \lambda) \mapsto E(\theta, \lambda),$$
is a continuous function as a function of two variables. Consequently, we obtain
$$\lim_{\theta \to 0} \frac{\sin(\theta)}{2\pi} \sum_j (\zeta_j(\theta) - \lambda)_- = \frac{1}{3\pi^2} \int_0^\infty (\mu_1(\xi) - \lambda)_-^{3/2} d\xi.$$

Notice that this formula is connected to the formula for the number of eigenvalues given in [?]:

$$\lim_{\theta\to 0}\big(\sin\theta\,\mathcal{N}(\lambda,\theta)\big)=\frac{1}{\pi}\int_0^\infty(\mu_1(\xi)-\lambda)_-^{3/2}d\xi,$$

where $\mathcal{N}(\lambda,\theta)=\mathrm{Card}\{\zeta_j(\theta)\ :\ \zeta_j(\theta)\leq\lambda\}$.

Remark 1.2.6. Assuming that the strength of the magnetic field is constant on the boundary, i.e. $|B|=b'$ on $\partial\Omega$, the asymptotic formula of Theorem **??** reads

$$\sum_j(e_j(h)-\Lambda h)_-=(b')^2\int_{\partial\Omega}E(\theta(x),\Lambda(b')^{-1})d\sigma(x)+o(1),\qquad\text{as}\quad h\to 0. \tag{1.2.12}$$

Using the technique to go from energies to densities (see [?] for details), we can differentiate both sides of (**??**) with respect to Λh and get an asymptotic formula for the number of eigenvalues of $\mathcal{P}_h$ below Λh. This is stated in the next corollary.

Corollary 1.2.7. *Let $\Lambda\in[0,b)$ such that (σ is the surface measure on $\partial\Omega$):*

$$\sigma\big(\{x\in\partial\Omega\ :\ \theta(x)\in(0,\pi/2),\quad\Lambda|\mathbf{B}(x)|^{-1}\in\mathrm{Spec}\,\mathcal{L}(\theta(x))\}\big)=0\,. \tag{1.2.13}$$

The following asymptotic formula holds true,

$$\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega)=h^{-1}\int_{\partial\Omega}|\mathbf{B}(x)|n(\theta(x),\Lambda|\mathbf{B}(x)|^{-1})d\sigma(x)+o(h^{-1})\quad(h\to 0_+)\,. \tag{1.2.14}$$

Here, if $\lambda\in[0,1)$, then $n(\theta,\lambda)$ is given by

$$n(\theta,\lambda)=\begin{cases}\dfrac{1}{2\pi^2}\displaystyle\int_0^\infty(\mu_1(\xi)-\lambda)_-^{1/2}d\xi & \text{if}\quad\theta=0,\\ \dfrac{\sin(\theta)\mathcal{N}(\lambda;\mathcal{L}(\theta),\mathbb{R}^2_+)}{2\pi} & \text{if}\quad\theta\in(0,\pi/2].\end{cases}$$

Remark 1.2.8. The condition in (**??**) is satisfied when Ω is the unit ball, the magnetic field $\mathbf{B}$ is constant of unit length and Λ is sufficiently close to the universal constant Θ_0. Details are given in Subsection **??**.

1.3 Perspectives

We list some natural questions for future research:

1. Inspection of the number $\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega)$ when the condition in (**??**) is violated.

2. Theorem **??** is established when the domains Ω has a smooth boundary. An interesting question is to study the case when the domain Ω has corners or wedges (see [?]). In two dimensions, this is done [?].

3. The inspection of the effect of the boundary conditions might be interesting. Theorem **??** is established for the operator with Neumann boundary condition. A natural question is to consider the operator with Robin boundary condition

$$\nu\ .\ (-ih\nabla+\mathbf{A})u+\gamma u=0\quad\text{ on }\quad\partial\Omega,$$

where $\gamma\in L^\infty(\partial\Omega;\mathbb{R})$.

4. The asymptotic formula in Theorem **??** holds for the energy of the eigenvalues below the energy level b_0h with $b_0<1$. However, in two dimension, such a restriction on b_0 does not appear (b_0 is allowed to be 1). Removing the restriction on b_0 in three dimensions is an interesting question.

1.4 Organization of the dissertation

This thesis is organized as follows.

Chapter 2 contains basic tools in spectral theory that are needed in the subsequent chapters.

Chapter 3 is devoted to the spectral analysis of the model operator on a half-cylinder with Neumann boundary condition on one edge and Dirichlet boundary conditions on the other edges.

Chapter 4 is devoted to the construction of the function $E(\theta, \lambda)$ as the limit of the energy of the operator in the half-cylinder. Continuity properties of this function and explicit formulas of it are given.

Chapter 5 contains the expression of the operator relative to local coordinates near the boundary of the domain Ω.

Chapter 6 concludes with the proof of Theorem **??** and Corollary **??**.

Chapter 2

Spectral theory

The aim of this chapter is to review standard facts regarding the spectrum of semi-bounded self-adjoint operators. In Section **??**, we recall the min-max principle. In Section **??**, we recall variational principles to compute the sum of negative eigenvalues of semi-bounded operators. In section **??**, we recall the Cwikel-Lieb-Rosenblum and Lieb-Thirring estimates for Schrödinger operators on $L^2(\mathbb{R}^3)$. Section **??** is devoted to the analysis of the harmonic oscillator on a half-axis. In Section **??**, we review some of the fundamental properties of the two-dimensional operator in the half-plane. The model operators on the half-axis and half-plane are fundamental in understanding the spectral analysis in three dimensional domains. Gauge invariance for magnetic Schroödinger operators is recalled in Section **??**. Finally, the essential spectrum of the magnetic Schrödinger operator (defined in (**??**)) is discussed in Section **??**.

2.1 The min-max theorem

The celebrated min-max principle is recalled in the next theorem. The proof is given in standard spectral theory textbooks, e.g. [**?**, Theorem XIII.1], [**?**, p. 75] and [**?**, Sections 1&2].

Theorem 2.1.1. *Let $\mathcal{H}$ be a self-adjoint operator corresponding to a semi bounded quadratic form $\mathcal{Q}(\Psi) = \langle \Psi, \mathcal{H}\Psi \rangle$ with form domain $\mathcal{D}(\mathcal{Q})$. Let us define*

$$\mu_n = \inf_{\substack{V \subset \mathcal{D}(\mathcal{Q}) \\ \dim V = n}} \max_{\substack{\Psi \in V \\ \|\Psi\| = 1}} \mathcal{Q}(\Psi). \tag{2.1.1}$$

Then, for each fixed n, we have the alternative (a) or (b) :

(a) There are n eigenvalues (counted with multiplicity) below the bottom of the essential spectrum, and μ_n is the n-th eigenvalue counted with multiplicity.

(b) The value μ_n is the bottom of the essential spectrum, and in that case $\mu_n = \mu_{n+1} = \cdots$ and there are at most $n-1$ eigenvalues (counting multiplicities) below μ_n.

Remark 2.1.2. The value of μ_n in (**??**) can be expressed in the following form as well :

$$\mu_n = \sup_{\Psi_1, \cdots, \Psi_{n-1} \in \mathcal{D}(\mathcal{Q})} \inf_{\substack{\Psi \in \mathrm{span}[\Psi_1, \cdots, \Psi_{n-1}]^\perp \\ \Psi \in \mathcal{D}(\mathcal{Q}),\ \|\Psi\| = 1}} \mathcal{Q}(\Psi). \tag{2.1.2}$$

Next, we recall a useful application of the min-max principle in comparing the number of eigenvalues of two operators. This is taken from [**?**, Lemma 5.1].

Lemma 2.1.3. *Let* $(\mathfrak{h}_1, \mathcal{Q}_1, \mathcal{D}(\mathcal{Q}_1))$ *and* $(\mathfrak{h}_2, \mathcal{Q}_2, \mathcal{D}(\mathcal{Q}_2))$ *be two closed quadratic forms such that*

$$j : \mathcal{D}(\mathcal{Q}_1) \hookrightarrow \mathcal{D}(\mathcal{Q}_2)$$

is an isometric embedding with respect to the norms of the Hilbert spaces $\mathfrak{h}_1$ *and* $\mathfrak{h}_2$*. Suppose that there exist constants* C_1 *and* C_2 *such that, for all* $f \in \mathfrak{h}_1$*,*

$$\mathcal{Q}_1(f) \geq C_1 \mathcal{Q}_2(j(f)) - C_2 \|f\|^2_{\mathfrak{h}_1}. \tag{2.1.3}$$

Denote by $\mathcal{N}_1$ *and* $\mathcal{N}_2$ *the spectral counting functions associated with* $\mathcal{Q}_1$ *and* $\mathcal{Q}_2$*, then we have :*

$$\forall\, \lambda \geq 0, \qquad \mathcal{N}_1(\lambda) \leq \mathcal{N}_2\Big(\frac{\lambda + C_2}{C_1}\Big).$$

Proof. Suppose that $\mathcal{N}_2\big(\frac{\lambda+C_2}{C_1}\big)$ is finite, otherwise there is nothing to prove. Denote by $\{\mu_j(\mathcal{Q}_1)\}_j$ and $\{\mu_j(\mathcal{Q}_2)\}_j$ the eigenvalues, defined by Theorem **??**, of the self-adjoint operators associated with the closed quadratic forms $\mathcal{Q}_1$ and $\mathcal{Q}_2$. Put

$$m := \mathcal{N}_2\big(\frac{\lambda + C_2}{C_1}\big) + 1, \tag{2.1.4}$$

and consider a vector space $V \subset \mathcal{D}(\mathcal{Q}_1)$ of dimension m. Then, for all $\varphi \in V$, we have in view of (**??**) and Theorem **??** that

$$\begin{aligned}
\max_{\varphi \in V} \frac{\mathcal{Q}_1(\varphi)}{\|\varphi\|^2_{\mathfrak{h}_1}} &\geq C_1 \max_{\varphi \in V} \frac{\mathcal{Q}_2(j(\varphi))}{\|\varphi\|^2_{\mathfrak{h}_1}} - C_2 \\
&= C_1 \max_{j(\varphi) \in j(V)} \frac{\mathcal{Q}_2(j(\varphi))}{\|j(\varphi)\|^2_{\mathfrak{h}_2}} - C_2 \\
&\geq C_1 \mu_m(\mathcal{Q}_2) - C_2 \\
&\geq C_1 \frac{\lambda + C_2}{C_1} - C_2 = \lambda.
\end{aligned}$$

Since this is true for any vector space V of dimension m, it follows from Theorem **??** that,

$$\mu_m(\mathcal{Q}_1) \geq \lambda. \tag{2.1.5}$$

Recalling (**??**), the lemma follows easily from (**??**). □

2.2 Eigenvalues sum

In this section, we recall variational principles to compute the sum of negative eigenvalues of a semi-bounded self-adjoint operator $\mathcal{H}$ on $L^2(\mathbb{R}^3)$. We will assume that

$$\inf \operatorname{Spec}_{\text{ess}}(\mathcal{H}) \geq 0, \tag{2.2.1}$$

and let $(\mathcal{H})_- = -\mathbf{1}_{(-\infty,0)}(\mathcal{H})\mathcal{H}$ denote the negative part of $\mathcal{H}$.

The principle stated in Lemma **??** provides a useful characterization of $\operatorname{Tr}(\mathcal{H})_-$. In finite dimensional spaces, it appears in [?] and [?, Section 8.6]. The proof we present is taken from [?].

Lemma 2.2.1. *Let* $\mathcal{H}$ *be a self-adjoint semi-bounded operator satisfying the hypothesis* (**??**) *and* $\{\nu_j\}_{j=1}^\infty$ *its min-max values defined in Theorem* **??***. Then, we have,*

$$-\sum_{j=1}^{\infty} (\nu_j)_- = \inf \sum_{j=1}^{N} \big\langle \psi_j, \mathcal{H}\psi_j \big\rangle, \tag{2.2.2}$$

where the infimum is taken over all $N \in \mathbb{N}$ *and orthonormal families* $\{\psi_1, \psi_2, \cdots, \psi_N\} \subset \mathcal{D}(\mathcal{H})$*.*

Proof. Let $\{\psi_j\}_{j=1}$ be an orthonormal family in $\mathcal{D}(\mathcal{H})$. We may assume that all $\langle \psi_j, \mathcal{H}\psi_j \rangle < 0$ otherwise we remove all the non-negative terms. We will prove that

$$\sum_{j=1}^{N} \nu_j \le \sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle, \tag{2.2.3}$$

for all $N \in \mathbb{N}$. Let us show (**??**) by induction. The case $N = 1$ follows directly from the min-max Theorem **??**, i.e.,

$$\langle \psi_1, \mathcal{H}\psi_1 \rangle \ge \nu_1.$$

Assume that (**??**) holds for $N-1$. Choose $\varphi_N \in \operatorname{span}[\psi_1, \cdots, \psi_N]$ normalized such that

$$\langle \varphi_N, \mathcal{H}\varphi_N \rangle = \max_{\substack{\psi \in \operatorname{span}[\psi_1, \cdots \psi_N] \\ \|\psi\|=1}} \langle \psi, \mathcal{H}\psi \rangle.$$

Note that the function φ_N exists, since we are taking the max of a continuous function over the unit ball in a finite dimensional normed vector space, where the unit ball is compact.

By the min-max Theorem in **??**, it follows that

$$\nu_N \le \langle \varphi_N, \mathcal{H}\varphi_N \rangle.$$

Now, we supplement φ_N to an orthonormal basis $\varphi_1, \cdots, \varphi_N$ for $\operatorname{span}[\psi_1, \cdots, \psi_N]$.By unitary invariance of the trace we then find

$$\sum_{j=1}^{N} \langle \varphi_j, \mathcal{H}\varphi_j \rangle = \sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge \nu_N + \sum_{j=1}^{N-1} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge \nu_n + \sum_{j=1}^{N-1} \nu_j$$

where in the last step we have used the induction assumption. This proves (**??**).

Suppose that $\mathcal{H}$ has only finite negative eigenvalues. Denote these eigenvalues by $\nu_1, \cdots, \nu_M$ (counting multiplicities). If $M \le N$, we apply (**??**) with $N' = M$. Hence

$$\sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge \sum_{j=1}^{M} \nu_j.$$

If $M > N$, we apply (**??**) with $N' = N$ and obtain

$$\sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge \sum_{j=1}^{N} \nu_j \ge \sum_{j=1}^{N} \nu_j + \sum_{j=N+1}^{M} \nu_j = \sum_{j=1}^{M} \nu_j. \tag{2.2.4}$$

Assume now that $\mathcal{H}$ has an infinite number of negative eigenvalues below 0. Choose $M > N$ and let $\nu_1, \cdots, \nu_M$ be the first M eigenvalues. We proceed as (**??**) and find

$$\sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge \sum_{j=1}^{N} \nu_j \ge \sum_{j=1}^{M} \nu_j,$$

for all $M > N$.

Thus, in all cases, we have

$$\sum_{j=1}^{N} \langle \psi_j, \mathcal{H}\psi_j \rangle \ge -\sum_{j=1}^{\infty} (\nu_j)_-,$$

for all $N \in \mathbb{N}$.

We turn to prove a lower bound. By the spectral theorem, it follows that for a given integer N we can find an orthonormal family $\{\phi_n\}_{n=1}^N$ such that the numbers $\langle \phi_j, \mathcal{H}\phi_j \rangle$, are arbitrary close to ν_j. It is therefore clear that $-\sum_j (\nu_j)_-$ can be approximated well (also when it is $-\infty$) by $\sum_{j=1}^N \langle \phi_j, \mathcal{H}\phi_j \rangle$. The statement of the lemma is thus proved. $\square$

Remark 2.2.2. We will often use the notation

$$\mathrm{Tr}(\mathcal{H})_- := \sum_j (\nu_j)_-,$$

since the quantity on the right hand side will be always finite in the cases we consider in this report.

The next lemma states another variational principle. It is used in several papers, e.g. [**?**].

Lemma 2.2.3. *Let $\mathcal{H}$ be a self-adjoint semi-bounded operator satisfying the hypothesis* (**??**)*. Suppose in addition that $(\mathcal{H})_-$ is trace class. For any orthogonal projection γ with range belonging to the domain of $\mathcal{H}$ and such that $\mathcal{H}\gamma$ is trace class, we have,*

$$-\,\mathrm{Tr}(\mathcal{H})_- \leq \mathrm{Tr}(\mathcal{H}\gamma), \tag{2.2.5}$$

Proof. Let us denote by $\{\lambda_k\}_k$ the sequence of strictly negative eigenvalues (counting multiplicities) of $\mathcal{H}$, and let $\{f_k^-\}_{k\in\mathbb{Z}^-}$ be the orthonormal basis of eigenfunctions associated with $\{\lambda_k\}_k$. Furthermore, we denote by $P_- = \mathbf{1}_{(-\infty,0)}(\mathcal{H})$ (resp. $P_+ = \mathrm{Id} - P_-$) the orthogonal projection on the eigenspaces of strictly negative (resp. positive) eigenvalues of $\mathcal{H}$. Since the operator $\mathcal{H}\gamma$ is trace class, we have,

$$\mathrm{Tr}(\mathcal{H}\gamma) = \mathrm{Tr}(\mathcal{H}\gamma P_+) + \mathrm{Tr}(\mathcal{H}\gamma P_-). \tag{2.2.6}$$

Since the trace is cyclic, it follows that

$$\mathrm{Tr}(\mathcal{H}\gamma P_+) = \mathrm{Tr}(P_+\mathcal{H}\gamma).$$

Taking into account that P_+ is a projector commuting with $\mathcal{H}$, we get

$$\mathrm{Tr}(P_+\mathcal{H}\gamma) = \mathrm{Tr}(P_+P_+\mathcal{H}\gamma) = \mathrm{Tr}(P_+\mathcal{H}P_+\gamma). \tag{2.2.7}$$

The last term is clearly positive since $\gamma \geq 0$ and the operator P_+HP_+ is positive. Indeed, since the trace is cyclic, we see that

$$\mathrm{Tr}(P_+\mathcal{H}P_+\gamma) = \mathrm{Tr}(P_+\mathcal{H}P_+\gamma^2) = \mathrm{Tr}(\gamma P_+\mathcal{H}P_+\gamma) \geq 0,$$

Therefore, the proof amounts to show that $\mathrm{Tr}(P_-\mathcal{H}\gamma) \geq -\mathrm{Tr}(\mathcal{H})_-$. As in (**??**), we have

$$\mathrm{Tr}(P_-\mathcal{H}\gamma) = \mathrm{Tr}(P_-\mathcal{H}P_-\gamma).$$

Next, consider the smallest closed space K defined as the direct sum of the eigenspaces associated with the strictly negative eigenvalues $\{\lambda_k\}_k$. Furthermore, let $\{f_k^-\}_{k\in\mathbb{Z}^-}$ be an orthonormal basis of K and $\{f_k^+\}_{k\in\mathbb{Z}^+}$ an orthonormal basis of $K^\perp$, such that $\{f_k^+ \cup f_k^-\}_{k\in\mathbb{Z}}$ form an orthonormal basis of $L^2(\mathbb{R}^3)$. Hence

$$\mathrm{Tr}(P_-\mathcal{H}P_-\gamma) = \sum_k \langle P_-\mathcal{H}P_-\gamma f_k^-, f_k^- \rangle + \sum_k \langle P_-\mathcal{H}P_-\gamma f_k^+, f_k^+ \rangle.$$

The second term on the right hand vanishes because

$$\sum_k \langle P_- \mathcal{H} P_- \gamma f_k^+, f_k^+ \rangle = \sum_k \langle \mathcal{H} P_- \gamma f_k^+, P_- f_k^+ \rangle = 0.$$

Using that $\mathcal{H}$ is self-adjoint, it follows that

$$\mathrm{Tr}(P_- \mathcal{H} P_- \gamma) = \sum_k \langle P_- \mathcal{H} P_- \gamma f_k^-, f_k^- \rangle = \sum_k \langle \gamma f_k^-, P_- \mathcal{H} P_- f_k^- \rangle = \sum_k \lambda_k \langle \gamma f_k^-, f_k^- \rangle.$$

Since $\lambda_k < 0$ and

$$0 \leq \langle \gamma f_k^-, f_k^- \rangle \leq \left\| f_k^- \right\|^2 = 1,$$

we deduce that

$$\lambda_k \leq \langle \lambda_k \gamma f_k^-, f_k^- \rangle \leq 0$$

Summing over k, we find

$$\sum_k \lambda_k \leq \sum_k \langle \lambda_k \gamma f_k^-, f_k^- \rangle.$$

Combining the foregoing relations, we obtain

$$-\mathrm{Tr}(\mathcal{H})_- := \sum_k \lambda_k \leq \mathrm{Tr}(\mathcal{H}\gamma).$$

The proof is thus complete. □

2.3 Eigenvalue bounds

Given a vector field $A \in L^2_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R}^3)$, the magnetic field, we consider the quadratic form

$$L^2(\mathbb{R}^3) \ni u \mapsto Q_0(u) = \int_{\mathbb{R}^3} |(-i\nabla + A)|^2 dx,$$

with form domain

$$\mathcal{D}(Q_0) = \{u \in L^2(\mathbb{R}^3) \ : \ (-i\nabla + A)u \in L^2(\mathbb{R}^3; \mathbb{R}^3)\}.$$

Since Q_0 is a semi-bounded closed quadratic form, it is associated to a self-adjoint operator,

$$H_0 = (-ih\nabla + A)^2,$$

with domain

$$\mathcal{D}(H_0) = \{u \in L^2(\mathbb{R}^3) \ : \ (-i\nabla + A)^2 u \in L^2(\mathbb{R}^3; \mathbb{R}^3)\}.$$

Next, let $V \in L^2_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{R})$ such that $(V)_- \in L^{3/2}(\mathbb{R}^3) \cap L^{5/2}(\mathbb{R}^3)$, and consider

$$H = H_0 + V$$

Under the assumptions on A and V, the operator H can be seen as a bounded perturbation of H_0. By Kato-Rellich Theorem, we deduce that H is self-adjoint, semi bounded from below with domain $\mathcal{D}(H_0)$. We recall in the next theorem a bound on the sum of negative eigenvalues of H in terms of the potential V. For proofs and details we refer the reader to [**?**, **?**].

Theorem 2.3.1 (Lieb-Thirring inequality)**.** *Suppose that the negative part $(V)_-$ of V satisfies $(V)_- \in L^{5/2}(\mathbb{R}^3)$ then H is bounded below and its eigenvalues μ_n satisfy the Lieb-Thirring inequality*

$$\sum_{n=1}^{\infty}(\mu_n)_- \leq C_{\mathrm{LT}} \int_{\mathbb{R}^3} (V(x))_-^{5/2} dx,$$

where C_{LT} is a universal constant independent of A and V.

Next, we state a bound on the number of negative eigenvalues of H, see [**?**] for details.

Theorem 2.3.2 (Cwikel-Rosenblum-Lieb)**.** *Let $(V)_- \in L^{3/2}(\mathbb{R}^3)$ and denote by $\mathcal{N}(V)$ the number of negative eigenvalues of H. We have the following estimate*

$$\mathcal{N}(V) \leq C_{\mathrm{CLR}} \int_{\mathbb{R}^3} (V(x))_-^{3/2} dx,$$

where C_{CLR} is a universal constant.

2.4 Harmonic Oscillator on a half-axis

Let $k \in \mathbb{N}$ and $I \subset \mathbb{R}$ is an interval, the space $B^k(I)$ is defined as :

$$B^k(I) = \{u \in L^2(I) \ : \ t^p u^{(q)}(t) \in L^2(I), \quad \forall p, q \quad \text{s.t.} \quad p + q \leq k\}, \tag{2.4.1}$$

where $u^{(q)}$ denote the distributional derivative of order q of u. In this section, we review some of the basic results concerning the Neumann realisation of the Harmonic Oscillator on $\mathbb{R}_+$.

Let $\mathfrak{q}[\xi]$ be the closed quadratic form associated with the Neumann realisation of the operator $\mathfrak{h}[\xi] = -\partial_t^2 + (t-\xi)^2$ in $L^2(\mathbb{R}_+)$. This form is given by

$$\mathfrak{q}[\xi] = \int_0^{\infty} \Big[|u'(t)|^2 + (t-\xi)^2|u|^2\Big] dt.$$

The domain of $\mathfrak{h}[\xi]$ is :

$$\mathcal{D}(\mathfrak{h}[\xi]) := \{u \in B^2(\mathbb{R}_+) \ : \ u'(0) = 0\}.$$

The operator $\mathfrak{h}[\xi]$ has compact resolvent since the embedding of $B^1(\mathbb{R}_+)$ into $L^2(\mathbb{R}_+)$ is compact. Hence the spectrum of $\mathfrak{h}[\xi]$ is purely discrete consisting of an increasing sequence of positive eigenvalues $\{\mu_j(\xi)\}_{j=1}^{\infty}$.

The eigenvalues of $\mathfrak{h}[\xi]$ are defined via the min-max principle by :

$$\mu_j(\xi) = \sup_{u_1, u_2, \cdots, u_{n-1}} \inf_{\left\{\begin{array}{l} u \in [\mathrm{span}(u_1, u_2, \cdots, u_{n-1})]^{\perp}; \\ u \in B^1(\mathbb{R}_+) \text{and} \ \|u\|_{L^2(\mathbb{R}_+)} = 1 \end{array}\right\}} \frac{\mathfrak{q}[\xi]u}{\|u\|^2_{L^2(\mathbb{R}_+)}}. \tag{2.4.2}$$

It follows from analytic perturbation theory (see [**?**]) that, for all $j \geq 1$, the function,

$$\mathbb{R} \ni \xi \mapsto \mu_j(\xi)$$

is analytic. The proof of the next lemma can be found in [**?**].

Lemma 2.4.1. *The lowest eigenvalue $\mu_1(\xi)$ is simple and the function φ_ξ is the unique L^2-normalized strictly positive eigenfunction associated to $\mu_1(\xi)$.*

The lowest eigenvalue $\mu_1(\xi)$ is studied in [**?**, **?**]. We collect in the following proposition some of the properties of $\mu_1(\xi)$ as a function of ξ.

Proposition 2.4.2. *The function $\mathbb{R} \ni \xi \mapsto \mu_1(\xi)$ is continuous and satisfies*

1. $\mu_1(\xi) > 0$, *for all* $\xi \in \mathbb{R}$.
2. *At* $-\infty$ *we have the limit*
$$\lim_{\xi \to -\infty} \mu_1(\xi) = +\infty. \tag{2.4.3}$$
3. *At the origin the value is*
$$\mu_1(0) = 1. \tag{2.4.4}$$
4. *At* $+\infty$ *we have*
$$\lim_{\xi \to +\infty} \mu_1(\xi) = 1. \tag{2.4.5}$$
5. μ_1 *admits a unique minimum* Θ_0 *at some* $\xi_0 \in (0, 1)$,
$$\Theta_0 := \inf_{\xi \in \mathbb{R}} \mu_1(\xi) = \mu_1(\xi_0) < 1. \tag{2.4.6}$$

The following assertion about the second eigenvalue $\mu_2(\xi)$ of $\mathfrak{h}[\xi]$ is taken from [**?**].

Lemma 2.4.3. *The second eigenvalue $\mu_2(\xi)$ satisfies,*

$$\mu_2(\xi) > 1, \qquad \forall \xi \in \mathbb{R}.$$

Remark 2.4.4. As a consequence of Proposition **??**, we have

$$\mu_1(\xi) < 1, \quad \forall \xi \in \mathbb{R}_+, \qquad \mu_1(\xi) > 1, \quad \forall \xi \in \mathbb{R}, \tag{2.4.7}$$

Moreover, the integral

$$\int_0^\infty (1 - \mu_1(\xi)) d\xi = \int_{\mathbb{R}} (\mu_1(\xi) - 1)_- d\xi, \tag{2.4.8}$$

is finite and positive.

For later reference, we include Agmon-type estimates on the eigenfunction $u_1(t; \xi)$ (cf. [**?**, Theorem 2.6.2]).

Lemma 2.4.5. *Let $\lambda \in [0, 1)$. For all $\epsilon \in (0, 1)$, there exists a constant C_ϵ such that, for all $\xi \in \mathbb{R}_+$ satisfying $\mu_1(\xi) \le \lambda$, we have*

$$\left\| e^{\frac{\epsilon(t-\xi)^2}{2}} u_1(t, \xi) \right\|^2_{H^1\left(\{t \in \mathbb{R}_+ \,:\, (t-\xi)^2 \ge C_\epsilon\}\right)} \le C_\epsilon. \tag{2.4.9}$$

Based on Proposition **??** and Remark **??**, we derive

Lemma 2.4.6. *Let $\mu_1(\xi)$ be defined as in (**??**). We have that*

$$\int_{\mathbb{R}^2} \left(\mu_1(\xi) + \tau^2 - \lambda\right)_- d\xi d\tau = \frac{4}{3} \int_0^\infty (\mu_1(\xi) - \lambda)_-^{3/2} d\xi$$

and that the integrals are finite for all $\lambda \in [0, 1]$.

Proof. In view of (**??**) and Lemma **??**, we observe that,

$$\int_{\mathbb{R}^2} \big(\mu_1(\xi)+\tau^2-\lambda\big)_- d\xi d\tau = \int_0^\infty \int_{-\sqrt{(\mu_1(\xi)-\lambda)_-}}^{\sqrt{(\mu_1(\xi)-\lambda)_-}} \big(\lambda-\mu_1(\xi)-\tau^2\big) d\tau d\xi$$

Performing the change of variable $\sigma = \dfrac{\tau}{\sqrt{(\mu_1(\xi)-\lambda)_-}}$, we find that

$$\int_{\mathbb{R}^2} \big(\mu_1(\xi)+\tau^2-\lambda\big)_- d\xi d\tau = \int_{-1}^{1}(1-\sigma^2)d\sigma \int_0^\infty \big(\mu_1(\xi)-\lambda\big)_-^{3/2} d\xi = \frac{4}{3}\int_0^\infty \big(\mu_1(\xi)-\lambda\big)_-^{3/2} d\xi. \tag{2.4.10}$$

Recall the constant Θ_0 from (**??**). It is easy to see that

$$\int_0^\infty (\mu_1(\xi)-\lambda)_-^{3/2} d\xi \leq (\lambda-\Theta_0)^{1/2} \int_0^\infty (\mu_1(\xi)-\lambda)_- d\xi < \infty.$$

Taking into account Remark **??** completes the proof of the lemma. □

2.5 Model operator in the half-plane

An important model operator that we meet frequently in this thesis is the operator $\mathcal{L}(\theta)$, $\theta \in [0,\pi/2]$, defined by

$$\mathcal{L}(\theta) := -\partial_t^2 - \partial_s^2 + (\cos(\theta)t - \sin(\theta)s)^2, \quad \text{in} \quad L^2(\mathbb{R}^2_+), \tag{2.5.1}$$

with Neumann boundary conditions at $t=0$. Let us recall some fundamental spectral properties of $\mathcal{L}(\theta)$ when $\theta \in (0,\pi/2)$ (see [**?**] for details and references). We denote by $\zeta_1(\theta)$ the infimum of the spectrum of $\mathcal{L}(\theta)$:

$$\zeta_1(\theta) := \inf \mathrm{Spec}(\mathcal{L}(\theta)). \tag{2.5.2}$$

The function $(0,\pi/2) \ni \theta \mapsto \zeta_1(\theta)$ is monotone increasing and the essential spectrum

$$\mathrm{Spec}_{\mathrm{ess}}\mathcal{L}(\theta) = [1,\infty).$$

Moreover, there exists a countable set of eigenvalues of $\mathcal{L}(\theta)$, $(\zeta_j(\theta))_{j\in\mathbb{N}}$ in $[\zeta_1(\theta),1)$. The associated normalized sequence of eigenfunctions will be denoted by $(u_{\theta,j})_{j\in\mathbb{N}}$ and satisfies,

$$\mathcal{L}(\theta)u_{\theta,j} = \zeta_j(\theta)u_{\theta,j}, \tag{2.5.3}$$

$$\langle u_{\theta,j}, u_{\theta,k}\rangle_{L^2(\mathbb{R}^2_+)} = \delta_{j,k}. \tag{2.5.4}$$

Let us denote by $\mathcal{N}(1,\mathcal{L}(\theta))$ the number of eigenvalues of $\mathcal{L}(\theta)$ strictly below 1. It was proved in [**?**] that $\mathcal{N}(1,\mathcal{L}(\theta))$ is finite for all $\theta \in (0,\pi/2)$ and that the number of eigenvalues below the essential spectrum is bounded.

Lemma 2.5.1. *Let $\theta \in (0,\pi/2]$. There exists a constant C such that*

$$\forall \theta \in (0,\pi/2), \quad \mathcal{N}(1,\mathcal{L}(\theta)) \leq \frac{C}{\sin(\theta)}.$$

*Here the constant Θ_0 is defined in (**??**).*

A lower bound on $\mathcal{N}(1, \mathcal{L}(\theta))$ was recently proved in [**?**] :

$$\forall \theta \in (0, \pi/2), \quad \mathcal{N}(1, \mathcal{L}(\theta)) \geq \frac{1 - \Theta_0 \cos\theta}{2\sin(\theta)} + \frac{1}{2}.$$

This was a direct consequence of the estimate

$$\zeta_j(\theta) \leq \Theta_0 \cos(\theta) + (2j-1)\sin(\theta),$$

which was also established in [**?**]. Using the technique of 'Agmon estimates', it is proved in [**?**, Theorem 1.1] that the eigenfunctions of $\mathcal{L}(\theta)$ decays exponentially at infinity. For later use, we record this as

Lemma 2.5.2. *Let $\theta \in (0, \pi/2)$. Given $\lambda \in (0,1)$ and $\alpha \in (0, \sqrt{1-\lambda})$, there exists a positive constant $C_{\theta,\alpha}$ such that, for all eigenpair $(\zeta(\theta), u_\theta)$ of $\mathcal{L}(\theta)$ with $\zeta(\theta) < \lambda$, we have*

$$\mathcal{Q}_\theta(e^{\alpha\sqrt{t^2+s^2}} u_\theta) \leq C_{\alpha,\theta} \|u_\theta\|^2_{L^2(\mathbb{R}_+)},$$

where $\mathcal{Q}_\theta$ is the quadratic form associated with $\mathcal{L}(\theta)$.

2.5.1 Discussion of the condition (**??**)

The condition (**??**) is closely related to the behaviour of the functions $(0, \pi/2) \ni \theta \mapsto \zeta_j(\theta)$. In this concern, we recall the following two results.

Lemma 2.5.3. *[**?**] The functions $\theta \mapsto \zeta_j(\theta)$ are increasing and continuous on $(0, \pi/2)$. Moreover,*

$$\zeta_1(0) = \Theta_0 \quad \text{and} \quad \forall\, \theta \in [0, \pi/2)\,, \quad \zeta_1(\theta) < 1\,.$$

The second Lemma is taken from [**?**].

Lemma 2.5.4. *Let $N \geq 1$ be an integer and suppose that there exists $\theta_* \in (0, \pi/2)$ such that the following assumptions are satisfied*

1. *$\zeta_N(\theta_*) < 1$;*
2. *The eigenvalues $\{\zeta_j(\theta_*)\}_{1 \leq n \leq N}$ are simple.*

Define

$$\theta_{\max,N} := \sup\{\theta \in (0, \pi/2],\ \zeta_N(\theta) < 1\}.$$

Then for all $1 \leq j \leq N$, the functions $\theta \mapsto \zeta_j(\theta)$ are strictly increasing on $(0, \theta_{\max,\mathrm{N}})$.

It is pointed in [**?**] that, to each N, there is θ_* such that the two conditions of Lemms **??** are satisfied. Thus, for every N, the conclusion of Lemma **??** is true. In particular, when $N = 2$ we get,

$$\delta = \min\left(\frac{\zeta_2(0) - \zeta_1(0)}{2}\,, \frac{1 - \Theta_0}{2}\right) > 0\,.$$

By continuity of the functions $\zeta_1(\theta)$ and $\zeta_2(\theta)$, there exists $\epsilon_0 \in (0, \theta_{\max,2})$ such that for all $\theta \in [0, \epsilon_0]$,

$$\zeta_2(\theta) \geq \zeta_1(\theta) + \delta \geq \Theta_0 + \delta.$$

Take $\Lambda \in (\Theta_0, \Theta_0 + \delta)$. That way we get that

$$\forall\, \theta \in [0, \pi/2]\,, \quad \zeta_2(\theta) \geq \Theta_0 + \delta > \Lambda\,,$$

and $\zeta_1(\theta) = \Lambda$ has at most one solution in $[0, \theta_{\max,1}]$. Notice here that $\theta_{\max,1} = \pi/2$ is a consequence of Lemma **??**.

Returning back the condition (**??**) and the above discussion, we see that when the magnetic field is constant of unit length and the domain Ω is the unit ball, the set

$$\Sigma = \{x \in \partial\Omega \; : \; \theta(x) \in (0, \pi/2), \quad \Lambda|\mathbf{B}(x)|^{-1} \in \operatorname{Spec} \mathcal{L}(\theta(x))\}$$

consists of at most one great circle (defined by the solution θ of $\zeta_1(\theta) = \Lambda$). That way the set Σ has measure zero relative to the surface measure and the condition (**??**) is satisfied.

2.6 Gauge invariance

Proposition 2.6.1. *(Gauge transformation) Let $\phi \in H^2(\Omega)$, $\mathbf{A}$ is a given magnetic potential and $\mathcal{P}_{h,\mathbf{A}} := (-ih\nabla + \mathbf{A})^2$. Then, we get the unitary equivalence of $\mathcal{P}_{h,\mathbf{A}}$ and $\mathcal{P}_{h,\mathbf{A}+\nabla\phi}$. Moreover, u is an eigenfunction of $\mathcal{P}^h_{\mathbf{A}}$ if and only if $e^{-i\phi/h}u$ is an eigenfunction of $\mathcal{P}^h_{\mathbf{A}+\nabla\phi}$, and the associated eigenvalues are equal.*

Proof. The proof follows easily by observing that $e^{-i\phi}\mathcal{P}_{h,\mathbf{A}}e^{i\phi} = \mathcal{P}_{h,\mathbf{A}+\nabla\phi}$. □

Remark 2.6.2. Suppose that $\mathbf{A}_1$ and $\mathbf{A}_2$ are two regular magnetic potentials satisfying

$$\operatorname{curl} \mathbf{A}_1 = \operatorname{curl} \mathbf{A}_2.$$

If Ω is simply connected, it follows that there exists $\phi \in H^2_{\mathrm{loc}}(\Omega)$ such that $\mathbf{A}_1 = \mathbf{A}_2 + \nabla\phi$, and the operators $\mathcal{P}_{h,\mathbf{A}_1}$ and $\mathcal{P}_{h,\mathbf{A}_2}$ are unitary equivalent. Consequently, we see that the magnetic field is unchanged by the change of gauge.

2.7 Essential spectrum of Schrödinger operators

Recall the Schrödinger operator $\mathcal{P}_h$ defined in (**??**). If Ω is the complement of a bounded domain of $\mathbb{R}^3$, the operator $\mathcal{P}_h$ can have an essential spectrum. In this case, we need to know the bottom of the essential spectrum of $\mathcal{P}_h$. Persson's Lemma gives a characterisation of the bottom of the essential spectrum of Schrödinger operators with magnetic field (see for instance [**?**, **?**]). The next theorem was proved in [**?**] in the case of domains with boundaries.

Theorem 2.7.1. *[Persson's Lemma] Let Ω be an unbounded domain with Lipschitz boundary. Then the bottom of the essential spectrum of the Neumann realisation of the Schrödinger operator can be expressed as:*

$$\begin{aligned}&\inf \operatorname{Spec}_{\mathrm{ess}}(\mathcal{P}_h + V) \\ &\quad = \sup_{\mathcal{K}\subset\mathbb{R}^d} \left[\inf_{\|\varphi\|_{L^2(\Omega)}=1, \varphi\neq 0} \left\{ \int_\Omega (|(-ih\nabla + \mathbf{A})\varphi|^2 + V|\varphi|^2)dx, \quad \varphi \in C_0^\infty(\overline{\Omega} \cap \mathcal{K}^c) \right\} \right], \end{aligned} \tag{2.7.1}$$

where the infimum is taken over all the compacts $\mathcal{K} \subset \mathbb{R}^d$ and $\mathcal{K}^c = \mathbb{R}^d \setminus \mathcal{K}$.

The following theorem has been established in [**?**, Theorem 3.1].

Theorem 2.7.2. *There exist constants C and $h_0 > 0$ such that, for all $h \in (0, h_0]$, we have :*

$$\int_\Omega |(h\nabla - i\mathbf{A})\varphi|^2 \geq \int_\Omega (h|\mathbf{B}(x)| - Ch^{5/4})|\varphi|^2 dx, \qquad \forall \varphi \in C_0^\infty(\Omega). \tag{2.7.2}$$

Combining Theorems **??** and **??**, we deduce

Corollary 2.7.3. *Let Ω be an exterior domain. Then, there exists a constant $C > 0$ such that for all $h \in (0, h_0]$, we have*

$$\inf \mathrm{Spec}_{\mathrm{ess}} \mathcal{P}_h \geq h(b - Ch^{1/4}),$$

where b is the constant introduced in (**??**).

Proof. Since Ω is an exterior domain, it is therefore the exterior of some compact domain $\mathcal{K}_0 \subset \mathbb{R}^3$, i.e. $\Omega = \mathcal{K}_0^c$. Applying Lemma **??** with $\mathcal{K} = \mathcal{K}_0$ and $V = 0$ yields the assertion of the corollary. ☐

Remark 2.7.4. If $\Lambda \in [0, b)$ then $\Lambda + Ch^{1/4} < b$ for h sufficiently small. Therefore, by Corollary **??**, it is easy to see that the spectrum of $\mathcal{P}_h$ below Λh is purely discrete.

Chapter 3

Model operator in the half-space

The main goal in this chapter is to establish sharp bounds on the number and the sum of eigenvalues of a magnetic Schrödinger operator in a three dimensional strip with infinite hight. The bounds will be valid when the area of the base of the domain tends to infinity. Preliminary results will be introduced in Section **??**. The aforementioned bounds will be presented in Section **??**.

3.1 Auxiliary Lemmas

The next lemma (cf. [**?**]) gives the infimum of the spectrum of the Schrödinger operator in $L^2(\mathbb{R}^3)$ with unit constant magnetic field.

Lemma 3.1.1. *Given* $\theta \in [0, \pi/2]$. *Let*

$$\mathcal{P}_\theta = -\partial_t^2 - \partial_s^2 + (-i\partial_r + t\cos(\theta) - s\sin(\theta))^2$$

be the self-adjoint operator in $L^2(\mathbb{R}^3)$ *generated by the quadratic form*

$$\mathcal{Q}_\theta(u) = \int_{\mathbb{R}^3} \left(|\partial_t u|^2 + |\partial_s u|^2 + |(-i\partial_r + t\cos(\theta) - s\sin(\theta))u|^2\right) drdsdt$$

Then,

$$\inf \operatorname{Spec} \mathcal{P}_\theta = 1.$$

Proof. Since $\operatorname{curl}\left\{(t\cos(\theta) - s\sin(\theta), 0, 0)\right\} = (0, \cos(\theta), \sin(\theta))$ is a normalized vector, we can perform a rotation of angle θ (in the (s,t) coordinates) in order to reduce the problem to that with magnetic vector potential $(t, 0, 0)$. It suffices then to look at the bottom of the spectrum of

$$\widetilde{\mathcal{P}}_\theta = -\partial_t^2 - \partial_s^2 + (-i\partial_r + t)^2$$

After a partial Fourier transform in the variables s and r, the operator $\widetilde{\mathcal{P}}_\theta$ can be thus written as the direct sum (see [**?**]) :

$$\int_{(\xi,\tau)\in\mathbb{R}^2}^{\oplus} -\partial_t^2 - \partial_s^2 + (\xi + t)^2 d\xi d\tau.$$

We are thus reduced to analyse the infimum over $(\xi, \tau) \in \mathbb{R}^2$ of the union of the spectra of the operators

$$\mathcal{P}_{\theta,\xi,\tau} = -\partial_t^2 + \tau^2 + (\xi + t)^2, \qquad (\xi, \tau) \in \mathbb{R}^2.$$

By translation $x = \xi + t$, this infimum is obtained as the infimum over $\tau \in \mathbb{R}$ of the union of the spectra of the operators

$$-\partial_x^2 + x^2 + \tau^2 \qquad \text{in} \quad L^2(\mathbb{R})$$

This is nothing but the infimum of the spectrum of the harmonic oscillator $-\partial_x^2 + x^2$ in $L^2(\mathbb{R})$ which is 1. The statement of the lemma is thus proved. □

We will henceforth use the following notations:

1. Given $\eta \in \mathbb{R}$ and a self-adjoint operator $\mathcal{H}$ and $E_{\mathcal{H}}(\eta)$ is the spectral measure associated with $\mathcal{H}$, we shall denote by
$$\mathcal{N}(\eta; \mathcal{H}, \Omega) := \dim \operatorname{ran} E_{\mathcal{H}}((-\infty, \eta)) \tag{3.1.1}$$
If the spectrum below η is discrete, then $\mathcal{N}(\eta; \mathcal{H}, \Omega)$ coincides with the number of eigenvalues (counting multiplicities) below η.

2. If the spectrum below η is discrete and $\{\lambda_j(\mathcal{H})\}_j$ are the eigenvalues of $\mathcal{H}$ below η, then we denote by
$$\mathcal{E}(\eta; \mathcal{H}, \Omega) := \operatorname{Tr}\big(\mathcal{H} - \eta\big)_- = \sum_j (\lambda_j(\mathcal{H}) - \eta)_- \tag{3.1.2}$$
the sum (the energy) of eigenvalues below η.

Based on the variational principle, we include

Lemma 3.1.2. *Let Ω be a subset of $\mathbb{R}^3$. Suppose that P is a positive self-adjoint operator on $L^2(\Omega)$ such that the spectrum below 1 is discrete. Let $\lambda \in [0, 1)$ and $\varsigma \in \mathbb{R}$ such that $-\lambda \leq \varsigma < 1 - \lambda$. Then we have*

$$\mathcal{E}(\lambda + \varsigma; P, \Omega) \leq \mathcal{E}(\lambda; P, \Omega) + \varsigma \mathcal{N}(\lambda + \varsigma; P, \Omega), \tag{3.1.3}$$

where $\mathcal{N}(\cdot; P, \Omega)$ and $\mathcal{E}(\cdot; P, \Omega)$ are introduced in (**??**) *and* (**??**) *respectively.*

Proof. Let $\{\lambda_k\}_{k=1}^N$ be the family of eigenvalues below $\lambda + \varsigma$ for P and $\{g_k\}_{k=1}^N$ are associated (normalized) eigenfunctions. Let us define the trial density matrix $\gamma : L^2(\Omega) \ni f \mapsto \gamma f \in L^2(\Omega)$,

$$\gamma f = \sum_{1 \leq k \leq N} \langle f, g_k \rangle g_k.$$

For all normalized $f \in L^2(\Omega)$, it follows by Bessel's inequality that

$$0 \leq \langle \gamma f, f \rangle_{L^2(\Omega)} \leq \|f\|^2_{L^2(\Omega)} = 1.$$

By Lemma **??**, we deduce that

$$-\mathcal{E}(\lambda; P, \Omega) := -\operatorname{Tr}\big(P - \lambda\big)_- \leq \operatorname{Tr}\big((P - \lambda)\gamma\big). \tag{3.1.4}$$

It is easy to see that

$$\operatorname{Tr}\big((P - \lambda)\gamma\big) = \sum_{1 \leq k \leq N} (\lambda_k - \lambda) = \sum_{1 \leq k \leq N} (\lambda_k - \lambda - \varsigma) + \varsigma \sum_{1 \leq k \leq N} 1. \tag{3.1.5}$$

Therefore, (**??**) reads

$$\operatorname{Tr}\big((P - \lambda)\gamma\big) = -\mathcal{E}(\lambda + \varsigma; P, \Omega) + \varsigma \mathcal{N}(\lambda + \varsigma; P, \Omega). \tag{3.1.6}$$

Inserting this into (**??**), we finally get,

$$-\mathcal{E}(\lambda; P, \Omega) \leq -\mathcal{E}(\lambda + \varsigma; P, \Omega) + \varsigma \mathcal{N}(\lambda + \varsigma; P, \Omega)$$

which is the assertion of the lemma. □

In order to state Lemma **??** below, we need to define the reflected magnetic Schrödinger operator in $L^2(\mathbb{R}^3)$ associated with the Neumann Schrödinger operator in $L^2(\mathbb{R}^3_+)$.

Given $\theta \in [0, \pi/2]$, we consider the magnetic field

$$\widetilde{\mathbf{F}}_\theta(r,s,t) := (0,0,|t|\cos(\theta) - s\sin(\theta)), \qquad (r,s,t) \in \mathbb{R}^3. \tag{3.1.7}$$

Let

$$\widetilde{\mathcal{P}}_\theta = (-i\nabla + \widetilde{\mathbf{F}}_\theta)^2 \qquad \text{in} \qquad L^2(\mathbb{R}^3), \tag{3.1.8}$$

be the self-adjoint operator generated by the quadratic form

$$\widetilde{\mathcal{Q}}_\theta(u) := \int_{\mathbb{R}^3} |(-i\nabla + \widetilde{\mathbf{F}}_\theta)u|^2 drdsdt, \tag{3.1.9}$$

with form domain

$$\mathcal{D}(\widetilde{\mathcal{Q}}_\theta) := \left\{ u \in L^2(\mathbb{R}^3) \ : \ (-i\nabla + \widetilde{\mathbf{F}}_\theta)u \in L^2(\mathbb{R}^3) \right\}. \tag{3.1.10}$$

We let $\beta = (0, \cos(\theta), \sin(\theta))$ denote the constant magnetic field generated by the vector potential :

$$\mathbf{F}_\theta(r,s,t) = (0,0,t\cos(\theta) - s\sin(\theta)), \qquad (r,s,t) \in \mathbb{R}^3_+. \tag{3.1.11}$$

Furthermore, let

$$\mathcal{P}^N_\theta = (-i\nabla + \mathbf{F}_\theta)^2 \qquad \text{in} \qquad L^2(\mathbb{R}^3_+), \tag{3.1.12}$$

be the self-adjoint (Neumann) Schrödinger operator associated with the quadratic form

$$\mathcal{Q}^N_\theta(u) := \int_{\mathbb{R}^3_+} |(-i\nabla + \mathbf{F}_\theta)u|^2 drdsdt, \tag{3.1.13}$$

defined for all functions u in the form domain

$$\mathcal{D}(\mathcal{Q}^N_\theta) := \left\{ u \in L^2(\mathbb{R}^3_+) \ : \ (-i\nabla + \mathbf{F}_\theta)u \in L^2(\mathbb{R}^3_+) \right\}. \tag{3.1.14}$$

The next lemma allows us to compare the eigenvalue counting function and the energy of eigenvalues for a perturbation of $\mathcal{P}^N_\theta$ in the half space $\mathbb{R}^3_+$ with the corresponding functions for $\widetilde{\mathcal{P}}_\theta$ in the whole space $\mathbb{R}^3$.

Lemma 3.1.3. *Let $\mathcal{U}$ be a positive bounded potential in $L^2(\mathbb{R}^3)$ verifying $\mathcal{U}(\cdot,\cdot,-t) = \mathcal{U}(\cdot,\cdot,t)$. Assume that the spectrum of $\mathcal{P}^N_\theta + \mathcal{U}$ below λ is discrete. Then, we have*

$$\mathcal{N}(\lambda; \mathcal{P}^N_\theta + \mathcal{U}, \mathbb{R}^3_+) \le C_{\mathrm{CLR}} \int_{\mathbb{R}^3} (\mathcal{U}_-)^{3/2} drdsdt$$

and

$$\mathcal{E}(\lambda; \mathcal{P}^N_\theta + \mathcal{U}, \mathbb{R}^3_+) \le C_{\mathrm{LT}} \int_{\mathbb{R}^3} (\mathcal{U}_-)^{5/2} drdsdt$$

Proof. Given $n \in \mathbb{N}$. Let $\{u_j\}_{j=1}^n$ be an orthonormal family of eigenfunctions with corresponding eigenvalues $\{\mu_j\}_{j=1}^n$ associated with the operator $\mathcal{P}^N_\theta + \mathcal{U}$ in $L^2(\mathbb{R}^3_+)$. We define the extension to $\mathbb{R}^3$ of the function u_j by :

$$\widetilde{u}_j(r,s,t) = \begin{cases} \frac{1}{\sqrt{2}} u_j(r,s,t) & t \ge 0 \\ \frac{1}{\sqrt{2}} u_j(r,s,-t) & t < 0. \end{cases} \tag{3.1.15}$$

Since $\{u_j\}_{j=1}^n$ are normalized and pairwise orthogonal, we get for all $1 \leq j,k \leq n$,

$$\langle \widetilde{u}_j, \widetilde{u}_k \rangle_{L^2(\mathbb{R}^3)} = \langle u_j, u_k \rangle_{L^2(\mathbb{R}^3_+)} = \delta_{j,k}, \tag{3.1.16}$$

where $\delta_{j,k}$ is the Kronecker symbol.

The bilinear form associated with $\widetilde{\mathcal{Q}}_\theta + \mathcal{U}$ is defined on the form domain by:

$$\widetilde{a}_{\theta,\mathcal{U}}(u,v) = \int_{\mathbb{R}^3} \Big((-i\nabla + \widetilde{\mathbf{F}}_\theta) u \overline{(-i\nabla + \widetilde{\mathbf{F}}_\theta) v} + \mathcal{U} u \overline{v} \Big)\, drdsdt.$$

Here the magnetic field $\widetilde{\mathbf{F}}_\theta$ is the same as in (**??**).

It is easy to see that the functions $\{\widetilde{u}_j\}_j$ belong to the form domain $\mathcal{D}(\widetilde{\mathcal{Q}}_\theta)$. Indeed, by construction we have

$$\widetilde{\mathcal{Q}}_\theta(\widetilde{u}_j) = \mathcal{Q}_\theta^N(u_j). \tag{3.1.17}$$

Using the definition of $\widetilde{u}_j$ in (**??**) and the fact that the potential $\mathcal{U}$ is symmetric in the t-variable, we obtain for all $1 \leq j,k \leq n$,

$$\widetilde{a}_{\theta,\mathcal{U}}(\widetilde{u}_j, \widetilde{u}_k) = \langle u_j, (\mathcal{P}_\theta^N + \mathcal{U}) u_k \rangle_{L^2(\mathbb{R}^3_+)}. \tag{3.1.18}$$

Since the $\{u_j\}_{j=1}^n$ are eigenfunctions of $\mathcal{P}_\theta^N + \mathcal{U}$, we get using (**??**),

$$\widetilde{a}_{\theta,\mathcal{U}}(\widetilde{u}_j, \widetilde{u}_k) = \delta_{j,k} \mu_k, \tag{3.1.19}$$

for all $1 \leq j,k \leq n$.

Let $\widetilde{\mu}_n$ be the n-th eigenvalue of $\widetilde{\mathcal{P}}_\theta + \mathcal{U}$ defined by the min-max principle. Owing to (**??**) and (**??**) we find,

$$\widetilde{\mu}_n = \inf_{v_1,\cdots v_n \in \mathcal{D}(\widetilde{\mathcal{Q}}_\theta)} \max_{\substack{v \in [v_1,\cdots,v_n] \\ \|v\|=1}} \widetilde{a}_{\theta,\mathcal{U}}(v,v) \leq \max_{v \in [\widetilde{u}_1,\cdots,\widetilde{u}_n]} \widetilde{a}_{\theta,\mathcal{U}}(v,v) = \mu_n,$$

This yields

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^N + \mathcal{U}, \mathbb{R}^3_+) \leq \mathcal{N}(\lambda; \widetilde{\mathcal{P}}_\theta + \mathcal{U}, \mathbb{R}^3), \tag{3.1.20}$$

and

$$\mathcal{E}(\lambda; \mathcal{P}_\theta^N + \mathcal{U}, \mathbb{R}^3_+) \leq \mathcal{E}(\lambda; \widetilde{\mathcal{P}}_\theta + \mathcal{U}, \mathbb{R}^3). \tag{3.1.21}$$

The lemma follows by applying Theorem **??** (resp. Theorem **??**) to the right-hand side of (**??**) (resp. (**??**)). $\square$

3.2 Schrödinger operator in a half-cylinder

Consider a positive real numbers L, and define the domain

$$\Omega^L = \Big(-\frac{L}{2}, \frac{L}{2} \Big)^2 \times \times \mathbb{R}_+. \tag{3.2.1}$$

In this section, we will analyse the magnetic Schrödinger operator

$$\mathcal{P}_\theta^L = (-i\nabla + \mathbf{F}_\theta)^2 \quad \text{in} \quad L^2(\Omega^L) \tag{3.2.2}$$

with Neumann boundary conditions at $t = 0$, and Dirichlet boundary conditions at $r \in \{-\frac{L}{2}, \frac{L}{2}\}$ and $s \in \{-\frac{L}{2}, \frac{L}{2}\}$. Here, for $\theta \in [0, \pi/2]$, $\mathbf{F}_\theta$ is the magnetic potential introduced in (**??**).

The operator $\mathcal{P}_\theta^L$ is the Friedrich's extension in $L^2(\Omega^L)$ associated with the semi-bounded quadratic form

$$\mathcal{Q}_\theta^L(u) = \int_{\Omega^L} |(-i\nabla + \mathbf{F}_\theta)u|^2 drdsdt\,. \tag{3.2.3}$$

The form domain of $\mathcal{Q}_\theta^L$ is :

$$\mathcal{D}(\mathcal{Q}_\theta^L) = \Big\{u \in L^2(\Omega^L) \,:\, (-i\nabla + \mathbf{F}_\theta)u \in L^2(\Omega^L), \quad u\Big(-\frac{L}{2},\cdot,\cdot\Big) = u\Big(\frac{L}{2},\cdot,\cdot\Big) = 0,$$
$$u\Big(\cdot,-\frac{L}{2},\cdot\Big) = u\Big(\cdot,\frac{L}{2},\cdot\Big) = 0\Big\}. \tag{3.2.4}$$

The following lemma rules out the existence of essential spectrum of $\mathcal{P}_\theta^L$ below some $\lambda \in [0,1)$.

Lemma 3.2.1. *Let $\theta \in (0,\pi/2]$. The infimum of the essential spectrum of $\mathcal{P}_\theta^L$ satisfies*

$$\inf \mathrm{Spec}_{\mathrm{ess}} \mathcal{P}_\theta^L \geq 1.$$

Here, it is used the convention that the infimum of an empty set is $+\infty$ in the case of purely discrete spectrum.

Proof. Since any compactly supported function $u \in C_0^\infty(\Omega^L)$ can be extended by 0 to $\mathbb{R}^3$, we get by Lemma **??** the following inequality

$$\int_{\Omega^L} |(-i\nabla + \mathbf{F}_\theta)u|^2 drdsdt \geq \int_{\Omega^L} |u|^2 drdsdt, \qquad \forall u \in C_0^\infty(\Omega^L).$$

Apply then Lemma **??** with $\mathcal{K} = [-L/2, L/2] \times [-L/2, L/2] \times \{0\}$ leads to the desired conclusion. □

The next lemma establishes super-additivity properties of the counting function and the sum of eigenvalues for $\mathcal{P}_\theta^L$.

Lemma 3.2.2. *For all $n \in \mathbb{N}$, $\lambda \in [0,1)$ and $L > 0$, we have,*

$$\frac{\mathcal{N}(\lambda; \mathcal{P}_\theta^{nL}, \Omega^{nL})}{n^2L^2} \geq \frac{\mathcal{N}(\lambda; \mathcal{P}_\theta^{L}, \Omega^{L})}{L^2} \tag{3.2.5}$$

and

$$\frac{\mathcal{E}(\lambda; \mathcal{P}_\theta^{nL}, \Omega^{nL})}{n^2L^2} \geq \frac{\mathcal{E}(\lambda; \mathcal{P}_\theta^{L}, \Omega^{L})}{L^2}. \tag{3.2.6}$$

Proof. Let $j,k \in \mathbb{N}$ such that $0 \leq j,k \leq n-1$. Let us define the domain

$$\Omega_{j,k}^L := \Big(\frac{(-n+2j)L}{2}, \frac{(-n+2j+2)L}{2}\Big) \times \Big(\frac{(-n+2k)L}{2}, \frac{(-n+2k+2)L}{2}\Big) \times \mathbb{R}_+.$$

We next consider the self-adjoint operator $\mathcal{P}_{\theta,j,k}^L$ generated by the quadratic form

$$\mathcal{Q}_{\theta,j,k}^L(u) = \int_{\Omega_{j,k}^L} |(-i\nabla + \mathbf{F}_\theta)u|^2 drdsdt, \tag{3.2.7}$$

with domain,

$$\mathcal{D}(\mathcal{Q}_{\theta,j,k}^L) = \Big\{u \in L^2(\Omega^L) \,:\, (-i\nabla + \mathbf{F}_\theta)u \in L^2(\Omega_{j,k}^L),$$
$$u\Big(\frac{(-n+2j)L}{2},\cdot,\cdot\Big) = u\Big(\frac{(-n+2j+2)L}{2},\cdot,\cdot\Big) = 0,$$
$$u\Big(\cdot,\frac{(-n+2k)L}{2},\cdot\Big) = u\Big(\cdot,\frac{(-n+2k+2)L}{2},\cdot\Big) = 0\Big\}. \tag{3.2.8}$$

Taking boundary conditions into account, we observe that for all $u = \sum_{j,k} u_{j,k} \in \oplus_{j,k}\mathcal{D}(\mathcal{Q}^L_{\theta,j,k})$,

$$\mathcal{Q}^{nL}_\theta(u) = \sum_{j,k} \mathcal{Q}^L_{\theta,j,k}(u_{i,j}).$$

This implies that, in the sense of quadratic forms,

$$\mathcal{P}^{nL}_\theta \leq \bigoplus\nolimits_{j,k} \mathcal{P}^L_{\theta,j,k}. \tag{3.2.9}$$

Hence, we get by the min-max principle that,

$$\sum_{j,k} \mathcal{N}(\lambda; \mathcal{P}^L_{\theta,j,k}, \Omega^L_{j,k}) \leq \mathcal{N}(\lambda; \mathcal{P}^{nL}_\theta, \Omega^{nL}), \qquad \forall\, 1 \leq j,k \leq n. \tag{3.2.10}$$

Since the operator $\mathcal{P}^L_{\theta,j,k}$ is unitarily equivalent to $\mathcal{P}^L_\theta$ by magnetic translation invariance, we have that,

$$\mathcal{N}(\lambda; \mathcal{P}^L_{\theta,j,k}, \Omega^L_{j,k}) = \mathcal{N}(\lambda; \mathcal{P}^L_\theta, \Omega^L), \qquad \forall\, 1 \leq j,k \leq n.$$

Therefore, the inequality (**??**) becomes,

$$n^2 \mathcal{N}(\lambda; \mathcal{P}^L_\theta, \Omega^L) \leq \mathcal{N}(\lambda; \mathcal{P}^{nL}_\theta, \Omega^{nL}).$$

This gives (**??**) upon dividing both sides by L^2.

Similarly, the inequality (**??**) follows from (**??**) and magnetic translation invariance. $\square$

We show in the next lemma a rough bound on the number and the sum of eigenvalues of $\mathcal{P}^L_\theta$ in terms of L^2.

Lemma 3.2.3. *Let $L > 0$. There exists a constant C such that for all $\lambda \in [0,1)$ and $\theta \in [0, \pi/2]$, it holds true that*

$$\frac{\mathcal{N}(\lambda; \mathcal{P}^L_\theta, \Omega_L)}{L^2} \leq \frac{C}{\sqrt{1-\lambda}}, \tag{3.2.11}$$

and

$$\frac{\mathcal{E}(\lambda; \mathcal{P}^L_\theta, \Omega_L)}{L^2} \leq \frac{C}{\sqrt{1-\lambda}}, \tag{3.2.12}$$

where $\mathcal{N}(\lambda; \mathcal{P}^L_\theta, \Omega_L)$ and $\mathcal{E}(\lambda; \mathcal{P}^L_\theta, \Omega_L)$ are defined in (**??**) *and* (**??**) *respectively.*

Proof. Let $(\psi_1(t), \psi_2(t))$ be a partition of unity on $\mathbb{R}_+$ with $\psi_1^2(t) + \psi_2^2(t) = 1$ and:

$$\begin{cases} \psi_1(t) = 1 & \text{if} \quad 0<\text{t}<1, \\ \psi_1(t) = 0 & \text{if} \quad \text{t}>2. \end{cases} \tag{3.2.13}$$

Let $T > 1$ be a large number to be chosen later. We consider the following two sets

$$\Omega_1^T = \Big\{(r,s,t) \in \Big(-\frac{L}{2}, \frac{L}{2}\Big)^2 \times \mathbb{R}_+ \,:\, 0 < t < 2T\Big\},$$

and

$$\Omega_2^T = \Big\{(r,s,t) \in \Big(-\frac{L}{2}, \frac{L}{2}\Big)^2 \times \mathbb{R}_+ \,:\, t > T\Big\}.$$

We define the partition of unity $(\psi_{1,T}(t), \psi_{2,T}(t))$ by

$$\psi_{1,T}(t) = \psi_1\left(\frac{t}{T}\right), \qquad \psi_{2,T}(t) = \psi_2\left(\frac{t}{T}\right)$$

We have $\psi'_{k,T}(t) = \frac{1}{T}\psi'_k(\frac{t}{T})$. Thus we deduce that there exists a constant $C_0 > 0$ so that

$$\sum_{k=1}^{2} |\psi'_k(t)|^2 \leq \frac{C_0}{T^2}. \tag{3.2.14}$$

By the IMS formula, we find for all $u \in \mathcal{D}(\mathcal{Q}_\theta^L)$

$$\mathcal{Q}_\theta^L(u) = \sum_{k=1}^{2} \mathcal{Q}_\theta^L(\psi_{k,T}u) - \int_{\Omega^L} \mathcal{U}_T(t)|u|^2 drdsdt, \tag{3.2.15}$$

where

$$\mathcal{U}_T(t) = \sum_{k=1}^{2} |\psi'_{k,T}(t)|^2.$$

Using (**??**), we further get

$$\mathcal{Q}_\theta^L(u) \geq \sum_{k=1}^{2} \mathcal{Q}_\theta^L(\psi_{k,T}u) - \frac{C_0}{T^2}\int_{\Omega^L} |u|^2 drdsdt. \tag{3.2.16}$$

Let us denote by $\mathcal{P}_{\theta,1}^L$ and $\mathcal{P}_{\theta,2}^L$ the self-adjoint operators associated with the following quadratic forms :

$$\mathcal{Q}_{\theta,1}^L(u) = \int_{\Omega_1^T} \Big[|\partial_t u|^2 + |\partial_s u|^2 + |(-i\partial_r + t\cos(\theta) - s\sin(\theta))u|^2\Big] drdsdt, \tag{3.2.17}$$

$$\begin{aligned}\mathcal{D}(\mathcal{Q}_{\theta,1}^L) := \big\{ u \in L^2(\Omega_1^T) \ : \ (-i\nabla + \mathbf{F}_\theta)u \in L^2(\Omega_1^T), \quad u(2T,\cdot,\cdot) = 0,\\ \Big(-\frac{L}{2},\cdot,\cdot\Big) = u\Big(\frac{L}{2},\cdot,\cdot\Big) = 0, \quad u\Big(\cdot,-\frac{L}{2},\cdot\Big) = u\Big(\cdot,\frac{L}{2},\cdot\Big) = 0\big\}, \end{aligned} \tag{3.2.18}$$

and

$$\mathcal{Q}_{\theta,2}^L(u) = \int_{\Omega_2^T} \Big[|\partial_t u|^2 + |\partial_s u|^2 + |(-i\partial_r + t\cos(\theta) - s\sin(\theta))u|^2\Big] drdsdt, \tag{3.2.19}$$

$$\begin{aligned}\mathcal{D}(\mathcal{Q}_{\theta,2}^L) := \big\{ u \in L^2(\Omega_2^T) \ : \ (-i\nabla + \mathbf{F}_\theta)u \in L^2(\Omega_2^T), \quad u(T,\cdot,\cdot) = 0,\\ \Big(-\frac{L}{2},\cdot,\cdot\Big) = u\Big(\frac{L}{2},\cdot,\cdot\Big) = 0, \quad u\Big(\cdot,-\frac{L}{2},\cdot\Big) = u\Big(\cdot,\frac{L}{2},\cdot\Big) = 0\big\}, \end{aligned} \tag{3.2.20}$$

respectively.

It is clear from (**??**) that,

$$\mathcal{Q}_\theta^L(u) \geq \mathcal{Q}_{\theta,1}^L(\psi_{1,T}u) + \mathcal{Q}_{\theta,2}^L(\psi_{2,T}u) - \frac{C_0}{T^2}\int_{\Omega^L} |u|^2 drdsdt. \tag{3.2.21}$$

Consider the isometry

$$j : L^2(\Omega^L) \mapsto L^2(\Omega_1^T) \oplus L^2(\Omega_2^T) \tag{3.2.22}$$

$$u \mapsto (\psi_{1,T}u, \psi_{2,T}u). \tag{3.2.23}$$

Let us define the quadratic form q_θ^L on $\mathcal{D}(\mathcal{Q}_{\theta,1}^L) \oplus \mathcal{D}(\mathcal{Q}_{\theta,2}^L)$ by

$$q_\theta^L(u_1, u_2) = \mathcal{Q}_{\theta,1}^L(u_1) + \mathcal{Q}_{\theta,1}^L(u_2).$$

Then, (**??**) reads

$$\mathcal{Q}_\theta^L(u) \geq q_\theta^L(j(u)) - \frac{C_0}{T^2}\int_{\Omega^L} |u|^2 drdsdt.$$

Applying Lemma **??** yields

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^L, \Omega^L) \leq \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L \oplus \mathcal{P}_{\theta,2}^L, \Omega^L). \tag{3.2.24}$$

It follows that

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^L, \Omega^L) \leq \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L, \Omega_1^T) + \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,2}^L, \Omega_2^T). \tag{3.2.25}$$

The Dirichlet boundary conditions imposed at $r \in \{-\frac{L}{2}, \frac{L}{2}\}$, $s \in \{\frac{L}{2}, \frac{L}{2}\}$ and $t = T$ ensures that the estimate (**??**) remains true if we replace Ω_2^T by $\mathbb{R}^3$ in the definition of $\mathcal{Q}_{\theta,2}^L$. More precisely,

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^L; \Omega^L) \leq \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L, \Omega_1^T) + \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_\theta, \mathbb{R}^3) \tag{3.2.26}$$

where $\mathcal{P}_\theta$ is the self-adjoint operator introduced in Lemma **??**.

By Lemma **??**, we know that the first eigenvalue of the Schrödinger operator with constant unit magnetic field in $L^2(\mathbb{R}^3)$ is equal to 1. We thus have

$$\begin{aligned}\mathcal{Q}_\theta(u) &= \int_{\mathbb{R}^3} \left[|\partial_t u|^2 + |\partial_s u|^2 + |(-i\partial_r + t\cos(\theta) - s\sin(\theta))u|^2\right] drdsdt \\ &\geq \int_{\mathbb{R}^3} |u|^2 drdsdt.\end{aligned} \tag{3.2.27}$$

Choose $T = 2\sqrt{\dfrac{C_0}{1-\lambda}}$, it holds that $1 > \lambda + C_0 T^{-2}$ and

$$\mathcal{Q}_\theta(u) > (\lambda + C_0 T^{-2}) \int_{\mathbb{R}^3} |u|^2 drdsdt.$$

This clearly gives $\mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_\theta, \mathbb{R}^3) = 0$. Thus, it remains to estimate $\mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L, \Omega_1^T)$. To do this, we introduce a potential V satisfying

$$\begin{cases} V \geq 0, \\ \text{supp } V \subset \mathbb{R}_+^3 \setminus \Omega_1^T. \end{cases} \tag{3.2.28}$$

Under these assumptions on V, we may write for all $u \in D(\mathcal{Q}_{\theta,1}^L)$,

$$\int_{\Omega_1^T} \left|(-i\nabla + \mathbf{F}_\theta)u\right|^2 drdsdt = \int_{\Omega_1^T} \left|(-i\nabla + \mathbf{F}_\theta)u\right|^2 drdsdt + \int_{\mathbb{R}_+^3} V(x)|u|^2 drdsdt. \tag{3.2.29}$$

Here, we have extended u by 0 to the whole of $\mathbb{R}_+^3$ in the last integral. Therefore, it follows from the min-max principle that :

$$\mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L, \Omega_1^T) = \mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L + V, \Omega_1^T). \tag{3.2.30}$$

Since any function u that belongs to the form domain of $\mathcal{Q}_\theta^{L_1,L_2}$ can be extended by 0 to the half space $\mathbb{R}_+^3$, we get using the bound in (**??**) and the min-max principle that

$$\mathcal{N}(\lambda + C_0 T^{-2}; \mathcal{P}_{\theta,1}^L + V, \Omega_1^T) \leq \mathcal{N}(\lambda; \mathcal{P}_\theta^N + V_1, \mathbb{R}_+^3), \tag{3.2.31}$$

where

$$V_1 = V - \frac{C_0}{T^2}.$$

Define the potential in $\mathbb{R}^3_+$

$$V(r,s,t) := \left(1 + \frac{C_0}{T^2}\right) \mathbf{1}_{\mathbb{R}^3_+ \setminus \Omega_1^T}.$$

It is easy to check that V satisfies the assumptions in (**??**). To V we associate the reflected potential in $\mathbb{R}^3$ defined by

$$\widetilde{V}(r,s,t) := \left(1 + \frac{C_0}{T^2}\right) \mathbf{1}_{\mathbb{R}^3 \setminus \widetilde{\Omega}_1^T},$$

with

$$\widetilde{\Omega}_1^T = \Big\{(r,s,t) \in \Big(-\frac{L}{2}, \frac{L}{2}\Big)^2 \times \mathbb{R} \,:\, |t| < 2T\Big\}.$$

In view of Lemma **??**, we have,

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^N + V_1, \mathbb{R}^3_+) \leq C_{\mathrm{CLR}} \int_{\mathbb{R}^3} (\lambda - \widetilde{V}_1)_+^{3/2} drdsdt \tag{3.2.32}$$

where

$$\widetilde{V}_1 = \widetilde{V} - \frac{C_0}{T^2}.$$

Next, we compute the integral

$$\int_{\mathbb{R}^3} (\lambda - \widetilde{V}_1)_+^{3/2} drdsdt = 2\lambda^{3/2} \int_{\widetilde{\Omega}_1^T} drdsdt = 4\lambda^{3/2} L^2 T.$$

Inserting this in (**??**), we obtain

$$\mathcal{N}(\lambda; \mathcal{P}_\theta^N + V_1, \mathbb{R}^3_+) \leq 4 C_{\mathrm{CLR}} \lambda^{3/2} L^2 T. \tag{3.2.33}$$

Combining the estimates (**??**),(**??**),(**??**) and (**??**) gives (**??**) upon inserting the choice $T = 2\sqrt{\frac{C_0}{1-\lambda}}$.

In a similar fashion, we can prove (**??**) by following the steps of the proof of (**??**), and using Lemma **??** (the energy case). $\square$

Chapter 4

The large area limit

Consider $\theta \in [0, \pi/2]$ and a positive L. Recall the self-adjoint operator $\mathcal{P}_\theta^L$ defined in (??). In accordance with the definition of $\mathcal{E}$ in (??), we write, for $\lambda \in [0, 1)$,

$$\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L) = \sum_j \left(\zeta_j^L(\theta) - \lambda\right)_-,$$

where $\{\zeta_j^L(\theta)\}_j$ denote the eigenvalues of $\mathcal{P}_\theta^L$.

In Section ??, we are interested in the behaviour of $\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L)$ as L approach ∞. We will obtain a function $E(\theta, \lambda)$ (see Theorem ?? below) such that the leading order asymptotics

$$\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L) \sim E(\theta, \lambda) L^2$$

holds true as $L \to \infty$. The approach we use is borrowed from [?, ?], where several limiting functions related to the Ginzburg-Landau functional are constructed. In Section ??, we derive a few properties of the limiting function found in Section ??. Explicit formulas are computed in Section ?? using the spectral decomposition of the model operators of the half-axis and the half-plane.

4.1 The function $E(\theta, \lambda)$

In this section, we prove the following theorem.

Theorem 4.1.1. *Let $\theta \in [0, \pi/2]$ and $\lambda \in [0, 1)$. There exists a constant $E(\theta, \lambda)$ such that*

$$\liminf_{L\to\infty} \frac{\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L)}{L^2} = \limsup_{L\to\infty} \frac{\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L)}{L^2} = E(\theta, \lambda). \tag{4.1.1}$$

Moreover, for all $\lambda_0 \in [0, 1)$, there exist constants L_0 and C_0 such that,

$$E(\theta, \lambda) - \frac{2C_0}{L^{2/3}} \le \frac{\mathcal{E}(\lambda; \mathcal{P}_\theta^L, \Omega^L)}{L^2} \le E(\theta, \lambda), \tag{4.1.2}$$

for all $\theta \in [0, \pi/2]$, $\lambda \in [0, \lambda_0]$, $L \ge 2L_0$.

Remark 4.1.2. The constants C_0 and L_0 are independent of the $(\lambda, \theta, L) \in [0, \lambda_0] \times [0, \pi/2] \times [2L_0, \infty)$.

Remark 4.1.3. We point out that explicit formulas of $E(\theta,\lambda)$ will be given ahead in Section **??**. This was an alternative approach before we are able to compute it explicitly. The reason we keep it is that it helps in studying properties of $E(\theta,\lambda)$.

The proof of Theorem **??** relies on the following lemma, which is proved in [**?**, Lemma 2.2].

Lemma 4.1.4. *Consider a decreasing function $d : (0,\infty) \to (-\infty, 0]$ such that the function $f : (0,\infty) \ni L \mapsto \frac{d(L)}{L} \in \mathbb{R}$ is bounded.*

Suppose that there exist constants $C > 0$, $L_0 > 0$ such that the estimate

$$f(nL) \geq f((1+a)L) - C\left(a + \frac{1}{a^2L^2}\right), \tag{4.1.3}$$

holds true for all $a \in (0,1)$, $n \in \mathbb{N}$, $L \geq L_0$. Then $f(L)$ has a limit A as $L \to \infty$. Furthermore, for all $L \geq 2L_0$, the following estimate holds true,

$$f(L) \leq A + \frac{2C}{L^{2/3}}\,. \tag{4.1.4}$$

In order to use the result of Lemma **??**, we establish the estimate in the Lemma **??** below.

Lemma 4.1.5. *Let $\lambda_0 \in [0,1)$, $\theta \in [0,\pi/2]$. There exist constants $C_0 > 0$ and $L_0 \geq 1$ such that, for all $L \geq L_0$, $\lambda \in [0,\lambda_0]$, $n \in \mathbb{N}$ and $a \in (0,1)$, we have,*

$$\frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL})}{n^2L^2} \leq \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L})}{(1+a)^2L^2} + C_0\left(\frac{1}{a^2L^2} + a\right).$$

Furthermore, the function

$$L \mapsto \mathcal{E}(\lambda;\mathcal{P}_\theta^{L},\Omega^{L})$$

is monotone increasing.

Proof. Let $n \geq 2$ be a natural number. If $a \in (0,1)$ and $j = (j_1,j_2) \in \mathbb{Z}^2$, let

$$K_{a,j} = I_{j_1} \times I_{j_2}\,,$$

where

$$\forall\, p \in \mathbb{Z}\,, \quad I_p = \left(\frac{2p+1-n}{2} - \frac{(1+a)}{2}\,,\ \frac{2p+1-n}{2} + \frac{(1+a)}{2}\right).$$

Consider a partition of unity $(\chi_j)_j$ of $\mathbb{R}^2$ such that:

$$\sum_j |\chi_j|^2 = 1\,, \quad 0 \leq \chi_j \leq 1 \quad \text{in } \mathbb{R}^2\,, \quad \operatorname{supp}\chi_j \subset K_{a,j}\,, \quad |\nabla\chi_j| \leq \frac{C}{a}\,, \tag{4.1.5}$$

where C is a universal constant. We define $\chi_{j,L}(r,s) = \chi_j\left(\frac{r}{L},\frac{s}{L}\right)$. We thus obtain a new partition of unity $\{\chi_{j,L}\}_{j\in\mathcal{J}}$ such that $\operatorname{supp}\chi_{j,L} \subset \mathcal{K}_{a,j,L}$, with

$$\mathcal{K}_{a,j,L} = \{(Lr, Ls) \ :\ (r,s) \in K_{a,j}\}\,.$$

Let $\mathcal{J} = \{j = (j_1,j_2) \in \mathbb{Z}^2 \ :\ 0 \leq j_1, j_2 \leq n-1\}$ and $K^{nL} = \left(-\frac{nL}{2},\frac{nL}{2}\right)^2$. Then the family $\{\mathcal{K}_{a,j,L}\}_{j\in\mathcal{J}}$ is a covering of K^{nL}, and is formed of exactly n^2 squares with side length L.

We restrict the partition of unity $\{\chi_{j,L}\}_{j\in\mathcal{J}}$ to the set $K^{nL} = \big(-\frac{nL}{2}, \frac{nL}{2}\big)^2$. Let $\mathcal{Q}_\theta^{nL}$ be the quadratic form defined in (**??**) and $\{f_{k,n}\}_{k=1}^N$ be any orthonormal set in $\mathcal{D}(\mathcal{Q}_\theta^{nL})$. By the IMS formula and the fact that $\sum_j \chi_{j,L}^2 = 1$, we have

$$\begin{aligned}&\sum_{k=1}^N \Big(\mathcal{Q}_\theta^{nL}(f_{k,n}) - \lambda \|f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big)\\ &\qquad = \sum_{k=1}^N\sum_{j\in\mathcal{J}} \bigg\{ \Big(\mathcal{Q}_\theta^{nL}(\chi_{j,L}f_{k,n}) - \lambda \|\chi_{j,L}f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big) - \|\,|\nabla\chi_{j,L}|\,f_{k,n}\|^2_{L^2(\Omega^{nL})}\bigg\} \end{aligned} \tag{4.1.6}$$

where $\Omega^{nL} = K^{nL}\times\mathbb{R}_+$ is as defined in (**??**). Using the bound on $|\nabla\chi_j|$ in (**??**) we obtain

$$\sum_{k=1}^N \Big(\mathcal{Q}_\theta^{nL}(f_{k,n}) - \lambda \|f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big) \geq \sum_{k=1}^N\sum_{j\in\mathcal{J}} \Big(\mathcal{Q}_\theta^{nL}(\chi_{j,L}f_{k,n}) - \big(\lambda + \frac{C}{a^2L^2}\big) \|\chi_{j,L}f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big). \tag{4.1.7}$$

For $j\in\mathcal{J}$, we define the trial density matrix $\gamma : L^2(\mathcal{K}_{a,j,L}) \ni f \mapsto \gamma_j f \in L^2(\mathcal{K}_{a,j,L})$,

$$\gamma_j f = \chi_{j,L}\sum_{k=1}^N \langle \chi_{j,L} f, f_{k,n}\rangle f_{k,n}.$$

We will show that $0\leq\gamma_j\leq 1$ in the sense of quadratic forms. Indeed, we have

$$\langle\gamma_j f, f\rangle_{L^2(\mathcal{K}_{a,j,L})} = \sum_{k=1}^N \big|\langle f, \chi_{j,L}f_{k,n}\rangle\big|^2 \geq 0$$

On the other hand, using that $\{f_{k,n}\}_k$ is an orthonormal set in $L^2(\Omega^{nL})$, it follows that for any normalized $f\in L^2(\Omega^{nL})$ we have

$$\begin{aligned}\langle\gamma_j f, f\rangle_{L^2(\mathcal{K}_{a,j,L})} &= \sum_{k=1}^N \big|\langle f, \chi_{j,L}f_{k,n}\rangle\big|^2\\ &\leq \|\chi_{j,L}f\|^2\\ &\leq \|f\|^2 = 1.\end{aligned}$$

Moreover, we note that γ_j is a finite-rank operator constructed so that we can write

$$\mathrm{Tr}\Big[\Big(\mathcal{P}_\theta^{nL} - (\lambda + \frac{C}{L^2a^2})\Big)\gamma_j\Big] = \sum_{k=1}^N \Big(\mathcal{Q}_\theta^{nL}(\chi_{j,L}f_{k,n}) - (\lambda + \frac{C}{L^2a^2})\|\chi_{j,L}f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big). \tag{4.1.8}$$

In view of the definition of the energy in (**??**), we have

$$-\mathcal{E}\Big(\lambda + \frac{C}{L^2a^2}; \mathcal{P}_\theta^{(1+a)L}, \Omega^{(1+a)L}\Big) = -\mathrm{Tr}\Big(\mathcal{P}_\theta^{(1+a)L} - (\lambda + \frac{C}{L^2a^2})\Big)_-.$$

Notice that each $\chi_{j,L}$ is supported in a square with side length $(1+a)L$. Hence, using magnetic translation invariance and Lemma **??**, we deduce that

$$-\mathcal{E}\Big(\lambda + \frac{C}{L^2a^2}; \mathcal{P}_\theta^{(1+a)L}, \Omega^{(1+a)L}\Big) \leq \mathrm{Tr}\Big[\Big(\mathcal{P}_\theta^{nL} - \big(\lambda + \frac{C}{L^2a^2}\big)\Big)\gamma_j\Big], \quad \forall\, j\in\mathcal{J}. \tag{4.1.9}$$

Combining (**??**), (**??**) and (**??**), we obtain

$$\sum_{k=1}^{N}\Big(\mathcal{Q}_\theta^{nL}(f_{k,n})-\lambda\,\|f_{k,n}\|^2_{L^2(\Omega^{nL})}\Big)\geq -n^2\mathcal{E}\Big(\lambda+\frac{C}{L^2a^2};\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\Big) \tag{4.1.10}$$

for all orthonormal family $\{f_{k,n}\}_{k=1}^N$ and $N\in\mathbb{N}$. Therefore we conclude, in view of Lemma **??**, that

$$\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL})\leq n^2\mathcal{E}\Big(\lambda+\frac{C}{L^2a^2};\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\Big). \tag{4.1.11}$$

Let $L_0\geq C/(a\sqrt{1-\lambda_0})$, then $\lambda+Ca^{-2}L^{-2}<1$ for all $L\geq L_0$. Applying Lemma **??** with $\varsigma=\dfrac{C}{a^2L^2}$, we find,

$$\mathcal{E}\Big(\lambda+\frac{C}{a^2L^2};\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\Big)-\mathcal{E}\big(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\big)\leq\frac{C}{L^2a^2}\mathcal{N}\Big(\lambda+\frac{C}{a^2L^2};\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\Big),$$

for all $L\geq L_0$. By (**??**), it follows that

$$\mathcal{E}\Big(\lambda+\frac{C}{a^2L^2};\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\Big)\leq\mathcal{E}\big(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\big)+\frac{C}{a^2},$$

for all $L\geq L_0$ and $\lambda\in[0,\lambda_0]$. Inserting this into (**??**), we get,

$$\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL})\leq n^2\mathcal{E}\big(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\big)+\frac{Cn^2}{a^2}, \tag{4.1.12}$$

Dividing both sides by n^2L^2, we find

$$\frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL})}{n^2L^2}\leq\frac{\mathcal{E}\big(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\big)}{L^2}+\frac{C}{L^2a^2}, \tag{4.1.13}$$

We infer from (**??**) the following upper bound,

$$\frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL})}{n^2L^2}\leq\frac{\mathcal{E}\big(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L}\big)}{(1+a)^2L^2}+C\left(a+\frac{1}{a^2L^2}\right), \tag{4.1.14}$$

for all $L\geq L_0$ and $\lambda\in[0,\lambda_0]$. This proves the first assertion of the lemma.

To obtain monotonicity of $\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega_L)$, we consider $L'\geq L>0$. Since the extension by zero of a function in the form domain $\mathcal{P}_\theta^L$ is contained in the form domain of $\mathcal{P}_\theta^{L'}$ and the values of both forms coincide for such a function, we may write in the sense of quadratic forms

$$\mathcal{P}_\theta^{L'}\leq\mathcal{P}_\theta^L.$$

On account of Lemma **??**, it follows that,

$$-\mathrm{Tr}\big(\mathcal{P}_\theta^{L'}-\lambda\big)_-\leq-\mathrm{Tr}\big(\mathcal{P}_\theta^L-\lambda\big)_-.$$

This shows that $\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)$ is monotone increasing with respect to L, thereby proving the statement of the lemma. $\square$

Proof of Theorem **??**. Let $f(L) = -\frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2}$. Thanks to Lemma **??**, we know that the functions $f(L)$ and $d(L) = -\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)$ satisfy the assumptions in Lemma **??**. Consequently, $f(L)$ has a limit as $L \to \infty$. Let us define

$$E(\theta,\lambda) := -\lim_{L\to\infty} f(L).$$

By Lemma **??**, there exists $L_0 > 0$ such that

$$E(\theta;\lambda) \leq \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2} + \frac{2C_0}{L^{2/3}}, \tag{4.1.15}$$

for all $L \geq 2L_0$ and $\lambda \in [0,\lambda_0]$.

It remains to establish the upper bound. According to Lemma **??**, we know that the energy satisfies

$$\frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^{nL},\Omega^{nL_1,nL_2})}{n^2L^2} \geq \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2}.$$

Letting $n \to \infty$ gives us

$$E(\theta,\lambda) \geq \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2}.$$

This, together with (**??**), completes the proof of Theorem **??**. □

4.2 Properties of the function $E(\theta,\lambda)$

Let $\mathcal{P}_\theta^L$, $\mathcal{Q}_\theta^L$ and Ω^L be as defined in (**??**), (**??**) and (**??**) respectively. In Theorem **??**, we proved the existence of a limiting function $E(\theta,\lambda) \in [0,\infty)$ defined for $\theta \in [0,\pi/2]$ and $\lambda \in [0,1)$. We aim in this section to study the properties of $E(\theta,\lambda)$ as a function of θ and λ.

Lemma 4.2.1. *Let $\lambda_0 \in [0,1)$. There exists $L^* > 0$ such that for all $L \geq L^*$, the function*

$$[0,\pi/2]\times[0,\lambda_0] \ni (\theta,\lambda) \mapsto \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2}$$

is continuous. Moreover, to every $\delta > 0$ there corresponds $\eta, L^* > 0$ such that for all $L \geq L^*$, $(\epsilon,\nu) \in (0,\eta)\times(0,\eta)$ and $(\theta,\lambda) \in [0,\pi/2]\times[0,\lambda_0]$ satisfying $(\theta+\epsilon,\lambda+\nu) \in [0,\pi/2]\times[0,\lambda_0]$, there holds,

$$\Big|\frac{\mathcal{E}(\lambda+\nu;\mathcal{P}_{\theta+\epsilon}^L,\Omega^L)}{L^2} - \frac{\mathcal{E}(\lambda;\mathcal{P}_\theta^L,\Omega^L)}{L^2}\Big| \leq \delta/2.$$

Proof. We introduce a partition of unity of $\mathbb{R}$,

$$\zeta_1^2 + \zeta_2^2 = 1, \qquad \operatorname{supp}\zeta_1 \subset [0,1], \qquad \operatorname{supp}\zeta_2 \subset [1/2,\infty) \tag{4.2.1}$$

and

$$|\zeta_p'| \leq C', \qquad p = 1,2. \tag{4.2.2}$$

Let $\delta > 0$. For reasons that will be clarified later, we set

$$L^* = \max\left\{\Big(\frac{4C'}{1-\lambda_0}\Big)^{1/2}, \Big(\frac{4C'C}{\delta\sqrt{(1-\lambda_0))/2}}\Big)^{1/2}\right\}, \tag{4.2.3}$$

where C' and C are the constants appearing in (**??**) and (**??**) respectively. We put further,

$$\zeta_{p,L^*}(r,s,t) = \zeta_p(t/L^*), \qquad p = 1,2, \qquad (r,s,t) \in \mathbb{R}^3_+.$$

Next, let $\{f_k\}_{k=1}^N$ be an orthonormal family of compactly supported functions in $\mathcal{D}(\mathcal{Q}_{\theta+\epsilon}^{L^*})$. We have the following IMS decomposition formula

$$\begin{aligned}\sum_{k=1}^{N}&\Big(\mathcal{Q}_{\theta+\epsilon}^{L^*}(f_k)-(\lambda+\nu)\,\|f_k\|^2_{L^2(\Omega^{L^*})}\Big)\\&=\sum_{k=1}^{N}\sum_{p=1}^{2}\bigg\{\Big(\mathcal{Q}_{\theta+\epsilon}^{L^*}(\zeta_{p,L^*}f_k)-(\lambda+\nu)\,\|\zeta_{p,L^*}f_k\|^2_{L^2(\Omega^{L^*})}\Big)-\|\,|\nabla\zeta_{p,L^*}|\;f_k\|^2_{L^2(\Omega^{L^*})}\bigg\}.\end{aligned}\tag{4.2.4}$$

To estimate the last term we use the bound on $\nabla\zeta_p$ in (**??**), and get, after inserting $\zeta_{1,L^*}^2+\zeta_{2,L^*}^2=1$, that

$$\sum_{k=1}^{N}\Big(\mathcal{Q}_{\theta+\epsilon}^{L^*}(f_k)-(\lambda+\nu)\,\|f_k\|^2\Big)\geq\sum_{k=1}^{N}\sum_{p=1}^{2}\Big(\mathcal{Q}_{\theta+\epsilon}^{L^*}(\zeta_{p,L^*}f_k)-(\lambda+\nu+C'(L^*)^{-2})\,\|\zeta_{p,L^*}f_k\|^2\Big)\,.\tag{4.2.5}$$

Since the function $\varphi=\zeta_{2,L^*}f_k\in C_0^\infty(\Omega^{L^*})$ is compactly supported in Ω^{L^*}, it can be extended by zero to all of $\mathbb{R}^3$. Therefore, selecting

$$|\nu|<\frac{\lambda_0-\lambda}{4},$$

we infer from Lemma **??** and the choice of L^* in (**??**) that the following inequality holds

$$\mathcal{Q}_{\theta+\epsilon}^{L^*}(\zeta_{2,L^*}f_k)\geq\int_{\Omega^{L^*}}|\zeta_{2,L^*}f_k|^2drdsdt>(\lambda+\nu+C'(L^*)^{-2})\int_{\Omega^{L^*}}|\zeta_{2,L^*}f_k|^2drdsdt.\tag{4.2.6}$$

Consequently, we find that the term corresponding to $p=2$ on the right hand side of (**??**) is strictly positive and can be neglected for a lower bound. What remains is to estimate the term corresponding to $p=1$ in (**??**). Using the pointwise inequality (with ϱ arbitrary)

$$|(-i\nabla+\mathbf{F}_{\theta+\epsilon})\zeta_{1,L^*}f_k|^2\geq(1-\varrho)|(-i\nabla+\mathbf{F}_\theta)\zeta_{1,L^*}f_k|^2-\varrho^{-1}|(\mathbf{F}_\theta-\mathbf{F}_{\theta+\epsilon})\zeta_{1,L^*}f_k|^2,$$

where $\mathbf{F}_\theta$ is the same as in (**??**), we obtain,

$$\begin{aligned}&\mathcal{Q}_{\theta+\epsilon}^{L^*}(\zeta_{1,L^*}f_k)\\&\quad\geq(1-\varrho)\int_{\Omega^{L^*}}|(-i\nabla+\mathbf{F}_{\theta+\epsilon})\zeta_{1,L^*}f_k|^2drdsdt-\varrho^{-1}\int_{\Omega^{L^*}}|(\mathbf{F}_{\theta+\epsilon}-\mathbf{F}_\theta)\zeta_{1,L_1}f_k|^2drdsdt.\end{aligned}\tag{4.2.7}$$

Using the bounds

$$|\cos(\theta+\epsilon)-\cos(\theta)|\leq|\epsilon|\,,\quad|\sin(\theta+\epsilon)-\sin(\theta)|\leq|\epsilon|\,,$$

we get

$$|\mathbf{F}_{\theta+\epsilon}(r,s,t)-\mathbf{F}_\theta(r,s,t)|\leq|\epsilon|\,(|s|+|t|)\,,\quad\forall\;(r,s,t)\in\mathbb{R}^3_+\,.$$

Taking the support of ζ_{1,L^*} into consideration, we infer from (**??**) the following bound,

$$\mathcal{Q}_{\theta+\epsilon}^{L^*}(\zeta_{1,L^*}f_k)\geq(1-\varrho)\int_{\Omega^{L^*}}|(-i\nabla+\mathbf{F}_\theta)\zeta_{1,L^*}f_k|^2drdsdt-\varrho^{-1}\epsilon^2(L^*)^2\int_{\Omega^{L^*}}|\zeta_{1,L^*}f_k|^2drdsdt.$$

Inserting this into (**??**), we get, using the bound on $|\zeta'_{1,L^*}|$, that

$$\sum_{k=1}^{N}\Big(\mathcal{Q}_{\theta+\epsilon}^{L_1,L^*}(f_k)-(\lambda+\nu)\,\|f_k\|^2_{L^2(\Omega^{L_1,L^*})}\Big)$$
$$\geq \sum_{k=1}^{N}\Big((1-\varrho)\mathcal{Q}_{\theta}^{L_1,L^*}(\zeta_{1,L^*}f_k)-(\lambda+\nu+\epsilon^2\varrho^{-1}(L^*)^2+C'(L^*)^{-2})\,\|\zeta_{1,L^*}f_k\|^2_{L^2(\Omega^{L_1,L^*})}\Big)\,. \tag{4.2.8}$$

We choose $\varrho=|\epsilon|$ and define the trial density matrix $L^2(\mathbb{R}^3)\ni\mapsto\gamma f\in L^2(\mathbb{R}^3)$,

$$\gamma f=\sum_{k=1}^{N}\langle f,\zeta_{1,L^*}f_k\rangle\zeta_{1,L^*}f_k.$$

It is clear that $0\leq\gamma\leq 1$ in the sense of quadratic forms. By Lemma **??** we see that

$$-\,\mathcal{E}\Big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|};\mathcal{P}_\theta^{L^*},\Omega^{L^*}\Big)$$
$$\leq \mathrm{Tr}\Big[\Big(\mathcal{P}_\theta^{L^*}-\big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|}\big)\Big)\gamma\Big]$$
$$:=\Big(\mathcal{Q}_\theta^{L^*}(\zeta_{1,L^*}f_k)-\big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|}\big)\,\|\zeta_{1,L^*}f_k\|_{L^2(\Omega^{L^*})}\Big) \tag{4.2.9}$$

Inserting this into (**??**), we obtain

$$\sum_{k=1}^{N}\Big(\mathcal{Q}_{\theta+\epsilon}^{L^*}(f_k)-(\lambda+\nu)\,\|f_k\|_{L^2(\Omega_{L^*})}\Big)$$
$$\geq -(1-|\epsilon|)\mathcal{E}\Big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|};\mathcal{P}_\theta^{L^*},\Omega^{L^*}\Big). \tag{4.2.10}$$

Consequently, it follows from Lemma **??** that,

$$\mathcal{E}(\lambda+\nu;\mathcal{P}_{\theta+\epsilon}^{L^*},\Omega^{L^*})\leq(1-|\epsilon|)\mathcal{E}\Big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|};\mathcal{P}_\theta^{L^*},\Omega^{L^*}\Big). \tag{4.2.11}$$

Fix $|\epsilon|<\frac{1-\lambda_0}{4(1+(L^*)^2)}$. Applying Lemma **??** with $\varsigma=\dfrac{|\epsilon|((L^*)^2+\lambda)+\nu+C'(L^*)^{-2}}{1-|\epsilon|}$, we get,

$$\mathcal{E}\Big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|};\mathcal{P}_\theta^{L^*},\Omega^{L^*}\Big)\leq\mathcal{E}(\lambda;\mathcal{P}_\theta^{L^*},\Omega^{L^*})$$
$$+\frac{|\epsilon|((L^*)^2+\lambda)+\nu+C'(L^*)^{-2}}{1-|\epsilon|}\mathcal{N}\Big(\frac{\lambda+\nu+|\epsilon|(L^*)^2+C'(L^*)^{-2}}{1-|\epsilon|};\mathcal{P}_\theta^{L^*},\Omega^{L^*}\Big). \tag{4.2.12}$$

Plugging (**??**) into (**??**), we obtain from (**??**) that

$$\mathcal{E}(\lambda+\nu;\mathcal{P}_{\theta+\epsilon}^{L^*},\Omega^{L^*})\leq(1-|\epsilon|)\mathcal{E}(\lambda;\mathcal{P}_\theta^{L^*},\Omega^{L^*})$$
$$+\frac{C}{\sqrt{(1-\lambda_0)/2}}(|\epsilon|(\lambda+(L^*)^2)+\nu+C'(L^*)^{-2})(L^*)^2, \tag{4.2.13}$$

where C is the constant from (**??**). Interchanging the roles of θ and $\theta+\epsilon$ we arrive at

$$\begin{aligned}&\left|\mathcal{E}(\lambda+\nu;\mathcal{P}^{L^*}_{\theta+\epsilon},\Omega^{L^*})-\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})\right|\\&\qquad\le|\epsilon|\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})+\frac{C}{\sqrt{(1-\lambda_0)/2}}(|\epsilon|(\lambda+(L^*)^2)+|\nu|+C'(L^*)^{-2})(L^*)^2.\end{aligned}\tag{4.2.14}$$

Dividing both sides by $(L^*)^2$, we get,

$$\begin{aligned}&\left|\frac{\mathcal{E}(\lambda+\nu;\mathcal{P}^{L^*}_{\theta+\epsilon},\Omega^{L^*})}{(L^*)^2}-\frac{\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})}{(L^*)^2}\right|\\&\qquad\le|\epsilon|\frac{\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})}{(L^*)^2}+\frac{C(|\epsilon|((L^*)^2+\lambda)+|\nu|+C'(L^*)^{-2})}{\sqrt{(1-\lambda_0)/2}}\\&\qquad\le\eta\frac{\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})}{L_1L^*}+\frac{C(\eta((L^*)^2+\lambda+1)+C'(L^*)^{-2})}{\sqrt{(1-\lambda_0)/2}}.\end{aligned}$$

Using the estimate in (**??**), we further obtain

$$\left|\frac{\mathcal{E}(\lambda+\nu;\mathcal{P}^{L^*}_{\theta+\epsilon},\Omega^{L^*})}{(L^*)^2}-\frac{\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*}}{(L^*)^2}\right|\le\frac{C(\eta((L^*)^2+\lambda+2)+C'(L^*)^{-2})}{\sqrt{(1-\lambda_0)/2}}.\tag{4.2.15}$$

Selecting $\eta<\frac{\delta\sqrt{(1-\lambda_0)/2}}{4C(\lambda+2+(L^*)^2)}$, we conclude that (recall the choice of L^* in (**??**)),

$$\left|\frac{\mathcal{E}(\lambda+\nu;\mathcal{P}^{L^*}_{\theta+\epsilon},\Omega^{L^*})}{(L^*)^2}-\frac{\mathcal{E}(\lambda;\mathcal{P}^{L^*}_{\theta},\Omega^{L^*})}{(L^*)^2}\right|\le\delta/2,$$

thereby proving the assertion of the lemma. □

We have the following corollary of Lemma **??**.

Corollary 4.2.2. *Given* $\lambda_0\in[0,1)$*, the function*

$$[0,\pi/2]\times[0,\lambda_0]\ni(\theta,\lambda)\mapsto E(\theta;\lambda)$$

is continuous.

Proof. In view of Theorem **??**, there exist constants C_0 and L_0 such that for all $L\ge 2L_0$ and (ν,ϵ) satisfying $\lambda+\nu\in[0,\lambda_0]$ and $\theta+\epsilon\in[0,\pi/2]$, one has

$$|E(\theta+\epsilon,\lambda+\nu)-E(\theta,\lambda)|\le\frac{|\mathcal{E}(\lambda+\nu;\mathcal{P}^{L}_{\theta+\epsilon},\Omega^{L})-\mathcal{E}(\lambda;\mathcal{P}^{L}_{\theta},\Omega^{L})|}{L^2}+\frac{2C_0}{L^{2/3}}.\tag{4.2.16}$$

Choose $L\ge\max\{2L_0,L^*,(4C_0/\delta)^{3/2}\}$ with L^* from (**??**). Hence, we infer from Lemma **??** that there exists $\eta>0$ such that for all $|(\epsilon,\nu)|\le\eta$ satisfying $\theta+\epsilon\in[0,\pi/2]$ and $\lambda+\nu\in[0,\lambda_0]$, we have

$$|E(\theta+\epsilon,\lambda+\nu)-E(\theta,\lambda)|\le\delta/2+\delta/2=\delta.$$

This completes the proof. □

We will prove

Lemma 4.2.3. *Let $\theta \in [0, \pi/2]$. The function*

$$[0,1) \ni \lambda \mapsto E(\theta, \lambda)$$

is locally Lipschitz. More precisely, given $\lambda_0 > 0$, there exists a constant C_0 (independent of θ) such that,

$$\forall\ \theta \in [0, \pi/2], \quad \forall\ \lambda_1, \lambda_2 \in [0, \lambda_0]\,, \quad |E(\lambda_1, \theta) - E(\lambda_2, \theta)| \le C_0 |\lambda_1 - \lambda_2|\,.$$

Proof. Fix $\lambda_0 \in [0,1)$, and let $\lambda_1, \lambda_2 \in [0, \lambda_0]$ be such that $\lambda_1 < \lambda_2$. Let $L > 0$ and $\mathcal{P}_\theta^L$ be as defined in (**??**). We infer from Lemma **??** that

$$\mathcal{E}(\lambda_2; \mathcal{P}_\theta^L, \Omega^L) - \mathcal{E}(\lambda_1; \mathcal{P}_\theta^L, \Omega^L) \le (\lambda_2 - \lambda_1) \mathcal{N}(\lambda_2; \mathcal{P}_\theta^L, \Omega^L).$$

In view of (**??**), there exists a constant C_0 independent of θ such that

$$\mathcal{N}(\lambda_2; \mathcal{P}_\theta^L, \Omega^L) \le C_0 L^2.$$

This implies

$$\mathcal{E}(\lambda_2; \mathcal{P}_\theta^L, \Omega^L) - \mathcal{E}(\lambda_1; \mathcal{P}_\theta^L, \Omega^L) \le C_0 L^2 (\lambda_2 - \lambda_1). \tag{4.2.17}$$

According to Theorem **??**, we have

$$E(\theta, \lambda) = \lim_{L \to \infty} \frac{\mathcal{E}(\lambda_2; \mathcal{P}_\theta^L, \Omega^L)}{L^2}.$$

Dividing both sides of (**??**) by L^2, we get, after taking $L \to \infty$,

$$E(\theta, \lambda_2) - E(\theta, \lambda_1) \le C_0 (\lambda_2 - \lambda_1). \tag{4.2.18}$$

Interchanging the roles of λ_1 and λ_2, we further get

$$|E(\theta, \lambda_2) - E(\theta, \lambda_1)| \le C_0 |\lambda_2 - \lambda_1|, \tag{4.2.19}$$

which gives the assertion of the lemma. ☐

Remark 4.2.4. Another alternative proof of the Lipschitz property uses the explicit formula of $E(\theta, \lambda)$ appearing in the statement of Theorem **??**. The proof of these formulas will be given ahead in the next section. In fact, when $\theta \in (0, \pi/2)$, the spectrum of $\mathcal{L}(\theta)$ (the two-dimesional operator defined in (**??**)) strictly below 1 is purely discrete then the function

$$[0,1) \ni \lambda \mapsto E(\theta, \lambda) = \frac{\sin(\theta)}{2\pi} \sum_j (\zeta_j(\theta) - \lambda)_-$$

can be seen as a finite sum of affine functions in λ, from which the Lipschitz property follows easily.

4.3 Explicit formulas of $E(\theta, \lambda)$

Recall the constant $E(\theta, \lambda)$ defined in (**??**). The aim of this section is to provide an explicit formula for $E(\theta, \lambda)$ using the eigenvalues of the Neumann Schrödinger operator on the half-space $\mathbb{R}^3_+$ defined in (**??**). We shall consider the cases $\theta = 0$ and $\theta \in (0, \pi/2]$ independently. Indeed, the construction of eigenprojectors in the case $\theta = 0$ is similar in spirit to the two-dimensional case (cf. [**?**, Section 4]), whereas in the case $\theta \in (0, \pi/2]$, the projectors are constructed using the spectral decomposition of the two-dimensional model operator on the half-space (see (**??**) below for the precise definition).

4.3.1 $E(\theta,\lambda)$ in the case $\theta = 0$

We start by recalling the family of one-dimensional harmonic oscillators $\mathfrak{h}[\xi]$, $\xi \in \mathbb{R}$, defined by :

$$\mathfrak{h}[\xi)] = -\partial_t^2 + (t-\xi)^2 \qquad \text{in} \qquad L^2(\mathbb{R}_+). \tag{4.3.1}$$

on their common Neumann domain:

$$\big\{v \in H^2(\mathbb{R}_+),\ (t-\xi)^2 v \in L^2(\mathbb{R}_+),\ v'(0) = 0\big\}.$$

The spectral properties related to this operator are discussed in Section **??**.

We denote by $(u_j(\cdot;\xi))_{j=1}^{\infty}$ the orthonormal family of real-valued eigenfunctions of the operator $\mathfrak{h}[\xi]$, i.e.,

$$\begin{cases} \mathfrak{h}[\xi] u_j(t;\xi) = \mu_j(\xi) u_j(t;\xi), \\ \quad u_j'(0;\xi) = 0, \\ \quad \displaystyle\int_{\mathbb{R}_+} u_j(t;\xi)^2 dt = 1. \end{cases} \tag{4.3.2}$$

Here μ_j are defined via the min-max principle in (**??**).

Next, we consider the Schrödinger operator (**??**) in the particular case $\theta = 0$, i.e.,

$$\mathcal{P}_0^N = -\partial_t^2 - \partial_s^2 + (-i\partial_r + t)^2 \qquad \text{in} \qquad \mathrm{L}^2(\mathbb{R}_+^3). \tag{4.3.3}$$

with Neumann boundary conditions at $t = 0$.

Let $(\xi,\tau) \in \mathbb{R}^2$. We denote by $\mathcal{F}_{r\to\xi}$ (resp. $\mathcal{F}_{s\to\tau}$) the unitary partial Fourier transform with respect to the r variable (resp. s variable).

We define the bounded function $\mathbb{R}_+^3 \ni (r,s,t) \mapsto v_j(r,s,t;\xi,\tau)$ by :

$$v_j(r,s,t;\xi,\tau) = \frac{1}{\sqrt{2\pi}} e^{-i\xi r} e^{-i\tau s} u_j(t;\xi). \tag{4.3.4}$$

Next, we introduce the operators $\Pi_j(\xi,\tau)$ on the functions v_j:

$$L^2(\mathbb{R}_+^3) \ni \varphi \mapsto (\Pi_j(\xi,\tau)\varphi)(r,s,t) = v_j(r_1,s_1,t_1;\xi,\tau)\int_{\mathbb{R}_+^3} \overline{v_j(r_2,s_2,t_2;\xi,\tau)}\varphi(r_2,s_2,t_2) dr_2 ds_2 dt_2 \tag{4.3.5}$$

In terms of quadratic forms, we write

$$\begin{aligned} \big\langle \varphi, \Pi_j(\xi,\tau)\varphi\big\rangle_{L^2(\mathbb{R}_+^3)} &= \Big|\big\langle \varphi, v_j(\cdot;\xi,\tau)\big\rangle_{L^2(\mathbb{R}_+^3)}\Big|^2 \\ &= 2\pi\Big|\big\langle \mathcal{F}_{r\to -\xi}\big[\big(\mathcal{F}_{s\to-\tau}\varphi(\cdot,\cdot,t)\big)(-\tau)\big](-\xi), u_j(t;\xi)\big\rangle_{L^2(\mathbb{R}_+)}\Big|^2 \end{aligned} \tag{4.3.6}$$

We state in the next lemma useful properties of the family $\{\Pi_j(\xi,\tau)\}_{(j,\xi,\tau)\in\mathbb{N}\times\mathbb{R}^2}$.

Lemma 4.3.1. *For all $\varphi \in L^2(\mathbb{R}_+^3)$, we have*

$$\big\langle \mathcal{P}_0^N \Pi_j(\xi,\tau)\varphi, \varphi\big\rangle_{L^2(\mathbb{R}_+^3)} = (\mu_j(\xi) + \tau^2)\big\langle \Pi_j(\xi,\tau)\varphi, \varphi\big\rangle_{L^2(\mathbb{R}_+^3)}, \tag{4.3.7}$$

$$\sum_j \int_{\mathbb{R}^2} \big\langle \varphi, \Pi_j(\xi,\tau)\varphi\big\rangle_{L^2(\mathbb{R}_+^3)} d\xi d\tau = 2\pi \left\|\varphi\right\|_{L^2(\mathbb{R}_+^3)}^2. \tag{4.3.8}$$

Moreover, for any cut-off function $\chi \in C_0^\infty(\mathbb{R}^2)$, we have

$$\mathrm{Tr}(\chi \Pi_{\theta,j}\chi) = (2\pi)^{-1}\int_{\mathbb{R}^2} \chi^2(r,s) dr ds. \tag{4.3.9}$$

Proof. Let $(\tau,\xi)\in\mathbb{R}^2$. By the definition of v_j in (**??**), we find,

$$\mathcal{P}_0^N v_j(r,s,t;\xi,\tau)=(\mu_j(\xi)+\tau^2)v_j(r,s,t;\xi,\tau).$$

Using the definition in (**??**) immediately gives (**??**).

Using the fact that $u_j(\cdot;\xi)$ is an orthonormal basis of $L^2(\mathbb{R}_+)$ for all $\xi\in\mathbb{R}$, we find, using the representation in (**??**),

$$\sum_j\left\langle\varphi,\Pi_j(\xi,\tau)\varphi\right\rangle_{L^2(\mathbb{R}^3_+)}=2\pi\int_{\mathbb{R}_+}\left|\mathcal{F}_{r\to-\xi}\big[\big(\mathcal{F}_{s\to-\tau}\varphi(\cdot,\cdot,t)\big)(-\tau)\big](-\xi)\right|^2dt.$$

Integrating in ξ and τ, it follows that

$$\int_{\mathbb{R}^2}\sum_j\left\langle\varphi,\Pi_j(\xi,\tau)\varphi\right\rangle_{L^2(\mathbb{R}^3_+)}d\xi d\tau=2\pi\left\|\varphi\right\|^2_{L^2(\mathbb{R}^3_+)},$$

upon applying Plancherel identity twice.

It remains to prove (**??**). In fact, we have

$$\mathrm{Tr}\big(\chi\Pi_{\theta,j}\chi\big)=(2\pi)^{-1}\int_{\mathbb{R}^3_+}\chi^2(r,s)|u_j(t;\xi)|^2drdsdt=(2\pi)^{-1}\int_{\mathbb{R}^2}\chi^2(r,s)drds.$$

The proof of the lemma is thus complete. ☐

We will prove

Theorem 4.3.2. *Given $\lambda\in(0,1)$, the following formula holds true:*

$$E(0,\lambda)=\frac{1}{3\pi^2}\int_0^\infty(\mu_1(\xi)-\lambda)_-^{3/2}d\xi,\tag{4.3.10}$$

where $\mu_1(\xi)$ is defined in (**??**).

Proof. We start by obtaining an upper bound on $E(0,\lambda)$. Let $L>0$. Pick an arbitrary positive integer N and let $\{f_1,\cdots,f_N\}$ be any L^2 orthonormal set in $\mathcal{D}(\mathcal{P}_0^L)$. In view of (**??**) and (**??**), we have the following splitting (recall the domain Ω^L from (**??**)),

$$\begin{aligned}\sum_{j=1}^N\big\langle f_j,(\mathcal{P}_0^L-\lambda)f_j\big\rangle_{L^2(\Omega^L)}&=\frac{1}{2\pi}\sum_{j=1}^N\sum_{p=1}^\infty\int_{\mathbb{R}^2}\left\langle f_j,(\mathcal{P}_0^N-\lambda)\Pi_p(\xi,\tau)f_j\right\rangle_{L^2(\mathbb{R}^3_+)}d\xi d\tau\\&=\frac{1}{2\pi}\sum_{j=1}^N\sum_{p=1}^\infty\int_{\mathbb{R}^2}(\mu_p(\xi)+\tau^2-\lambda)\big\langle f_j,\Pi_p(\xi,\tau)f_j\big\rangle_{L^2(\mathbb{R}^3_+)}d\xi d\tau\,,\end{aligned}$$

where we have extended f_j by 0 to $\mathbb{R}^3_+\setminus\overline{\Omega^L}$. Since $\lambda<1$, Lemma **??** gives that $\mu_p(\xi)+\tau^2>\lambda$ for $p\geq 2$ and $(\tau,\xi)\in\mathbb{R}^2$. Hence, we obtain

$$\sum_{j=1}^N\big\langle f_j,(\mathcal{P}_0^L-\lambda)f_j\big\rangle_{L^2(\Omega^L)}\geq-\frac{1}{2\pi}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_-\sum_{j=1}^N\big\langle f_j,\Pi_1(\xi,\tau)f_j\big\rangle_{L^2(\mathbb{R}^3_+)}.\tag{4.3.11}$$

Since $\{f_j\}_{j=1}^N$ is an orthonormal family in $L^2(\Omega^L)$, we deduce that

$$\begin{aligned}\sum_{j=1}^{N}\big\langle f_j,\Pi_1(\xi,\tau)f_j\big\rangle_{L^2(\mathbb{R}^3_+)} &= \sum_{j=1}^{N}\Big|\langle v_1,f_j\rangle\Big|^2 \leq \int_{\Omega^L}|v_1(r,s,t)|^2drdsdt\\ &= \frac{1}{2\pi}\int_{\Omega^L}|u_1(t;\xi)|^2drdsdt = \frac{1}{2\pi}L^2.\end{aligned} \tag{4.3.12}$$

The last equality comes from the fact that the function $u_1(\cdot;\xi)$ is normalized in $L^2(\mathbb{R}_+)$ for all ξ. Substituting (**??**) into (**??**) yields

$$\sum_{j=1}^{N}\big\langle f_j,(\mathcal{P}_0^L-\lambda)f_j\big\rangle_{L^2(\Omega^L)} \geq -\frac{L^2}{4\pi^2}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_{-}d\xi d\tau,$$

uniformly with respect to N and the orthonormal family $\{f_j\}_{j=1}^N$. Then, on account of Definition (**??**) and Lemma **??**, we have

$$\frac{\mathcal{E}(\lambda,\mathcal{P}_0^L;\Omega^L)}{L^2} \leq \frac{1}{4\pi^2}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_{-}d\xi d\tau.$$

Letting $L\to\infty$, we infer from (**??**) and Lemma **??** the following upper bound,

$$E(0,\lambda) \leq \frac{1}{3\pi^2}\int_0^{\infty}(\mu_1(\xi)-\lambda)_{-}^{3/2}d\xi. \tag{4.3.13}$$

We give the proof of the lower bound on $E(0,\lambda)$. Let $M(\xi,\tau)$ be the characteristic function of the set

$$\Big\{(\xi,\tau)\in\mathbb{R}^2\ :\ \lambda-\mu_1(\xi)-\tau^2\geq 0\Big\}$$

We consider the trial density matrix

$$\gamma = \int_{\mathbb{R}^2}M(\xi,\tau)\Pi_1(\xi,\tau)d\xi d\tau.$$

It is clear that $\gamma\geq 0$. We will prove that $\gamma\leq 2\pi$. Consider $g\in L^2(\Omega^L)$. Using that $0\leq M\leq 1$, we see that

$$\big\langle g,\gamma g\big\rangle_{L^2(\mathbb{R}^3_+)} \leq \int_{\mathbb{R}^2}\big|\langle g,v_1\rangle\big|^2d\xi d\tau \leq \sum_j\int_{\mathbb{R}^2}\big|\langle g,v_j\rangle\big|^2d\xi d\tau = 2\pi\left\|g\right\|^2.$$

The last step follows by Plancherel's identity and the that fact that $u_j(\cdot,\xi)$ is an orthonormal basis of $L^2(\mathbb{R}_+)$ for all ξ.

Recall the quadratic form Q_θ^L from (**??**), it easy to check that

$$\mathcal{Q}_0^L(v_1) = \frac{L^2}{2\pi}(\mu_1(\xi)+\tau^2). \tag{4.3.14}$$

We calculate, using (**??**),

$$\begin{aligned}\mathrm{Tr}\big[(\mathcal{P}_0^L-\lambda)\gamma\big] &= \int_{\mathbb{R}^2}M(\xi,\tau)\big(\mathcal{Q}_0^L(v_1)-\lambda\left\|v_1\right\|^2_{L^2(\Omega^L)}\big)d\xi d\tau\\ &= \frac{L^2}{2\pi}\int_{\mathbb{R}^2}M(\xi,\tau)(\mu_1(\xi)+\tau^2-\lambda)d\xi d\tau\\ &= -\frac{L^2}{2\pi}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_{-}d\xi d\tau.\end{aligned}$$

In view of Lemma **??**, we get

$$-\mathrm{Tr}\big(\mathcal{P}_0^L-\lambda\big)_- \le \frac{1}{2\pi}\mathrm{Tr}\big((\mathcal{P}_0^L-\lambda)\gamma\big) = -\frac{L^2}{4\pi^2}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_- d\xi d\tau.$$

This gives

$$\frac{\mathcal{E}(\lambda;\mathcal{P}_0^L,\Omega^L)}{L^2} \ge \frac{1}{4\pi^2}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-\lambda\big)_- d\xi d\tau.$$

Letting $L\to\infty$, it follows from Lemma **??** that

$$E(0,\lambda) \ge \frac{1}{3\pi^2}\int_0^\infty (\mu_1(\xi)-\lambda)_-^{3/2} d\xi. \tag{4.3.15}$$

Combining this with (**??**) proves the desired formula.

□

4.3.2 $E(\theta,\lambda)$ in the case $\theta\in(0,\pi/2]$

The purpose of this subsection is to provide an explicit formula for $E(\theta,\lambda)$ in the case $\theta\in(0,\pi/2]$ ($\lambda\in[0,1)$). However, we have not been able to compute it directly like in the case $\theta=0$. Our approach is to find alternative limiting functions (see below (**??**)), which can be constructed and computed explicitly using the eigenprojectors on the eigenfunctions of the two-dimensional model operator from (**??**). Afterwards, what remains is to establish a connection with $E(\theta,\lambda)$.

Let us define the function $\mathbb{R}^3_+\ni(r,s,t)\mapsto v_{\theta,j}(r,s,t;\xi)$ by

$$v_{\theta,j}(r,s,t;\xi) = \frac{1}{\sqrt{2\pi}}e^{i\xi r}u_{\theta,j}\Big(s-\frac{\xi}{\sin(\theta)},t\Big), \tag{4.3.16}$$

where $\{u_{\theta,j}\}_j$ are the eigenfunctions from (**??**). We define the projectors $\pi_{\theta,j}$ by

$$\big(\pi_{\theta,j}(\xi)\big)\varphi(s_1,t_1) = u_{\theta,j}\Big(s_1-\frac{\xi}{\sin(\theta)},t_1\Big)\int_{\mathbb{R}^2_+}\overline{u_{\theta,j}\Big(s_2-\frac{\xi}{\sin(\theta)},t_2\Big)}\varphi(s_2,t_2)ds_2dt_2. \tag{4.3.17}$$

We then introduce a family of operators $\Pi_{\theta,j}$ by

$$\begin{aligned} L^2(\mathbb{R}^3_+)\ni f\mapsto \Pi_{\theta,j}f(r_1,s_1,t_1)& \\ = \int_{\mathbb{R}} v_{\theta,j}(r_1,s_1,t_1;\xi)&\Big\{\int_{\mathbb{R}^3_+}\overline{v_{\theta,j}(r_2,s_2,t_2;\xi)}f(r_2,s_2,t_2)dr_2ds_2dt_2\Big\}d\xi \end{aligned} \tag{4.3.18}$$

In terms of quadratic forms, we have

$$\begin{aligned} L^2(\mathbb{R}^3_+)\ni f\mapsto \langle\Pi_{\theta,j}f,f\rangle_{L^2(\mathbb{R}^3_+)} &= \int_{\mathbb{R}}\Big|\langle v_{\theta,j}(\cdot,\xi),f\rangle_{L^2(\mathbb{R}^3_+)}\Big|^2 d\xi \\ &= \int_{\mathbb{R}}\Big\langle \mathcal{F}^{-1}_{\xi\to r}\big(\pi_{j,\theta}(\xi)(\mathcal{F}_{r\to\xi}f(\cdot,s,t)(\xi))\big)(r), f(r,s,t)\Big\rangle_{L^2(\mathbb{R}^3_+)} d\xi, \end{aligned} \tag{4.3.19}$$

Since the Fourier transform is a unitary transform and $\pi_{\theta,j}(\xi)$ is a projection, it follows that the operators $\Pi_{\theta,j}$ are indeed projections.

Lemma 4.3.3. *Let $f \in L^2(\mathbb{R}^3_+)$ and $\mathcal{P}^N_\theta$ be the operator defined in (??). We have*

$$\big\langle \mathcal{P}^N_\theta \Pi_{\theta,j} f, f\big\rangle_{L^2(\mathbb{R}^3_+)} = \zeta_j(\theta)\big\langle \Pi_{\theta,j} f, f\big\rangle_{L^2(\mathbb{R}^3_+)}. \tag{4.3.20}$$

$$\Big\langle \sum_j \Pi_{\theta,j} f, f\Big\rangle_{L^2(\mathbb{R}^3_+)} \leq \|f\|^2_{L^2(\mathbb{R}^3_+)}\,. \tag{4.3.21}$$

Moreover, for any smooth cut-off function $\chi \in C_0^\infty(\mathbb{R}^2)$, it holds true that

$$\mathrm{Tr}(\chi \Pi_{\theta,j}\chi) = \frac{\sin(\theta)}{2\pi}\int_{\mathbb{R}^2} \chi^2(r,s)drds. \tag{4.3.22}$$

Proof. Applying the operator $\mathcal{P}^N_\theta$ to the function $v_{\theta,j}$, we find

$$\mathcal{P}^N_\theta v_{\theta,j}(r,s,t;\xi) = \zeta_j(\theta) v_{\theta,j}(r,s,t;\xi).$$

The assertion (??) then follows from the definition of $\Pi_{\theta,j}$ in (??).

To prove (??), we rewrite (??) as

$$\Big\langle \Pi_{\theta,j} f, f\Big\rangle_{L^2(\mathbb{R}^3_+)} = \int_{\mathbb{R}} \Big\langle \pi_{\theta,j}(\xi)\big(\mathcal{F}_{r\to\xi} f(\cdot,s,t)\big)(\xi), \big(\mathcal{F}_{r\to\xi} f(\cdot,s,t)(\xi)\big)\Big\rangle_{L^2(\mathbb{R}^2_+)} d\xi. \tag{4.3.23}$$

It can be easily shown that $\sum_j \pi_{\theta,j}$ is a projection. Hence, by Plancherel's identity, we see that

$$\Big\langle \sum_j \Pi_{\theta,j} f, f\Big\rangle_{L^2(\mathbb{R}^3_+)} \leq \int_{\mathbb{R}^2_+}\int_{\mathbb{R}} |\mathcal{F}_{r\to\xi} f(\cdot,s,t)|^2 d\xi ds dt = \int_{\mathbb{R}^3_+} |f(r,s,t)|^2 drdsdt.$$

We come to the proof of (??). For this, we notice that

$$\mathrm{Tr}\big(\chi\Pi_{\theta,j}\chi\big) = \frac{1}{2\pi}\int_{\mathbb{R}^3_+} \chi^2(r,s)\Big(\int_{\mathbb{R}} \big|e^{i\xi r} u_{\theta,j}\big(s - \frac{\xi}{\sin(\theta)}, t\big)\big|^2 d\xi\Big) drdsdt.$$

Performing the change of variable $\nu = s - \frac{\xi}{\sin\theta}$ and using that the functions $\{u_{\theta,j}\}_j$ are normalized, we get

$$\mathrm{Tr}\big(\chi\Pi_{\theta,j}\chi\big) = \frac{1}{2\pi}\sin(\theta)\int_{\mathbb{R}^2}\chi^2(r,s)drds\int_{\mathbb{R}^2_+}|u_{\theta,j}(\nu,t)|^2 d\nu dt = \frac{1}{2\pi}\sin(\theta)\int_{\mathbb{R}^2}\chi^2(r,s)drds. \tag{4.3.24}$$

Thereby completing the proof of the lemma. ∎

Let $a > 0$. In order to define $F(\theta,\lambda)$ below, we need to introduce the cut-off function $\chi_a \in C_0^\infty(\mathbb{R}^2)$, which satisfies

$$0 \leq \chi_a \leq 1, \text{ in } \mathbb{R}^2, \quad \mathrm{supp}\,\chi_a \in \Big(-\frac{1+a}{2}, \frac{1+a}{2}\Big)^2, \quad \chi_a = 1 \quad \text{in } \Big(-\frac{1}{2}, \frac{1}{2}\Big)^2, \ |\nabla\chi_a| \leq Ca^{-1}. \tag{4.3.25}$$

Let $L > 0$. Setting

$$\chi_{a,L}(r,s) = \chi_a\Big(\frac{r}{L}, \frac{s}{L}\Big), \quad (r,s) \in \mathbb{R}^2, \tag{4.3.26}$$

and,

$$\mu_a = \int_{\mathbb{R}^2} \chi_a^2(r,s)drds. \tag{4.3.27}$$

Recall that the negative part of a self-adjoint operator is defined via the spectral theorem and the function $\mathbb{R} \ni x \mapsto (x)_-$. We define

$$F_1(\theta,\lambda) := \liminf_{L\to\infty} \frac{\mathrm{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N - \lambda)\chi_{a,L}\big)_-}{L^2}, \quad F_2(\theta,\lambda) := \limsup_{L\to\infty} \frac{\mathrm{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N - \lambda)\chi_{a,L}\big)_-}{L^2} \tag{4.3.28}$$

where $\mathcal{P}_\theta^N$ is the self-adjoint operator given in (**??**). We now formulate the main theorem of this section.

Theorem 4.3.4. *Let $\theta \in (0, \pi/2]$, $\lambda \in [0, 1)$ and $E(\theta, \lambda)$ as introduced in* (**??**)*. We have the following explicit formula of $E(\theta,\lambda)$*

$$E(\theta,\lambda) = \frac{1}{2\pi}\sin(\theta)\sum_j (\zeta_j(\theta) - \lambda)_-, \tag{4.3.29}$$

where the $\{\zeta_j(\theta)\}_j$ are the eigenvalues from (**??**)*.*

The proof of Theorem **??** is split into two lemmas.

Lemma 4.3.5. *Let $a > 0$ be sufficiently small, $\lambda \in [0, 1)$ and $\theta \in (0, \pi/2]$. The following formula holds true*

$$F_1(\theta,\lambda) = F_2(\theta,\lambda) = \frac{1}{2\pi}\mu_a \sin(\theta)\sum_j (\zeta_j(\theta) - \lambda)_-, \tag{4.3.30}$$

where $F_1(\theta,\lambda)$, $F_2(\theta,\lambda)$ are the functions defined in (**??**) *and μ_a is the constant defined in* (**??**)*.*

Proof. Let $\mathcal{P}_\theta^N$ be the self-adjoint operator given in (**??**),and let $\{g_1, \cdots, g_N\}$ be any orthonormal set in $\mathcal{D}(\mathcal{P}_\theta^N)$. It follows from Lemma **??** that

$$\sum_{k=1}^N \big\langle \chi_{a,L} g_k, (\mathcal{P}_\theta^N - \lambda)\chi_{a,L} g_k\big\rangle_{L^2(\mathbb{R}^3_+)} \geq -\sum_j (\zeta_j(\theta) - \lambda)_- \sum_{k=1}^N \big\langle \chi_{a,L} g_k, \Pi_{\theta,j}\chi_{a,L} g_k\big\rangle_{L^2(\mathbb{R}^3_+)}. \tag{4.3.31}$$

Since $\{g_k\}_{k=1}^N$ is an orthonormal family in $L^2(\mathbb{R}^3_+)$ and performing a similar calculation to that in(**??**), we deduce that

$$\sum_{k=1}^N \big\langle \chi_{a,L} g_k, \Pi_{\theta,j}\chi_{a,L} g_k\big\rangle_{L^2(\mathbb{R}^3_+)} = \int_{\mathbb{R}} \sum_{k=1}^N \big|\langle g_k, v_{j,\theta}\chi_{a,L}\rangle_{L^2(\mathbb{R}^3_+)}\big|^2 d\xi \leq \frac{1}{2\pi}\mu_a L^2 \sin(\theta).$$

Implementing this in (**??**), we obtain

$$\sum_{k=1}^N \big\langle \chi_{a,L} g_k, (\mathcal{P}_\theta^N - \lambda)\chi_{a,L} g_k\big\rangle_{L^2(\mathbb{R}^3_+)} \geq -\frac{1}{2\pi}L^2 \mu_a \sin(\theta)\sum_j (\zeta_j(\theta) - \lambda)_-. \tag{4.3.32}$$

By the variational principle in Lemma **??**, we find

$$\mathrm{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N - \lambda)\chi_{a,L}\big)_- \leq \frac{1}{2\pi}L^2 \mu_a \sin(\theta)\sum_j (\zeta_j(\theta) - \lambda)_-. \tag{4.3.33}$$

Dividing by L^2 on both sides, we get after passing to the limit $L \to \infty$,

$$\limsup_{L\to\infty} \frac{\mathrm{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N - \lambda)\chi_{a,L}\big)_-}{L^2} \leq \frac{1}{2\pi}\mu_a \sin(\theta)\sum_j (\zeta_j(\theta) - \lambda)_-. \tag{4.3.34}$$

To prove a lower bound, we consider the density matrix

$$\gamma = \sum_{\{j\,:\,\zeta_j(\theta)\le\lambda\}} \Pi_{\theta,j}. \tag{4.3.35}$$

It is easy to see that $\gamma \ge 0$, and in view of (**??**), it follows that

$$\langle f, \gamma f\rangle_{L^2(\mathbb{R}^3_+)} \le \|f\|^2_{L^2(\mathbb{R}^3_+)}. \tag{4.3.36}$$

Next, we observe that

$$\begin{aligned}\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^N_\theta-\lambda)\chi_{a,L}\Pi_{\theta,j}\big) &= \int_{\mathbb{R}}\int_{\mathbb{R}^3_+}\Big(|(-i\nabla+\mathbf{F}_\theta)\chi_{a,L}v_{\theta,j}|^2-\lambda|\chi_{a,L}v_{\theta,j}|^2\Big)drdsdtd\xi\\ &\le \int_{\mathbb{R}}\int_{\mathbb{R}^3_+}\Big\{\chi^2_{a,L}(r,s)\Big(|(-i\nabla+\mathbf{F}_\theta)v_{\theta,j}|^2-\lambda|v_{\theta,j}|^2\Big)+|\nabla\chi_{a,L}(r,s)|^2|v_{\theta,j}|^2\Big\}drdsdtd\xi,\end{aligned} \tag{4.3.37}$$

where the last step follows by Cauchy Schwarz inequality. Performing the change of variable $\nu = s-\frac{\xi}{\sin(\theta)}$ in (**??**), we arrive at

$$\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^N_\theta-\lambda)\chi_{a,L}\gamma\big) \le \frac{\sin(\theta)}{2\pi}\sum_{\{j\,:\,\zeta_j(\theta)\le\lambda\}}\Big\{(\zeta_j(\theta)-\lambda)\mu_a L^2+\int_{\mathbb{R}^2}|\nabla\chi_a(r,s)|^2drds\Big\}, \tag{4.3.38}$$

where μ_a is the constant from (**??**). Dividing both sides by L^2 both sides, we see that

$$\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^N_\theta-\lambda)\chi_{a,L}\gamma\big)}{L^2} \le \frac{1}{2\pi}\sin(\theta)\sum_{\{j\,:\,\zeta_j(\theta)\le\lambda\}}\Big\{\mu_a(\zeta_j(\theta)-\lambda)+L^{-2}\int_{\mathbb{R}^2}|\nabla\chi_a|^2drds\Big\}. \tag{4.3.39}$$

Here we point out that the number $\mathcal{N}(\lambda;\mathcal{L}(\theta),\mathbb{R}^2_+)$ is controlled by $C/\sin(\theta)$ according to Lemma **??**. Using the variational principle, it follows that

$$-\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^N_\theta-\lambda)\chi_{a,L}\big)_-}{L^2} \le -\frac{1}{2\pi}\mu_a\sin(\theta)\sum_j(\zeta_j(\theta)-\lambda)_- + C(2\pi)^{-1}L^{-2}\int_{\mathbb{R}^2}|\nabla\chi_a|^2drds.$$

Taking the limit $L\to\infty$, we deduce that

$$\liminf_{L\to\infty}\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^N_\theta-\lambda)\chi_{a,L}\big)_-}{L^2} \ge \frac{1}{2\pi}\mu_a\sin(\theta)\sum_j(\zeta_j(\theta)-\lambda)_-.$$

This together with (**??**) and the definitions of $F_1(\theta,\lambda)$ and $F_2(\theta,\lambda)$ in (**??**) yields the desired formula. $\square$

Our next goal is to establish a connection between the functions $F_1(\theta,\lambda)$ and $F_2(\theta,\lambda)$ obtained in Lemma **??** and $E(\theta,\lambda)$ from (**??**).

Theorem 4.3.6. *Let $\theta\in(0,\pi/2]$ and $\lambda\in(0,1)$. It holds true that*

$$F_1(\theta,\lambda)=F_2(\theta,\lambda)=\mu_a E(\theta,\lambda).$$

*where μ_a is the constant from (**??**).*

Proof. Let $L \gg \ell \gg 1$. We consider the domain

$$\Omega_{j,k,\ell} = (j\ell, (j+1)\ell) \times (k\ell, (k+1)\ell) \times \mathbb{R}_+, \qquad (j,k) \in \mathbb{Z}^2.$$

We will denote by $\mathcal{N}_B$ the number of boxes of the form $\Omega_{j,k,\ell}$ intersecting $\operatorname{supp} \chi_{a,L}$:

$$\mathcal{N}_B = \sharp\{(j,k) \in \mathbb{Z}^2 \,:\, \operatorname{supp} \chi_{a,L} \cap \Omega_{j,k,\ell} \neq \emptyset\}. \tag{4.3.40}$$

Recall the magnetic field $\mathbf{F}_\theta$ defined in (**??**), we consider the self-adjoint operator $\mathcal{P}^\ell_{\theta,j,k}$ generated by the quadratic form

$$\mathcal{Q}^\ell_{\theta,j,k}(u) = \int_{\Omega_{j,k,\ell}} |(-i\nabla + \mathbf{F}_\theta)u|^2 drdsdt,$$

with domain,

$$\begin{aligned}\mathcal{D}(\mathcal{Q}^\ell_{\theta,j,k}) = \Big\{ & u \in L^2(\Omega_{j,k,\ell}) \,:\, (-i\nabla + \mathbf{F}_\theta)u \in L^2(\Omega_{j,k,\ell}), \\ & u(j\ell,\cdot,\cdot) = u((j+1)\ell,\cdot,\cdot) = 0, u(\cdot,k\ell,\cdot) = u(\cdot,(k+1)\ell,\cdot) = 0\Big\}.\end{aligned} \tag{4.3.41}$$

Since any function that belongs to the form domain $\bigoplus_{j,k} \mathcal{D}(\mathcal{Q}^\ell_{\theta,j,k})$ lies in the form domain $\mathcal{D}(\mathcal{Q}^N_\theta)$ and the values of both quadratic forms coincide for such a function, we have the operator inequality

$$\chi_{a,L}(\mathcal{P}^N_\theta - \lambda)\chi_{a,L} \leq \bigoplus_{j,k} \chi_{a,L}(\mathcal{P}^\ell_{\theta,j,k} - \lambda)\chi_{a,L}, \tag{4.3.42}$$

in the sense of quadratic forms. As a consequence, the min max principle allows us to write,

$$-\operatorname{Tr}(\chi_{a,L}(\mathcal{P}^N_\theta - \lambda)\chi_{a,L})_- \leq -\sum_{j,k} \operatorname{Tr}(\chi_{a,L}(\mathcal{P}^\ell_{\theta,j,k} - \lambda)\chi_{a,L})_-. \tag{4.3.43}$$

Let $S_{jk} \in \mathbb{N}$ be the number of eigenvalues of $\mathcal{P}^\ell_{\theta,j,k}$, $\{\lambda_m\}_{m=1}^{S_{jk}}$, that are below λ and let $\{f_s\}_{m=1}^{S_{jk}} \in \mathcal{D}(\mathcal{Q}^\ell_{\theta,j,k})$ be associated (normalized) eigenfunctions. We consider the density matrix

$$\gamma_{j,k} f = \sum_{m=1}^{S_{jk}} \langle f, f_m\rangle f_m, \quad f \in L^2(\Omega^\ell_{jk}).$$

Next, we compute

$$\begin{aligned}\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^\ell_{\theta,j,k} - \lambda)\chi_{a,L}\gamma_{j,k}\big) &= \sum_{m=1}^{S_{jk}} (\mathcal{Q}^\ell_{\theta,j,k}(\chi_{a,L}f_m) - \lambda\|\chi_{a,L}f_m\|^2) \\ &= \sum_{m=1}^{S_{jk}} \Big\{(\lambda_m - \lambda)\|\chi_{a,L}f_m\|^2 + \||\nabla\chi_{a,L}|f_m\|^2\Big\},\end{aligned} \tag{4.3.44}$$

where the last step follows since $\{f_m\}_{m=1}^{S_{jk}}$ are eigenfunctions.

Let us denote by $x^\star_{j,k,\ell}$ the point belonging to the interval $(j\ell, (j+1)\ell) \times (k\ell, (k+1)\ell)$ where the function $\chi^2_{a,L}$ attains its minimum :

$$\chi^2_{a,L}(x^\star_{j,k,\ell}) = \min_{(r,s)\in(j\ell,(j+1)\ell)\times(k\ell,(k+1)\ell)} \chi^2_{a,L}(r,s).$$

It follows that

$$\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{\ell}_{\theta,j,k}-\lambda)\chi_{a,L}\gamma_{j,k}\big)\leq \chi^2_{a,L}(x^{\star}_{j,k,\ell})\sum_{m=1}^{S_{jk}}(\lambda_m-\lambda)+\sum_{m=1}^{S_{jk}}\||\nabla\chi_{a,L}|f_m\|^2, \tag{4.3.45}$$

where have used that the term $\sum_{m=1}^{S_{jk}}(\lambda_m-\lambda)$ is negative. Inserting this into (**??**) and using the bound $|\nabla\chi_{a,L}|\leq C(aL)^{-1}$, we find

$$\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{\ell}_{\theta,j,k}-\lambda)\chi_{a,L}\gamma_{j,k}\big)\leq \chi^2_{a,L}(x^{\star}_{j,k,\ell})\sum_{m=1}^{S_{jk}}(\lambda_m-\lambda)+S_{jk}C(aL)^{-2}.$$

By (**??**), we have $S_{jk}\leq C\ell^2$. Using (**??**), we obtain

$$\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{\ell}_{\theta,j,k}-\lambda)\chi_{a,L}\gamma_{j,k}\big)\leq \chi^2_{a,L}(x^{\star}_{j,k,\ell})(-E(\theta,\lambda)+C\ell^{-2/3})\ell^2+C\ell^2(aL)^{-2}. \tag{4.3.46}$$

By (**??**) and Lemma **??**, it follows that

$$\begin{aligned}-\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-&\leq\sum_{j,k}\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\gamma_{j,k}\big)\\&\leq\Big\{\sum_{j,k}\chi^2_{a,L}(x^{\star}_{j,k,\ell})\ell^2\Big\}(-E(\theta,\lambda)+C\ell^{-2/3})+C\mathcal{N}_B\ell^2(aL)^{-2}.\end{aligned} \tag{4.3.47}$$

The sum $\sum_{j,k}\chi^2_{a,L}(x^{\star}_{j,k,\ell})\ell^2$ is a (lower) Riemannian sum. Thus, we have

$$\Big|\sum_{j,k}\chi^2_{a,L}(x^{\star}_{j,k,\ell})\ell^2-\int_{\mathbb{R}^2}\chi^2_{a,L}(r,s)drds(=\mu_aL^2)\Big|\leq C\ell L.$$

Substituting this into (**??**), we obtain

$$-\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-\leq E(\theta,\lambda)L^2\big(-\mu_a+C\ell L^{-1}\big)+C\ell^{-2/3}(\mu_aL^2+C\ell L)+C\mathcal{N}_B\ell^2(aL)^{-2}.$$

Dividing both sides by L^2, we get

$$-\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-}{L^2}\leq E(\theta,\lambda)\big(-\mu_a+C\ell L^{-1}\big)+C\ell^{-2/3}(\mu_a+C\ell L^{-1})+C\mathcal{N}_B\ell^{-2}a^{-2}L^{-4}.$$

We make the following choice of ℓ,

$$\ell=L^{\eta},\quad \eta<1.$$

Since $\mathcal{N}_B\sim((1+a))^2L^2\ell^{-2}$ as $L\to\infty$, we get, after taking $L\to\infty$ the following lower bound

$$\liminf_{L\to\infty}\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-}{L^2}\geq E(\theta,\lambda)\mu_a. \tag{4.3.48}$$

It remains to prove the upper bound. By the variational principle and the fact that the trace is cyclic, we see that

$$-\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-=\inf_{0\leq\gamma\leq1}\operatorname{Tr}\big((\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\gamma\chi_{a,L}\big).$$

Since the function $\chi_{a,L}$ is supported in $\big(-\frac{(1+a)L}{2},\frac{(1+a)L}{2}\big)^2$, it follows that

$$-\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}^{N}_{\theta}-\lambda)\chi_{a,L}\big)_-\geq\inf_{0\leq\widetilde{\gamma}\leq1}\operatorname{Tr}\big[(\mathcal{P}^{(1+a)L}_{\theta}-\lambda)\widetilde{\gamma}\big]. \tag{4.3.49}$$

By Theorem **??**, we know that

$$\inf_{0\le\widetilde{\gamma}\le 1}\operatorname{Tr}\big[(\mathcal{P}_\theta^{(1+a)L}-\lambda)\widetilde{\gamma}\big]=-\mathcal{E}(\lambda;\mathcal{P}_\theta^{(1+a)L},\Omega^{(1+a)L})\ge-((1+a)L)^2E(\theta,\lambda).$$

Substituting in (**??**) yields that

$$-\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N-\lambda)\chi_{a,L}\big)_-\ge-((1+a)L)^2E(\theta,\lambda).$$

We conclude that, when $L\to\infty$,

$$\limsup_{L\to\infty}\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N-\lambda)\chi_{a,L}\big)_-}{L^2}\le E(\theta,\lambda)(1+a)^2. \tag{4.3.50}$$

Combining (**??**) and (**??**), we obtain

$$\begin{aligned}\mu_aE(\theta,\lambda)&\le\liminf_{L\to\infty}\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N-\lambda)\chi_{a,L}\big)_-}{L^2}\\&\le\limsup_{L\to\infty}\frac{\operatorname{Tr}\big(\chi_{a,L}(\mathcal{P}_\theta^N-\lambda)\chi_{a,L}\big)_-}{L^2}\le(1+a)^2E(\theta,\lambda)\end{aligned} \tag{4.3.51}$$

We select a sufficiently small so that $\mu_a\sim(1+a)^2$. Recall the definition of $F_1(\theta,\lambda)$ and $F_2(\theta,\lambda)$ in (**??**), we deduce that

$$F_1(\theta,\lambda)=F_2(\theta,\lambda)=\mu_aE(\theta,\lambda),$$

thereby completing the proof of Lemma **??**. □

Proof of Theorem **??**. The proof follows easily from Lemma **??** and Lemma **??**. □

4.3.3 Dilation

Let us define the unitary operator

$$U_{h,b}:L^2(\mathbb{R}^3_+)\ni u\mapsto U_{h,b}u(z)=h^{3/4}b^{-3/4}u(h^{1/2}b^{-1/2}z)\in L^2(\mathbb{R}^3_+), \tag{4.3.52}$$

Let $h,b>0$ and $\theta\in[0,\pi/2]$. We introduce the self-adjoint operator

$$\mathcal{P}^N_{\theta,h,b}=(-ih\nabla+b\mathbf{F}_\theta)^2,\quad\text{in}\quad L^2(\mathbb{R}^3_+), \tag{4.3.53}$$

with Neumann boundary conditions at $t=0$. With $\mathcal{P}_\theta^N$ being the operator from (**??**), it is easy to check that

$$\mathcal{P}^N_{\theta,h,b}=hbU_{h,b}\mathcal{P}^N_\theta U^{-1}_{h,b}. \tag{4.3.54}$$

For $j\in\mathbb{N}$ and $(\xi,\tau)\in\mathbb{R}^2$, we introduce the family of projectors

$$\Pi_j(\xi,\tau;h,b)=U_{h,b}\Pi_j(\xi,\tau)U^{-1}_{h,b} \tag{4.3.55}$$

and, for $\theta\in(0,\pi/2]$,

$$\Pi_{\theta,j}(h,b)=U_{h,b}\Pi_{\theta,j}U^{-1}_{h,b} \tag{4.3.56}$$

where, $\Pi_j(\xi,\tau)$ and $\Pi_{\theta,j}$ are introduced in (**??**) and (**??**) respectively. We deduce the following two generalizations of Lemma **??** and Lemma **??**.

Lemma 4.3.7. *For all $\varphi \in L^2(\mathbb{R}^3_+)$, we have*

$$\left\langle \mathcal{P}^N_{0,h,b}(\Pi_j(\xi,\tau;h,b)\varphi),\varphi\right\rangle_{L^2(\mathbb{R}^3_+)} = hb(\mu_j(\xi)+\tau^2)\left\langle \Pi_j(\xi,\tau;h,b)\varphi,\varphi\right\rangle_{L^2(\mathbb{R}^3_+)}, \tag{4.3.57}$$

$$\sum_j \int_{\mathbb{R}^2} \left\langle \varphi, \Pi_j(\xi,\tau;h,b)\varphi\right\rangle_{L^2(\mathbb{R}^3_+)} d\xi d\tau = 2\pi \left\|\varphi\right\|^2_{L^2(\mathbb{R}^3_+)}. \tag{4.3.58}$$

Moreover, for any smooth cut-off function $\chi \in C_0^\infty(\mathbb{R}^2)$, it holds true that

$$\mathrm{Tr}(\chi\Pi_j(\xi,\tau;h,b)\chi) = bh^{-1}(2\pi)^{-1}\int_{\mathbb{R}^2}\chi^2(r,s)drds. \tag{4.3.59}$$

Lemma 4.3.8. *Let $f \in L^2(\mathbb{R}^3_+)$, we have*

$$\left\langle \mathcal{P}^N_{\theta,h,b}\Pi_{\theta,j}(h,b)f,f\right\rangle_{L^2(\mathbb{R}^3_+)} = hb\zeta_j(\theta)\left\langle \Pi_{\theta,j}(h,b)f,f\right\rangle_{L^2(\mathbb{R}^3_+)}, \tag{4.3.60}$$

$$\Big\langle \sum_j \Pi_{\theta,j}(h,b)f,f\Big\rangle_{L^2(\mathbb{R}^3_+)} \leq \|f\|^2_{L^2(\mathbb{R}^3_+)}. \tag{4.3.61}$$

Moreover, for any smooth cut-off function $\chi \in C_0^\infty(\mathbb{R}^2)$, it holds true that

$$\mathrm{Tr}(\chi\Pi_{\theta,j}(h,b)\chi) = bh^{-1}(2\pi)^{-1}\sin(\theta)\int_{\mathbb{R}^2}\chi^2(r,s)drds. \tag{4.3.62}$$

Chapter 5

Boundary coordinates

The aim of this chapter is to approximate the quadratic form defined in (**??**):

$$\mathcal{D}(\mathcal{Q}_h) \ni u \mapsto \mathcal{Q}_h(u) := \int_\Omega |(-ih\nabla + \mathbf{A})u|^2 dx$$

under the assumption that u is supported near the boundary $\partial\Omega$ and the magnetic potential $\mathbf{A}$ is $C^\infty(\Omega; \mathbb{R}^3)$. To achieve this, we need to introduce a system of coordinates valid near a point of the boundary. This is the subject of Section **??**. These coordinates are used in [**?**] and then in [**?**] in order to estimate the ground state energy of a magnetic Schrödinger operator with large magnetic field (or with 'small' semi-classical parameter). In section **??**, we perform a rotation in order to obtain a reduced form of the metric (in the new coordinates). Having this in hand, we proceed to approximate the quadratic form in Section **??**.

5.1 Local coordinates

We denote the standard coordinates on $\mathbb{R}^3$ by $x = (x_1, x_2, x_3)$. The standard Euclidean metric is given by

$$g_0 = dx_1^2 + dx_2^2 + dx_3^2. \tag{5.1.1}$$

Consider a point $x_0 \in \partial\Omega$. Let $\mathcal{V}_{x_0}$ be a neighbourhood of x_0 such that there exist local boundary coordinates (r, s) in $W = \mathcal{V}_{x_0} \cap \partial\Omega$, i.e., there exist an open subset U of $\mathbb{R}^2$ and a diffeomorphism $\phi_{x_0} : W \to U$, $\phi_{x_0}(x) = (r, s)$, such that $\phi_{x_0}(x_0) = 0$ and $D\phi_{x_0}(x_0) = \mathrm{Id}_2$ where Id_2 is the 2×2 identity matrix. Then for $t_0 > 0$ small enough, we define the coordinate transformation $\Phi_{x_0}^{-1}$ as

$$U \times (0, t_0) \ni (r, s, t) \mapsto x := \Phi_{x_0}^{-1}(r, s, t) = \phi_{x_0}^{-1}(r, s) + t\nu, \tag{5.1.2}$$

where ν is the interior normal unit vector at the point $\phi_{x_0}^{-1}(r, s) \in \partial\Omega$. This defines a diffeomorphism of $U \times (0, t_0)$ onto $\mathcal{V}_{x_0}$ and its inverse Φ_{x_0} defines local coordinates on $\mathcal{V}_{x_0}$, $\mathcal{V}_{x_0} \ni x \mapsto \Phi_{x_0}(x) = (r(x), s(x), t(x))$ such that

$$t(x) = \operatorname{dist}(x, \partial\Omega).$$

It is easily to be seen that the Φ_{x_0} are constructed so that

$$\Phi_{x_0}(x_0) = 0, \qquad D\Phi_{x_0}(x_0) = \mathrm{Id}_3, \tag{5.1.3}$$

where Id_3 denotes the 3×3 identity matrix. For convenience, we will henceforth write (y_1, y_2, y_3) instead of (r, s, t). Let us consider the matrix

$$\begin{aligned} g &:= g_{x_0} = (g_{pq})_{p,q=1}^3, \\ g_{pq} &= \left\langle \frac{\partial x}{\partial y_p}, \frac{\partial x}{\partial y_q} \right\rangle \\ \langle X, Y \rangle &= \sum_{1 \le p,q \le 3} g_{pq} \widetilde{X}_p \widetilde{Y}_q, \end{aligned} \tag{5.1.4}$$

where $X = \sum_p \widetilde{X}_p \frac{\partial}{\partial y_p}$ and $Y = \sum_q \widetilde{Y}_q \frac{\partial}{\partial y_q}$.

We point out that we may express the matrix $g = (g_{pq})_{p,q=1}^3$, whose coefficients are defined in (**??**), as

$$g = (g_{pq})_{p,q=1}^3 = (D\Phi_{x_0}^{-1})^T (D\Phi_{x_0}^{-1}). \tag{5.1.5}$$

Next, we define the map :

$$y \mapsto \widetilde{u}(y) := u(\Phi_{x_0}^{-1}(y)) \,. \tag{5.1.6}$$

The Euclidean metric (**??**) transforms to

$$\begin{aligned} g_0 &= \sum_{1 \le p,q \le 3} g_{pq} dy_p \otimes dy_q \\ &= dy_3 \otimes dy_3 + \sum_{1 \le p,q \le 2} \big[G_{pq}(y_1, y_2) - 2y_3 K_{pq}(y_1, y_2) + y_3^2 L_{pq}(y_1, y_2) \big] dy_p \otimes dy_q, \end{aligned}$$

where

$$\begin{aligned} G &= \sum_{1 \le p,q \le 2} G_{pq} dy_p \otimes dy_q &&= \sum_{1 \le p,q \le 2} \left\langle \frac{\partial x}{\partial y_p}, \frac{\partial x}{\partial y_q} \right\rangle dy_p \otimes dy_q, \\ K &= \sum_{1 \le p,q \le 2} K_{pq} dy_p \otimes dy_q &&= \sum_{1 \le p,q \le 2} \left\langle \frac{\partial \nu}{\partial y_p}, \frac{\partial x}{\partial y_q} \right\rangle dy_p \otimes dy_q, \\ L &= \sum_{1 \le p,q \le 2} L_{pq} dy_p \otimes dy_q &&= \sum_{1 \le p,q \le 2} \left\langle \frac{\partial \nu}{\partial y_p}, \frac{\partial \nu}{\partial y_q} \right\rangle dy_p \otimes dy_q \end{aligned}$$

are the first, second and third fundamental forms on $\partial\Omega$.

Note that if $x \in \mathcal{V}_{x_0} \cap \partial\Omega$, i.e, $t(x) = 0$, g_0 reduces to

$$g_0 = dy_3 \otimes dy_3 + G. \tag{5.1.7}$$

Let us denote by $g^{-1} := (g^{pq})_{p,q=1}^3$ the matrix inverse of $(g_{pq})_{p,q=1}^3$. By virtue of (**??**), we may assume, by taking $\mathcal{V}_{x_0}$ small enough, that

$$\frac{1}{2} \,\mathrm{Id}_3 \le (g^{pq})_{p,q=1}^3 \le 2 \,\mathrm{Id}_3 \tag{5.1.8}$$

Let y_0 be such that $\Phi_{x_0}^{-1}(y_0) \in \mathcal{V}_{x_0} \cap \partial\Omega$. We will prove that there exists a uniform constant $c > 0$ such that

$$(1 - 2c|y - y_0|) g^{-1}(y_0) \le g^{-1}(y) \le (1 + 2c|y - y_0|) g^{-1}(y_0). \tag{5.1.9}$$

Proof of (**??**). By Taylor expansion, we have

$$g^{-1}(y) = g^{-1}(y_0) + \mathcal{R} \tag{5.1.10}$$

where $\mathcal{R}$ is given by

$$\mathcal{R} := \begin{pmatrix} \mathcal{O}(|y-y_0|) & \mathcal{O}(|y-y_0|) & 0 \\ \mathcal{O}(|y-y_0|) & \mathcal{O}(|y-y_0|) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5.1.11}$$

Notice that the constants implicit in (**??**) depends for instance on the point x_0 of the boundary, in particular on the derivatives $\partial^2_{x_i}\phi_{x_0}$, $i = 1, 2, 3$. In a neighbourhood of x_0, these derivatives are uniformly bounded. We thus get

$$|g^{-1}(y) - g^{-1}(y_0)| \leq \|\mathcal{R}\| \,\mathrm{Id}_3 = c_{y_0}|y - y_0|\mathrm{Id}_3\,, \tag{5.1.12}$$

with c_{x_0} a constant depending on the point x_0. However, since the boundary is compact, we can cover the boundary by a finite collection of neighbourhoods of points (x_j) (see Subsection **??** below). In each neighbourhood, we get an estimate of the type (**??**) with constant c_{x_j}. Defining $c = \max c_{x_j}$, we get,

$$|g(y) - g(y_0)| \leq c|y - y_0|\mathrm{Id}_3\,. \tag{5.1.13}$$

This way, c does not vary as the point x_0 traces $\partial\Omega$. Using (**??**), the claim follows from (**??**). □

Let $|g| = \det(g)$. The Lebesgue measure transforms to $dx = \det(g)^{1/2}dy$. The Taylor expansion of $\det(g)^{1/2}$ in $\mathcal{V}_{x_0}$ gives us :

$$(1 + 2c|y - y_0|)|g|^{1/2}(y_0) \leq |g|^{1/2}(y) \leq (1 + 2c|y - y_0|)|g|^{1/2}(y_0). \tag{5.1.14}$$

Again the constant c appearing in (**??**) can be chosen uniformly by compactness and regularity of $\partial\Omega$. The magnetic potential $\mathbf{A} = (\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3)$ is transformed to a magnetic potential in the new coordinates $\widetilde{\mathbf{A}} = (\widetilde{\mathbf{A}}_1, \widetilde{\mathbf{A}}_2, \widetilde{\mathbf{A}}_3)$ given by

$$\widetilde{\mathbf{A}}_p(y) = \sum_{k=1}^{3} \mathbf{A}_k(\Phi^{-1}_{x_0}(y))\frac{\partial x_k}{\partial y_p}, \quad p = 1, 2, 3. \tag{5.1.15}$$

The magnetic field is given by

$$B = \sum_{1\leq j<k\leq 3} \widetilde{B}_{jk}dy_j \wedge dy_k,$$

where

$$\widetilde{B}_{jk} = \frac{\partial \widetilde{\mathbf{A}}_k}{\partial y_j} - \frac{\partial \widetilde{\mathbf{A}}_j}{\partial y_k}$$

For $y \in \Phi_{x_0}(\mathcal{V}_{x_0})$, we define

$$\widetilde{\mathbf{B}}(y) = \mathbf{B}(\Phi^{-1}_{x_0}(y)).$$

By the fact that

$$\mathbf{A} = \mathbf{A}_1dx_1 + \mathbf{A}_2dx_2 + \mathbf{A}_3dx_3 = \widetilde{\mathbf{A}}_1dy_1 + \widetilde{\mathbf{A}}_2dy_2 + \widetilde{\mathbf{A}}_3dy_3,$$

it follows that

$$\sum_{1\leq j<k\leq 3} B_{jk}dx_j \wedge dx_k = \sum_{1\leq j<k\leq 3} \widetilde{B}_{jk}dy_j \wedge dy_k.$$

Consequently, we get

$$\widetilde{\mathbf{B}}(y) = |g|^{-1/2}(\widetilde{B}_{23}, \widetilde{B}_{31}, \widetilde{B}_{12}).$$

The approximation of the magnetic potential in the new coordinates is done by replacing $\widetilde{\mathbf{A}}$ by its linear part at y_0, which we denote $\widetilde{\mathbf{A}}^{\mathrm{lin}} = (\widetilde{\mathbf{A}}_1^{\mathrm{lin}}, \widetilde{\mathbf{A}}_2^{\mathrm{lin}}, \widetilde{\mathbf{A}}_3^{\mathrm{lin}})$, so that

$$|\widetilde{\mathbf{A}}_p(y) - \widetilde{\mathbf{A}}_p^{\mathrm{lin}}(y)| \leq C|y-y_0|^2, \tag{5.1.16}$$

for all $p = 1, 2, 3$, where

$$\widetilde{\mathbf{A}}^{\mathrm{lin}}(y) = \widetilde{\mathbf{A}}(y_0) + \sum_{p=1}^{3}(y_p - y_{0p})\frac{\partial \widetilde{\mathbf{A}}}{\partial y_p}(y_0). \tag{5.1.17}$$

The following identity (cf. [?, formula (7.23)]) gives the strength of the magnetic field expressed in the new coordinates,

$$|\widetilde{\mathbf{B}}(y_0)|^2 = |g(y_0)|^{-1}\left[\sum_{p,q=1}^{3} g_{pq}(y_0)\alpha_p\alpha_q\right], \tag{5.1.18}$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3)$ is given by

$$\begin{aligned}
\alpha_1 &= \frac{\partial \widetilde{\mathbf{A}}_3}{\partial y_2}(y_0) - \frac{\partial \widetilde{\mathbf{A}}_2}{\partial y_3}(y_0),\\
\alpha_2 &= \frac{\partial \widetilde{\mathbf{A}}_1}{\partial y_3}(y_0) - \frac{\partial \widetilde{\mathbf{A}}_3}{\partial y_1}(y_0),\\
\alpha_3 &= \frac{\partial \widetilde{\mathbf{A}}_2}{\partial y_1}(y_0) - \frac{\partial \widetilde{\mathbf{A}}_1}{\partial y_2}(y_0).
\end{aligned} \tag{5.1.19}$$

It follows from (??) that $\det\left(D\Phi_{x_0}^{-1}\right) = |g|^{1/2}$.

The next Lemma expresses, in terms of the new coordinates, the quadratic form and the L^2-norm of a function u supported in a neighbourhood of x_0.

Lemma 5.1.1. *Let $u \in \mathcal{D}(\mathcal{P}_h)$ such that $\operatorname{supp} u \subset \mathcal{V}_{x_0}$. We have*

$$\begin{aligned}
\mathcal{Q}_h(u) &= \int_{\mathcal{V}_{x_0}} |(-ih\nabla + \mathbf{A})u|^2 dx\\
&= \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\,\widetilde{u}\,\overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\,\widetilde{u}}\,|g|^{1/2}dy,
\end{aligned} \tag{5.1.20}$$

and,

$$\|u\|^2_{L^2(\Omega)} = \int_\Omega |u(x)|^2 dx = \int_{\mathbb{R}^3_+} |g|^{1/2}|\widetilde{u}(y)|^2 dy. \tag{5.1.21}$$

5.2 Diagonalization of the metric and gauge transformation

Recall the Jacobian matrix $g := g_{x_0}$ introduced in (??) and valid in $\mathcal{V}_{x_0}$. Let y_0 be such that $\Phi_{x_0}^{-1}(y_0) \in \mathcal{V}_{x_0} \cap \partial\Omega$. The goal in this section is to get a simplified expression of the quadratic form

$$L^2(\mathcal{V}_{x_0}) \ni u \mapsto \mathcal{Q}_h^{\mathrm{lin}}(u) := \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p^{\mathrm{lin}})\,\widetilde{u}\,\overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q^{\mathrm{lin}})\,\widetilde{u}}\,|g(y_0)|^{1/2}dy \tag{5.2.1}$$

where $\widetilde{\mathbf{A}}^{\text{lin}}$ is the magnetic potential from (**??**), and $\widetilde{u}$ is associated to u by (**??**).

The matrix $(g(y_0))$ being symmetric, in view of (**??**), it can be orthogonally diagonalized, and such a diagonalization amounts to a rotation of the coordinate system. Namely, there is an orthogonal matrix P (with $P^{-1} = P^T$) and a diagonal matrix D such that $g(y_0) = PDP^{-1}$. In other words, there are $a, b, \lambda_1, \lambda_2 \in \mathbb{R}$ such that

$$P := \begin{pmatrix} a_1 & a_2 & 0 \\ -a_2 & a_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.2.2}$$

with $a_1^2 + a_2^2 = 1$, and

$$D := \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{5.2.3}$$

By virtue of (**??**), it is easy to see that $\lambda_1, \lambda_2 > 0$.

Thus g can be written as

$$g := \begin{pmatrix} \lambda_1 a_1^2 + \lambda_2 a_2^2 & (-\lambda_1 + \lambda_2) a_1 a_2 & 0 \\ (-\lambda_1 + \lambda_2) a_1 a_2 & \lambda_2 a_1^2 + \lambda_1 a_2^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{5.2.4}$$

Let $y' = yP^{-1} = (a_1 y_1 + a_2 y_2, -a_2 y_1 + a_1 y_2, y_3)$ and

$$\widehat{\mathbf{A}}^{\text{lin}}(y') = P\widetilde{\mathbf{A}}^{\text{lin}}(y'P) = \begin{pmatrix} a_1 \widetilde{\mathbf{A}}_1^{\text{lin}}(y'P) + a_2 \widetilde{\mathbf{A}}_2^{\text{lin}}(y'P) \\ -a_2 \widetilde{\mathbf{A}}_1^{\text{lin}}(y'P) + a_1 \widetilde{\mathbf{A}}_2^{\text{lin}}(y'P) \\ \widetilde{\mathbf{A}}_3^{\text{lin}}(y'P) \end{pmatrix} \tag{5.2.5}$$

Easy manipulations leads to

$$\begin{aligned} \mathcal{Q}_h^{\text{lin}}(u) &= \int_{\mathbb{R}^3_+} \lambda_1^{-1} \big|(-ih\partial_{y_1'} + \widehat{\mathbf{A}}_1^{\text{lin}})\widetilde{u}(y'P)\big|^2 (\lambda_1\lambda_2)^{1/2} dy' \\ &+ \int_{\mathbb{R}^3_+} \lambda_2^{-1} \big|(-ih\partial_{y_2'} + \widehat{\mathbf{A}}_2^{\text{lin}})\widetilde{u}(y'P)\big|^2 (\lambda_1\lambda_2)^{1/2} dy' + \int_{\mathbb{R}^3_+} \big|(-ih\partial_{y_3'} + \widehat{\mathbf{A}}_3^{\text{lin}})\widetilde{u}(y'P)\big|^2 (\lambda_1\lambda_2)^{1/2} dy'. \end{aligned} \tag{5.2.6}$$

Recall (**??**), we have

$$\operatorname{curl}_y (\widetilde{\mathbf{A}}^{\text{lin}}(y)) = (\alpha_1, \alpha_2, \alpha_3).$$

where $\alpha_1, \alpha_2, \alpha_3$ are defined in (**??**). It follows that

$$P^{-1}\operatorname{curl}_y (\widetilde{\mathbf{A}}^{\text{lin}}(y)) := \begin{pmatrix} a_1\alpha_1 - a_2\alpha_2 \\ a_2\alpha_1 + a_1\alpha_2 \\ \alpha_3 \end{pmatrix} \tag{5.2.7}$$

It is straightforward to show that

$$\operatorname{curl}_{y'} (\widehat{\mathbf{A}}^{\text{lin}}(y')) = P^{-1}\operatorname{curl}_y (\widetilde{\mathbf{A}}^{\text{lin}}(y)).$$

This shows that the strength of the magnetic field is conserved under orthogonal diagonalization, i.e,

$$|\operatorname{curl}_{y'} (\widehat{\mathbf{A}}^{\text{lin}}(y'))| = |\operatorname{curl}_y (\widetilde{\mathbf{A}}^{\text{lin}}(y))| = (\alpha_1^2 + \alpha_2^2 + \alpha_3^2)^{1/2} = |\widetilde{\mathbf{B}}(y_0)|.$$

Moreover, by (**??**), we may work henceforth with the diagonalized form of the metric and assume that the matrix $(g_{x_0}(y_0))$ is a diagonal matrix, i.e.,

$$g(y_0) = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5.2.8}$$

It follows that $|g(y_0)|^{1/2} = \sqrt{\lambda_1 \lambda_2}$.

Next, we perform the change of variables $z = (z_1, z_2, z_3) = \left(\lambda_1^{1/2} y_1, \lambda_2^{1/2} y_2, y_3\right)$ and denote by

$$\breve{u}(z) := \widetilde{u}(y) = \widetilde{u}\big(\lambda_1^{-1/2} z_1, \lambda_2^{-1/2} z_2, z_3\big). \tag{5.2.9}$$

It is easy to check that

$$\int_{\mathbb{R}^3_+} |g(y_0)|^{1/2} |\widetilde{u}(y)|^2 dy = \int_{\mathbb{R}^3_+} |\breve{u}(z)|^2 dz. \tag{5.2.10}$$

Moreover, the quadratic form in (**??**) becomes

$$\mathcal{Q}_h^{\text{lin}}(u) = \sum_{p=1}^{3} \int_{\mathbb{R}^3_+} |(-ih\nabla_{z_p} + \mathbf{F}_p)\, \breve{u}|^2 \, dz \tag{5.2.11}$$

where $\mathbf{F} = (\mathbf{F}_1, \mathbf{F}_2, \mathbf{F}_3)$ is the magnetic potential given by

$$\begin{aligned} \mathbf{F}_1(z) &= \lambda_1^{-1/2} \widetilde{\mathbf{A}}_1^{\text{lin}}(\lambda_1^{-1/2} z_1, \lambda_2^{-1/2} z_2, z_3) \\ \mathbf{F}_2(z) &= \lambda_2^{-1/2} \widetilde{\mathbf{A}}_2^{\text{lin}}(\lambda_1^{-1/2} z_1, \lambda_2^{-1/2} z_2, z_3) \\ \mathbf{F}_3(z) &= \widetilde{\mathbf{A}}_3^{\text{lin}}(\lambda_1^{-1/2} z_1, \lambda_2^{-1/2} z_2, z_3). \end{aligned}$$

Let $\beta = (\beta_1, \beta_2, \beta_3) = \text{curl}_z(\mathbf{F}(z))$ and note that the coefficients of β and α (see (**??**)) are related by

$$\beta_1 = \lambda_2^{-1/2} \alpha_1, \qquad \beta_2 = \lambda_1^{-1/2} \alpha_2, \qquad \beta_3 = (\lambda_1 \lambda_2)^{-1/2} \alpha_3.$$

The relation (**??**) gives that

$$|\beta| = |\text{curl}_z(\mathbf{F}(z))| = (\beta_1^2 + \beta_2^2 + \beta_3^2)^{1/2} = |\widetilde{\mathbf{B}}|(y_0). \tag{5.2.12}$$

Recall the magnetic field from (**??**), and note that for any $\theta \in [0, \pi/2]$, we have

$$\text{curl}(\mathbf{F}_\theta) = (0, \cos(\theta), \sin(\theta)).$$

Next we perform a rotation in the (z_1, z_2)-variables chosen so that the image of $(\beta_1, \beta_2, \beta_3)$ is the vector $|\widetilde{\mathbf{B}}(y_0)|(0, \cos(\theta_0), \sin(\theta_0))$ where $\theta_0 := \widetilde{\theta}(y_0)$ is given by

$$\theta_0 := \widetilde{\theta}(y_0) = \arcsin\left(\frac{|\beta_3|}{|\beta|}\right). \tag{5.2.13}$$

We emphasize here that (**??**) is compatible with the definition of $\theta(x)$ given in (**??**), i.e., $\widetilde{\theta}(y_0) = \theta(\Phi_{x_0}^{-1}(y_0))$. Moreover, the image of the magnetic potential by the rotation in the (z_1, z_2)-variables, still denoted $\mathbf{F}(z)$, satisfies

$$\text{curl}_z \mathbf{F}(z) = |\widetilde{\mathbf{B}}(y_0)| \text{curl}_z \mathbf{F}_{\theta_0}(z).$$

From this relation and the discussion in Section **??**, it follows that there exists a smooth function ϕ_0 such that

$$\mathbf{F}(z) = b_0 \mathbf{F}_{\theta_0}(z) + \nabla \phi_0, \quad b_0 := |\widetilde{\mathbf{B}}(y_0)| \tag{5.2.14}$$

From this and (**??**), we deduce the following lemma.

Lemma 5.2.1. *Let $\mathcal{Q}_h^{\rm lin}$ be as defined in (??) and $u \in L^2(\mathcal{V}_{x_0})$. Then, there exists a function ϕ_0 such that*

$$\mathcal{Q}_h^{\rm lin}(u) = \int_{\mathbb{R}^3_+} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})\, e^{i\phi_0/h}\breve{u}|^2\, dz, \tag{5.2.15}$$

where, for $\theta \in [0, \pi/2]$, $\mathbf{F}_\theta$ is the magnetic potential defined in (??), $b_0 := |\widetilde{\mathbf{B}}(y_0)|$ and, to a function u we associate $\breve{u}$ by means of (??) and (??).

5.3 Approximation of the quadratic form

Let $\ell, T > 0$ (ℓ, T will depend on h and tend to 0 as $h \to 0$). Consider the sets

$$Q_{0,\ell,T} = (-\ell/2, \ell/2)^2 \times (0, T), \qquad Q_{0,\ell} = (-\ell/2, \ell/2)^2 \times \{0\}, \tag{5.3.1}$$

such that $\Phi_{x_0}^{-1}\big((-\ell/2, \ell/2)^2 \times (0, T)\big) \subset \mathcal{V}_{x_0}$. Consider a function $u \in L^2(\mathcal{V}_{x_0})$ such that $\widetilde{u}$, defined in (??), satisfies

$$\operatorname{supp} \widetilde{u} \in Q_{0,\ell,T}. \tag{5.3.2}$$

We will approximate $Q_h(u)$ from (??) via the quadratic form in the half-space corresponding to a constant magnetic field.

Lemma 5.3.1. *Let $\mathbf{F}_\theta$ be the magnetic potential given in (??) and let $y_0 \in Q_{0,\ell}$. There exists a constant $C > 0$ (independent of y_0) and a function $\phi := \phi_{y_0} \in C^\infty(\widetilde{Q}_{0,\ell,T})$ such that, for all $\varepsilon \in (0, 1]$ satisfying $\varepsilon \geq (\ell + T)$ and for all u satisfying (??) one has*

$$\begin{aligned}\Big|\mathcal{Q}_h(u) - \int_{\widetilde{Q}_{0,\ell,T}} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz\Big| \\ \leq C\varepsilon \int_{\widetilde{Q}_{0,\ell,T}} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz + C(\ell^2 + T^2)^2\varepsilon^{-1}\int_{\widetilde{Q}_{0,\ell,T}} |\breve{u}|^2\, dz,\end{aligned} \tag{5.3.3}$$

and,

$$(1 - C(\ell + T))\int_{\widetilde{Q}_{0,\ell,T}} |\breve{u}|^2\, dz \leq \|u\|^2_{L^2(\mathcal{V}_{x_0})} \leq (1 + C(\ell + T))\int_{\widetilde{Q}_{0,\ell,T}} |\breve{u}|^2\, dz. \tag{5.3.4}$$

Here $b_0 = |\widetilde{\mathbf{B}}(y_0)|$, $\theta_0 = \widetilde{\theta}(y_0)$, and to a function $v(x)$ we associate the function $\breve{v}(z)$ by means of (??) and (??).

Proof. By (??), we have

$$\mathcal{Q}_h(u) = \int_{Q_{0,\ell,T}} \sum_{p,q=1}^{3} g^{pq}(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\, \widetilde{u}\, \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\widetilde{u}}\, |g|^{1/2} dy.$$

Using (??) and (??), it follows that for some constant $c_1 > 0$

$$\begin{aligned}(1 - c_1(\ell + T))\Big\{\int_{Q_{0,\ell,T}} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\, \widetilde{u}\, \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\, \widetilde{u}}\, |g(y_0)|^{1/2} dy\Big\} \\ \leq \mathcal{Q}_h(u) \leq (1 + c_1(\ell + T))\Big\{\int_{Q_{0,\ell,T}} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\, \widetilde{u}\, \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\, \widetilde{u}}\, |g(y_0)|^{1/2} dy\Big\}.\end{aligned} \tag{5.3.5}$$

Let $H_p(y) = \widetilde{\mathbf{A}}_p(y) - \widetilde{\mathbf{A}}_p^{\rm lin}(y)$, we get using (**??**) that,

$$\int_{\mathbb{R}^3_+} |H_p u \overline{H_q u}||g(y_0)|^{1/2} dy \leq C(\ell^2+T^2)^4 \int_{\mathbb{R}^3_+} |u|^2 |g(y_0)|^{1/2} dy. \tag{5.3.6}$$

Writing $\widetilde{\mathbf{A}}_p = H_p + \widetilde{\mathbf{A}}_p^{\rm lin}$, we have the following estimate of Cauchy-Schwarz type

$$\begin{aligned}
&\left| 2\Re \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p^{\rm lin})\, \widetilde{u}\, \overline{H_q \widetilde{u}} dy \right| \\
&\qquad \leq \varepsilon \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p^{\rm lin})\, \widetilde{u} \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q^{\rm lin})\, \widetilde{u}} dy \\
&\qquad\qquad + \varepsilon^{-1} \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0) H_p\, \widetilde{u}\, \overline{H_q\, \widetilde{u}} dy,
\end{aligned} \tag{5.3.7}$$

for any $\varepsilon > 0$.

Recall the quadratic form $\mathcal{Q}_h^{\rm lin}$ defined in (**??**). Using (**??**) and (**??**), it follows that there exists a constant $c_2 > 0$ such that

$$\begin{aligned}
&(1-\varepsilon)\mathcal{Q}_h^{\rm lin}(u) - c_2(\ell^2+T^2)^2\varepsilon^{-1} \int_{\mathbb{R}^3_+} |\widetilde{u}|^2\, |g(y_0)|^{1/2} dy \\
&\qquad \leq \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\, \widetilde{u}\, \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\, \widetilde{u}}\, |g(y_0)|^{1/2} dy \\
&\qquad\qquad \leq (1+\varepsilon)\mathcal{Q}_h^{\rm lin}(u) + c_2(\ell^2+T^2)^2\varepsilon^{-1} \int_{\mathbb{R}^3_+} |\widetilde{u}|^2\, |g(y_0)|^{1/2} dy,
\end{aligned} \tag{5.3.8}$$

for any $\varepsilon > 0$.

From Lemma **??**, it follows that

$$\begin{aligned}
&(1-\varepsilon)\int_{\mathbb{R}^3_+} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz - c_2(\ell^2+T^2)^2 \int_{\mathbb{R}^3_+} |\breve{u}|^2 dz \\
&\qquad \leq \int_{\mathbb{R}^3_+} \sum_{p,q=1}^{3} g^{pq}(y_0)(-ih\nabla_{y_p} + \widetilde{\mathbf{A}}_p)\, \widetilde{u}\, \overline{(-ih\nabla_{y_q} + \widetilde{\mathbf{A}}_q)\, \widetilde{u}}\, |g(y_0)|^{1/2} dy \\
&\qquad \leq (1+\varepsilon)\int_{\mathbb{R}^3_+} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz + c_2(\ell^2+T^2)^2\varepsilon^{-1} \int_{\mathbb{R}^3_+} |\breve{u}|^2\, dz.
\end{aligned} \tag{5.3.9}$$

for any $\varepsilon > 0$. Choose $\varepsilon \geq (\ell + T)$. Inserting (**??**) into (**??**), we obtain that for some constant $c_4 > 0$

$$\begin{aligned}
&(1-c_3\varepsilon)\int_{\mathbb{R}^3_+} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz - c_3(\ell^2+T^2)^2\varepsilon^{-1} \int_{\mathbb{R}^3_+} |\breve{u}|^2 dz \\
&\quad \leq \mathcal{Q}_h(u) \leq (1+c_3\varepsilon)\int_{\mathbb{R}^3_+} |(-ih\nabla_z + b_0\mathbf{F}_{\theta_0})e^{i\phi_0/h}\, \breve{u}|^2\, dz + c_3(\ell^2+T^2)^2\varepsilon^{-1} \int_{\mathbb{R}^3_+} |\breve{u}|^2\, dz.
\end{aligned} \tag{5.3.10}$$

Thus establishing (**??**).

To prove (**??**), we use (**??**) and (**??**) and we see that for some constant $c_4 > 0$, we have

$$(1 - c_4(\ell + T)) \int_{Q_{0,\ell,T}} |g(y_0)|^{1/2} |\widetilde{u}|^2 dy \;\leq\; \|u\|^2_{L^2(\mathcal{V}_{x_0})} \;\leq\; (1 + c_4(\ell + T)) \int_{Q_{0,\ell,T}} |g(y_0)|^{1/2} |\widetilde{u}|^2 dy. \tag{5.3.11}$$

Now, (**??**) yields (**??**). Choose $C = \max\{c_3, c_4\}$. $\square$

Chapter 6

Proof of Theorem ??

Our goal in this chapter is to establish the asymptotics of the sum of eigenvalues of the operator $\mathcal{P}_h$ stated in Theorem **??**. This will be done by establishing matching lower and and upper bounds. The variational principle for the sum of eigenvalues discussed earlier in Chapter 2 will play a key role.

Section **??** is devoted to obtain a lower bound. We shall see that the bulk does not contribute to the principal term and the analysis is restricted to the boundary. Locally near a point of the boundary, the quadratic form can be approximated by a quadratic form of the half-space operator with constant magnetic field.

Section **??** is devoted to the proof of a matching upper bound. Finally, in Section **??**, we prove Corollary **??** which provide an asymptotic formula for the number of eigenvalues of the operator $\mathcal{P}_h$.

6.1 Lower bound

6.1.1 Splitting into bulk and surface terms

Let

$$h^{1/2} \ll \varsigma \ll 1. \tag{6.1.1}$$

be a positive number to be chosen later (see (**??**) below) as a positive power of h. We consider smooth real-valued functions ψ_1 and ψ_2 satisfying

$$\psi_1^2(x) + \psi_2^2(x) = 1 \qquad \text{in} \qquad \Omega, \tag{6.1.2}$$

where

$$\psi_1(x) := \begin{cases} 1 & \text{if} \quad \operatorname{dist}(x, \partial\Omega) < \varsigma/2 \\ 0 & \text{if} \quad \operatorname{dist}(x, \partial\Omega) > \varsigma, \end{cases} \tag{6.1.3}$$

and such that there exists a constant $C_1 > 0$ so that

$$\sum_{k=1}^{2} |\nabla \psi_k|^2 \le C_1 \varsigma^{-2}. \tag{6.1.4}$$

Let $\{f_j\}_{j=1}^N$ be any L^2 orthonormal set in $\mathcal{D}(\mathcal{P}_h)$ and Q_h be the quadratic form introduced in (**??**). To prove a lower bound for $\sum_j (e_j(h) - \Lambda h)_-$, we use the variational principle in Lemma **??**. Namely, we seek a uniform lower bound (with respect to N) of

$$\sum_{j=1}^{N} \big(\mathcal{Q}_h(f_j) - \Lambda h \big).$$

The following Lemma shows that the bulk contribution is negligible compared to the expected leading order term.

Lemma 6.1.1. *Let $\Lambda \in [0,b)$ with b from (**??**). The following lower bound holds true*

$$\sum_{j=1}^{N}\big(\mathcal{Q}_h(f_j)-\Lambda h\big) \geq \sum_{j=1}^{N}\Big(\mathcal{Q}_h(\psi_1 f_j)-(\Lambda h + C_1 h^2 \varsigma^{-2})\,\|\psi_1 f_j\|^2_{L^2(\Omega)}\Big)\,, \tag{6.1.5}$$

*where $\{f_j\}_{j=1}^N$ is an L^2 orthonormal set in $\mathcal{D}(\mathcal{P}_h)$ and ψ_1 is the function from (**??**).*

Proof. By the IMS formula, we find

$$\mathcal{Q}_h(f_j)=\sum_{k=1}^{2}\Big(\mathcal{Q}_h(\psi_k f_j)-h^2\,\||\nabla\psi_k|f_j\|^2_{L^2(\Omega)}\Big)\,.$$

Using the fact that $\psi_1^2+\psi_2^2=1$ and the bound on $|\nabla\psi_k|$ in (**??**), it follows that

$$\sum_{j=1}^{N}\big(\mathcal{Q}_h(f_j)-\Lambda h\big) \geq \sum_{k=1}^{2}\sum_{j=1}^{N}\Big(\mathcal{Q}_h(\psi_k f_j)-(\Lambda h + C_1 h^2 \varsigma^{-2})\,\|\psi_k f_j\|^2_{L^2(\Omega)}\Big)\,. \tag{6.1.6}$$

Let us now examine the term corresponding to $k=2$ in the right hand side of (**??**). Using the inequality (**??**) for $u:=\psi_2 f_j$, we see that

$$\int_\Omega |(-ih\nabla+\mathbf{A})\psi_2 f_j|^2 dx \geq h(b-Ch^{1/4})\int_\Omega |\psi_2 f_j|^2 dx.$$

We write

$$h(b-Ch^{1/4})\int_\Omega |\psi_2 f_j|^2 dx = h\Lambda\int_\Omega |\psi_2 f_j|^2 dx + h(b-\Lambda-Ch^{1/4})\int_\Omega |\psi_2 f_j|^2 dx.$$

This yields, in view of (**??**),

$$\mathcal{Q}_h(\psi_2 f_j) \geq (\Lambda h + C_1 h^2\varsigma^{-2})\int_\Omega |\psi_2 f_j|^2 dx. \tag{6.1.7}$$

This gives that the bulk term in (**??**) is positive, and the lemma follows. □

6.1.2 Partition of unity of the boundary

Recall the cut-off function ψ_1 from (**??**), which is supported near a neighborhood of the boundary $\partial\Omega$. Let

$$\mathcal{O}_1 := \operatorname{supp}\,\psi_1 = \{x\in\Omega\ :\ \operatorname{dist}(x,\partial\Omega)\leq\varsigma\}, \tag{6.1.8}$$

where ς is, as introduced in (**??**).

Given a point x of the boundary, we let Φ_x^{-1} be the coordinate transformation valid near a small neighbourhood of x (these coordinates are introduced in Section **??**). To each $x\in\partial\Omega$, there exists $\delta_x>0$ such that

$$\Phi_x^{-1}:\widetilde{\Omega}_{\delta_x}\to\mathcal{O}_x,$$

where,

$$\widetilde{\Omega}_{\delta_x}:=(-\delta_x,\delta_x)^2\times(0,\delta_x),\quad \mathcal{O}_x=\Phi_x^{-1}(\widetilde{\Omega}_{\delta_x}).$$

Next, we consider the subset Ω_{δ_x} of $\widetilde{\Omega}_{\delta_x}$ to be

$$\Omega_{\delta_x} := \left(-\frac{\delta_x}{2}, \frac{\delta_x}{2}\right)^2 \times (0, \delta_x),$$

and a covering of $\mathcal{O}_1$ by open sets $\{\mathcal{O}_x\}_{x\in\partial\Omega}$. Using the compactness of the boundary, it follows that there exist an integer K and an index set $J = \{1, \cdots, K\}$, such that the sets $\{\mathcal{O}_{x_l}\}_{l\in J}$ form a finite covering of $\mathcal{O}_1$. For ease of notation, we write δ_l (respectively $\mathcal{O}_l, \Phi_l$) instead of δ_{x_l} (respectively $\mathcal{O}_{x_l}, \Phi_{x_l}$). We emphasize here that the δ_l's are fixed and independent of h. Thus, by choosing $\varsigma = \varsigma(h)$ sufficiently small (see (**??**) below), we may assume that

$$\varsigma \ll \delta_0 := \min_{l\in J} \delta_l. \tag{6.1.9}$$

Next, we choose $\{\chi_l\}_{l\in J}$ to be non-negative, smooth, compactly supported functions such that

$$\sum_{l\in J} \chi_l^2(x) \equiv 1 \quad \text{in} \quad \mathcal{O}_1, \qquad \operatorname{supp} \chi_l \subset \mathcal{O}_l, \tag{6.1.10}$$

and such that there exists a constant $C_2 > 0$ (independent of h) so that

$$\sum_{l\in J} |\nabla\chi_l(x)|^2 \le C_2, \tag{6.1.11}$$

for all $x \in \Omega$.

Consider the lattice $\{F_\varsigma^m\}_{m\in\mathbb{Z}^2}$ of $\mathbb{R}^2$ generated by the square:

$$F_\varsigma = \Big(-\frac{\varsigma}{2}, \frac{\varsigma}{2}\Big)^2.$$

If $m \in \mathbb{Z}^2$, denote by $(r_m, s_m) = \varsigma m \in \mathbb{R}^2$ the center of the square F_ς^m so that we can write

$$F_\varsigma^m = \left(-\frac{\varsigma}{2} + r_m, \frac{\varsigma}{2} + r_m\right) \times \left(-\frac{\varsigma}{2} + s_m, \frac{\varsigma}{2} + s_m\right).$$

We let $\mathcal{I}_l = \{m \in \mathbb{Z}^2 \ : \ F_\varsigma^m \cap (-\frac{\delta_l}{2}, \frac{\delta_l}{2})^2 \neq \emptyset\}$. If $m \in \mathcal{I}_l$ and $\eta > 0$, we will write

$$F_\eta^{m,l} = \left(-\frac{\eta}{2} + r_m, \frac{\eta}{2} + r_m\right) \times \left(-\frac{\eta}{2} + s_m, \frac{\eta}{2} + s_m\right), \qquad Q_\eta^{m,l} := F_\eta^{m,l} \times (0, \varsigma). \tag{6.1.12}$$

Let $a \ll 1$ to be chosen later as a positive power of h (see (**??**) below). We introduce a new partition of unity of the square $(-\frac{\delta_l}{2}, \frac{\delta_l}{2})^2$ by smooth functions $\{\widetilde{\varphi}_{m,l}\}_{m\in\mathcal{I}_l}$ with the following properties

$$\sum_{m\in\mathcal{I}_l} \widetilde{\varphi}_{m,l}^2 \equiv 1 \qquad \text{in} \quad \Big(-\frac{\delta_l}{2}, \frac{\delta_l}{2}\Big)^2, \quad \operatorname{supp} \widetilde{\varphi}_{m,l} \subset F_{(1+a)\varsigma}^{m,l}, \quad \widetilde{\varphi}_{m,l} = 1 \quad \text{in} \quad F_{(1-a)\varsigma}^{m,l}, \tag{6.1.13}$$

and such that there exists a constant $C_3 > 0$ so that

$$\sum_{m\in\mathcal{I}_l} |\nabla\widetilde{\varphi}_{m,l}|^2 \le C_3 (a\varsigma)^{-2}. \tag{6.1.14}$$

Construction of the partition of unity. Let $a > 0$. We consider a non-negative function $\chi_a \in C_0^\infty(\mathbb{R}^2)$ satisfying the following properties

$$0 \le \chi_a \le 1, \quad \text{supp}\ \chi_a \subset \Big(-\frac{1}{2}-a, \frac{1}{2}+a\Big)^2 \quad \chi_a \equiv 1 \text{ in } \Big(-\frac{1}{2}+a, \frac{1}{2}-a\Big)^2, \quad |\nabla \chi_a| \le C.$$

We can construct $\widetilde{\varphi}_{m,l}$ in the following way. For each $m \in \mathcal{I}_l$, we consider the function $\gamma_m(r,s,t) = \chi_a\Big(\frac{(r-r_m, s-s_m)}{\varsigma}\Big)$. We then set

$$\widetilde{\varphi}_{m,l} := \frac{\gamma_m}{\sqrt{\sum_{k\in\mathcal{I}_l}\gamma_k^2}}.$$

It is easy to check that the functions $\widetilde{\varphi}_{m,l}$ satisfy the properties in (**??**). $\square$

We set

$$\varphi_{m,l}(x) = \widetilde{\varphi}_{m,l}(\Phi_l(x)).$$

Let $y_{m,l}$ be an arbitrary point of $Q^{m,l}_{(1+a)\varsigma}$. As we did in Section **??**, we may assume, after performing a diagonalization, that $g_l(y_{m,l})$ (g_l is a short notation for g_{x_l}) is a diagonal matrix given by

$$g_l(y_{m,l}) = \begin{pmatrix} \lambda_{m,l,1} & 0 & \\ 0 & \lambda_{m,l,2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{6.1.15}$$

For $y = (y_1, y_2, y_3) \in \mathbb{R}^3_+$, we denote $y^\perp = (y_1, y_2) \in \mathbb{R}^2$. Applying (**??**) with $y_0 := y_{m,l} = (y^\perp_{m,l}, 0) \in F^{m,l}_{(1+a)\varsigma} \times \{0\}$, we immediately see that

$$\big||g_l|^{1/2}(y) - \lambda^{1/2}_{m,l,1}\lambda^{1/2}_{m,l,2}\big| \le c\varsigma\lambda^{1/2}_{m,l,1}\lambda^{1/2}_{m,l,2}. \tag{6.1.16}$$

Similarly, we can show that for some constant $c' > 0$

$$\big||g_l|^{-1/2}(y) - \lambda^{-1/2}_{m,l,1}\lambda^{-1/2}_{m,l,2}\big| \le c'\varsigma\lambda^{-1/2}_{m,l,1}\lambda^{-1/2}_{m,l,2}. \tag{6.1.17}$$

We also note that we can approximate the function $\widetilde{\chi}_l^2$ within the domain $Q^{m,l}_{(1+a)\varsigma}$ by $\widetilde{\chi}_l^2(y_{m,l})$. Indeed, by Taylor expansion, we obtain that for some positive constant $c_5 > 0$

$$\big|\widetilde{\chi}_l^2(y) - \widetilde{\chi}_l^2(y_{m,l})\big| \le c_5\varsigma. \tag{6.1.18}$$

Put $z = (z_1, z_2, z_3) = (\lambda^{1/2}_{m,l,1}y_1, \lambda^{1/2}_{m,l,2}y_2, y_3)$ and denote by

$$\widetilde{Q}^{m,l}_{(1+a)\varsigma} := \Big(-\frac{\varsigma_{m,l,1}}{2}, \frac{\varsigma_{m,l,1}}{2}\Big) \times \Big(-\frac{\varsigma_{m,l,2}}{2}, \frac{\varsigma_{m,l,2}}{2}\Big) \times (0,\varsigma), \quad \varsigma_{m,l,k} = \frac{\lambda^{1/2}_{m,l,k}(1+a)\varsigma}{2}, \quad k = 1,2. \tag{6.1.19}$$

In the following lemma, we apply localization formulas to restrict the analysis into small boxes where we can approximate the quadratic form using Lemma **??**.

Lemma 6.1.2. *Let $\Lambda \in [0,b)$ with b from (**??**), $\mathbf{F}_\theta$ the magnetic potential given in (**??**) and $y_{m,l} \in F^{m,l}_{(1+a)\varsigma} \times \{0\}$. There exist a function $\phi_{m,l} := \phi_{y_{m,l}} \in C^\infty(\widetilde{Q}^{m,l}_{(1+a)\varsigma})$ and a constant $\widetilde{C} > 0$*

such that for all $\varepsilon \in (0,1]$ satisfying $\varepsilon \gg \varsigma$ one has

$$\sum_{j=1}^{N} \big(\mathcal{Q}_h(\psi_1 f_j) - \Lambda h\big)$$
$$\geq (1-\widetilde{C}\varepsilon)\sum_{j=1}^{N}\sum_{l\in J}\sum_{m\in\mathcal{I}_l}\Big\{\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})\, e^{i\phi_{m,l}/h}\breve{\varphi}_{m,l}\breve{\psi}_1\breve{\chi}_l\breve{f}_j|^2 dz$$
$$- \Lambda_1(h,a,\varsigma,\varepsilon)\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |\breve{\varphi}_{m,l}\breve{\psi}_1\breve{\chi}_l\breve{f}_j|^2\, dz\Big\}, \quad (6.1.20)$$

where

$$\Lambda_1(h,a,\varsigma,\varepsilon) = \frac{(\Lambda h + \widetilde{C}h^2(a\varsigma)^{-2})(1+\widetilde{C}\varsigma) + \widetilde{C}\varsigma^4\varepsilon^{-1}}{1-\widetilde{C}\varepsilon}, \quad (6.1.21)$$

$b_{m,l} = |\widetilde{\mathbf{B}}(y_{m,l})|$, $\theta_{m,l} = \widetilde{\theta}(y_{m,l})$ and to a function $v(x)$, we associate the function $\breve{v}(z)$ by means of (**??**).

Proof. According to Lemma **??**, the lemma follows if we can prove a lower bound on the right-hand side of (**??**). We start by estimating $\mathcal{Q}_h(\psi_1 f_j)$. Using the IMS decomposition formula, it follows that

$$\mathcal{Q}_h(\psi_1 f_j) = \sum_{l\in J}\Big(\mathcal{Q}_h(\chi_l\psi_1 f_j) - h^2\, \||\nabla\chi_l|\psi_1 f_j\|^2_{L^2(\Omega)}\Big)\,. \quad (6.1.22)$$

Using (**??**), and implementing (**??**), we get

$$\mathcal{Q}_h(\psi_1 f_j) - (\Lambda h + C_1 h^2\varsigma^{-2})\,\|\psi_1 f_j\|^2_{L^2(\Omega)}$$
$$\geq \sum_{l\in J}\Big(\mathcal{Q}_h(\psi_1\chi_l f_j) - \big(\Lambda h + (C_1+C_2)h^2\varsigma^{-2}\big)\,\|\psi_1\chi_l f_j\|^2_{L^2(\Omega)}\Big)\,, \quad (6.1.23)$$

where we used that $\varsigma^{-2} \gg 1$.

Applying the IMS formula once again, we find, using that $a \ll 1$,

$$\mathcal{Q}_h(\psi_1\chi_l f_j) = \sum_{m\in\mathcal{I}_l}\Big\{\mathcal{Q}_h(\varphi_{m,l}\psi_1\chi_l f_j) - h^2\,\||\nabla\varphi_{m,l}|\psi_1\chi_l f_j\|^2_{L^2(\Omega)}\Big\}$$
$$\geq \sum_{m\in\mathcal{I}_l}\Big\{\mathcal{Q}_h(\varphi_{m,l}\psi_1\chi_l f_j) - (C_1+C_2+C_3')h^2(a\varsigma)^{-2}\,\|\varphi_{m,l}\psi_1\chi_l f_j\|^2_{L^2(\Omega)}\Big\}. \quad (6.1.24)$$

The last inequality follows from (**??**) and $C_3' := C_3\sup_{l\in J}\|D\Phi_l\|^2$. Inserting this into (**??**), it follows that

$$\mathcal{Q}_h(\psi_1 f_j) - (\Lambda h + C_1 h^2\varsigma^{-2})\,\|\psi_1 f_j\|^2_{L^2(\Omega)}$$
$$\geq \sum_{l\in J}\sum_{m\in\mathcal{I}_l}\Big(\mathcal{Q}_h(\varphi_{m,l}\psi_1\chi_l f_j) - \big(\Lambda h + (C_1+C_2+C_3')h^2(a\varsigma)^{-2}\big)\,\|\varphi_{m,l}\psi_1\chi_l f_j\|^2_{L^2(\Omega)}\Big)\,, \quad (6.1.25)$$

Applying Lemma **??** with y_0 replaced by $y_{m,l}$, $u = \varphi_{m,l}\psi_1\chi_l f_j$, $\ell = (1+a)\varsigma$, $T = \varsigma$, we then deduce that there exists a function $\phi_{m,l} := \phi_{y_{m,l}} \in C^\infty(\widetilde{Q}^{m,l}_{(1+a)\varsigma})$ such that, for all $\varepsilon \in (0,1]$

satisfying $\varepsilon \gg \varsigma$, one has

$$
\begin{aligned}
&\mathcal{Q}_h(\psi_1 f_j) - (\Lambda h + C_1 h^2 \varsigma^{-2}) \|\psi_1 f_j\|^2_{L^2(\Omega)} \\
&\qquad \geq (1 - C\varepsilon) \sum_{l\in J} \sum_{m\in\mathcal{I}_l} \int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})\, e^{i\phi_{m,l}/h} \breve{\varphi}_{m,l}\breve{\psi}_1\breve{\chi}_l\breve{f}_j|^2 dz \\
&- \big((\Lambda h + (C_1 + C_2 + C_3')h^2(a\varsigma)^{-2})(1 + 3C\varsigma) + 25C\varsigma^4\varepsilon^{-1}\big) \sum_{l\in J} \sum_{m\in\mathcal{I}_l} \int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |\breve{\varphi}_{m,l}\breve{\psi}_1\breve{\chi}_l\breve{f}_j|^2\, dz,
\end{aligned}
\tag{6.1.26}
$$

where C is the constant from Lemma **??**. Put $\widetilde{C} = \max\{C_1 + C_2 + C_3', 25C\}$. Inserting (**??**) into (**??**) yields the desired estimate of the lemma. ☐

6.1.3 Leading order term

For $h, \mathfrak{b} > 0$ and $\theta \in [0, \pi/2]$, we recall the operator $\mathcal{P}^N_{\theta,h,\mathfrak{b}}$ from (**??**). Let us rewrite (**??**) as

$$
\sum_{j=1}^{N} (\mathcal{Q}_h(f_j) - \Lambda h) \geq I_1 + I_2,
\tag{6.1.27}
$$

where

$$
\begin{aligned}
&I_1 = (1 - \widetilde{C}\varepsilon)\times \\
&\quad \sum_{j=1}^{N} \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}\in(0,\pi/2]}} \big\langle e^{i\phi_{m,l}/h}\breve{\varphi}_{m,l}\breve{\chi}_l\breve{\psi}_1\breve{f}_j, \big(\mathcal{P}^N_{\theta_{m,l},h,b_{m,l}} - \Lambda_1(h,a,\varsigma,\varepsilon)\big) e^{i\phi_{m,l}/h}\breve{\varphi}_{m,l}\breve{\chi}_l\breve{\psi}_1\breve{f}_j\big\rangle,
\end{aligned}
\tag{6.1.28}
$$

and

$$
\begin{aligned}
&I_2 = (1 - \widetilde{C}\varepsilon)\times \\
&\quad \sum_{j=1}^{N} \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} \big\langle e^{i\phi_{m,l}/h}\breve{\varphi}_{m,l}\breve{\chi}_l\breve{\psi}_1\breve{f}_j, \big(\mathcal{P}^N_{\theta_{m,l},h,b_{m,l}} - \Lambda_1(h,a,\varsigma,\varepsilon)\big) e^{i\phi_{m,l}/h}\breve{\varphi}_{m,l}\breve{\chi}_l\breve{\psi}_1\breve{f}_j\big\rangle.
\end{aligned}
\tag{6.1.29}
$$

Below in (**??**), the parameters a, ς and ε are chosen so that, when h is sufficiently small, one has

$$
h^{-1}\Lambda_1(h,a,\varsigma,\varepsilon) < b,
\tag{6.1.30}
$$

where b is defined in (**??**).

We begin by estimating I_1. Using Lemma **??**, we see that

$$
\begin{aligned}
I_1 \geq -h(1 - \widetilde{C}\varepsilon) \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}\in[0,\pi/2)}} b_{m,l} \sum_{k} \big(\zeta_k(\theta_{m,l}) - h^{-1}b^{-1}_{m,l}\Lambda_1(h,a,\varsigma,\varepsilon)\big)_- \times \\
\sum_{j=1}^{N} \Big\langle e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j, \Pi_{\theta_{m,l},k}(h,b_{m,l}) e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j\Big\rangle_{L^2(\widetilde{Q}^{m,l}_{(1+a)\varsigma})}.
\end{aligned}
\tag{6.1.31}
$$

Here, for $\theta \in (0, \pi/2]$ and $\mathfrak{b} > 0$, $\{\zeta_k(\theta)\}_k$ are the eigenvalues from (??) and $\Pi_{\theta,k}(h, \mathfrak{b})$ is the projector defined in (??). Using (??) and that $dz = \lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}dy$, we obtain that for some constant $C_4 > 0$

$$\sum_{j=1}^{N}\left\langle e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j, \Pi_{\theta_{m,l},k}(h, b_{m,l})e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j\right\rangle_{L^2(\widetilde{Q}^{m,l}_{(1+a)\varsigma})}$$
$$\leq (1 + C_4\varsigma)\sum_{j=1}^{N}\langle f_j, H(m, l, k, h, b_{m,l}, \theta_{m,l})f_j\rangle_{L^2(\Omega)}. \quad (6.1.32)$$

Here $H(m, l, k, h, b_{m,l}, \theta_{m,l})$ is the positive operator given by,

$$H(m, l, k, h, b_{m,l}, \theta_{m,l}) := \psi_1\chi_l\varphi_{m,l}U_{\Phi_l}V_{z\to y}e^{i\phi_{m,l}}\Pi_{\theta_{m,l},k}(h, b_{m,l})e^{i\phi_{m,l}}V_{z\to y}^{-1}U_{\Phi_l}^{-1}\psi_1\chi_l\varphi_{m,l},$$

where, for a function v, $V_{z\to y}$ is defined by

$$(V_{z\to y}v)(y) = v(\lambda_{m,l,1}^{1/2}y_1, \lambda_{m,l,2}^{1/2}y_2, y_3), \quad (6.1.33)$$

and, for a function u, the transformation U_{Φ_l} is given by

$$(U_{\Phi_l}u)(x) = u(\Phi_l(x)). \quad (6.1.34)$$

Since $\{f_j\}_{j=1}^N$ is an orthonormal family in $L^2(\Omega)$, we deduce that

$$\sum_{j=1}^{N}\langle f_j, H(m, l, k, h, b_{m,l}, \theta_{m,l})f_j\rangle_{L^2(\Omega)} \leq \mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l})). \quad (6.1.35)$$

Combining (??), (??) and (??), and using that $\varepsilon \gg \varsigma$ (see (??) below), we obtain that for some constant $C_5 > 0$

$$I_1 \geq -(1 - C_5\varepsilon)h\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}} b_{m,l}\sum_k\big(\zeta_k(\theta_{m,l}) - h^{-1}b_{m,l}^{-1}\Lambda_1(h, a, \varsigma, \varepsilon)\big)_-\times$$
$$\mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l})). \quad (6.1.36)$$

It is straightforward to show that

$$\mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l}))$$
$$= b_{m,l}^{3/2}h^{-3/2}\int_{\mathbb{R}}\int_{\mathbb{R}^3_+}|g_l(y)|^{1/2}\widetilde{\psi}_1^2(y)\widetilde{\chi}_l^2(y)\widetilde{\varphi}_{m,l}^2(y_1, y_2, 0)|V_{z\to y}\big(v_{\theta_{m,l},k}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)|^2dyd\xi, \quad (6.1.37)$$

where, for $\theta \in [0, \pi/2]$, $v_{\theta,k}(\cdot, \xi)$ is the function defined in (??). Using (??) and (??), and that $|\psi_1(x)| \leq 1$ for all $x \in \Omega$, it follows that

$$\mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l})) \leq (2\pi)^{-1}(1 + c\varsigma)(\widetilde{\chi}_l^2(y_{m,l}) + c_5\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}h^{-3/2}b_{m,l}^{3/2}\times$$
$$\int_{\mathbb{R}}\int_{\mathbb{R}^3_+}\widetilde{\varphi}_{m,l}^2(y_1, y_2, 0)|u_{\theta_{m,l},k}(h^{-1/2}b_{m,l}^{1/2}\lambda_{m,l,2}^{1/2}y_2 - \frac{\xi}{\sin(\theta_{m,l})}, h^{-1/2}b_{m,l}^{1/2}y_3)|^2dyd\xi, \quad (6.1.38)$$

where, for $\theta \in [0, \pi/2]$, the functions $\{u_{\theta,k}\}_k$ are introduced in (**??**). Performing the translation $\nu = h^{-1/2} b_{m,l}^{1/2} \lambda_{m,l,2}^{1/2} y_2 - \frac{\xi}{\sin(\theta_{m,l})}$ and using that the function $u_{\theta_{m,l},k}$ is normalized, we find

$$\begin{aligned}
&\int_{\mathbb{R}} \int_{\mathbb{R}^3_+} \widetilde{\varphi}^2_{m,l}(y_1, y_2, 0) |u_{\theta_{m,l},k}(h^{-1/2} b_{m,l}^{1/2} \lambda_{m,l,2}^{1/2} y_2 - \frac{\xi}{\sin(\theta_{m,l})}, h^{-1/2} b_{m,l}^{1/2} y_3)|^2 dy d\xi \\
&= \sin(\theta_{m,l}) \int_{\mathbb{R}^2} \widetilde{\varphi}^2_{m,l}(y_1, y_2, 0) dy_1 dy_2 \int_{\mathbb{R}^2_+} |u_{\theta_{m,l},k}(\nu, h^{-1/2} b_{m,l}^{1/2} y_3)|^2 dy_3 d\nu \qquad (6.1.39) \\
&= h^{-1/2} b_{m,l}^{1/2} \sin(\theta_{m,l}) \int_{\mathbb{R}^2} |\widetilde{\varphi}_{m,l}|^2 dy_1 dy_2.
\end{aligned}$$

Inserting this into (**??**), we deduce that

$$\begin{aligned}
&\mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l})) \\
&\quad \leq (2\pi)^{-1} h^{-1} b_{m,l} \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} (\chi_l^2(y_{m,l}) + c_5 \varsigma)(1 + c\varsigma) \sin(\theta_{m,l}) \int_{\mathbb{R}^2} |\widetilde{\varphi}_{m,l}|^2 dy_1 dy_2. \qquad (6.1.40)
\end{aligned}$$

Using that the function $\widetilde{\varphi}_{m,l}$ is less than one and supported in the square $F^{m,l}_{(1+a)\varsigma}$ (the set defined in (**??**)), we see that

$$\begin{aligned}
&\mathrm{Tr}(H(m, l, k, h, b_{m,l}, \theta_{m,l})) \\
&\qquad \leq (2\pi)^{-1} h^{-1} b_{m,l} \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} \big(\chi_l^2(y_{m,l}) + c_5 \varsigma\big)(1 + c\varsigma) \sin(\theta_{m,l})(1 + a)^2 \varsigma^2. \qquad (6.1.41)
\end{aligned}$$

Substituting (**??**) into (**??**), we obtain that for some positive constant $C_6 > 0$

$$\begin{aligned}
I_1 \geq -(1 - C_6 \varepsilon)(1 + a)^2 &\sum_{l \in J} \sum_{\substack{m \in \mathcal{I}_l \\ \theta_{m,l} \in (0, \pi/2]}} \sum_k \big(\zeta_k(\theta_{m,l}) - h^{-1} b_{m,l}^{-1} \Lambda_1(h, a, \varsigma, \varepsilon)\big)_- \times \\
&\qquad b_{m,l}^2 \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} (\chi_l^2(y_{m,l}) + c_5 \varsigma) \varsigma^2. \qquad (6.1.42)
\end{aligned}$$

Recalling (**??**), this reads

$$\begin{aligned}
&I_1 \geq -(1 - C_6 \varepsilon)(1 + a)^2 \times \\
&\quad \sum_{l \in J} \sum_{\substack{m \in \mathcal{I}_l \\ \theta_{m,l} \in (0, \pi/2]}} E\Big(\theta_{m,l}, h^{-1} b_{m,l}^{-1} \Lambda_1(h, a, \varsigma, \varepsilon)\Big) b_{m,l}^2 \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} \big(\chi_l^2(y_{m,l}) + c_5 \varsigma\big) \varsigma^2. \qquad (6.1.43)
\end{aligned}$$

We now proceed in a similar manner to get a lower bound of I_2. By virtue of Lemma **??**, it follows that

$$\begin{aligned}
I_2 \geq -h(2\pi)^{-1}(1 - \widetilde{C}\varepsilon) &\sum_{l \in J} \sum_{\substack{m \in \mathcal{I}_l \\ \theta_{m,l} = 0}} b_{m,l} \int_{\mathbb{R}^2} \sum_k \big(\mu_k(\xi) + \tau^2 - h^{-1} b_{m,l}^{-1} \Lambda_1(h, a, \varsigma, \varepsilon)\big)_- \times \\
&\sum_{j=1}^N \Big\langle e^{i\phi_{m,l}/h} \breve{\psi}_1 \breve{\chi}_l \breve{\varphi}_{m,l} \breve{f}_j, \Pi_k(h, b_{m,l}; \xi, \tau) e^{i\phi_{m,l}/h} \breve{\psi}_1 \breve{\chi}_l \breve{\varphi}_{m,l} \breve{f}_j \Big\rangle_{L^2(\widetilde{Q}^{m,l}_{(1+a)\varsigma})} d\xi d\tau, \qquad (6.1.44)
\end{aligned}$$

where, for $(\xi,\tau)\in\mathbb{R}^2$ and $\mathfrak{b}>0$, $\{\mu_k(\xi)\}_k$ are the eigenvalues from (**??**) and $\Pi_1(\xi,\tau;h,\mathfrak{b})$ is the projector defined in (**??**). Using Lemma **??**, it follows that

$$I_2 \geq -h(2\pi)^{-1}(1-\widetilde{C}\varepsilon)\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}} b_{m,l}\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\big)_-\times$$
$$\sum_{j=1}^{N}\Big\langle e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j,\Pi_1(h,b_{m,l};\xi,\tau)e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j\Big\rangle_{L^2(\widetilde{Q}^{m,l}_{(1+a)\varsigma})}d\xi d\tau. \quad (6.1.45)$$

Using (**??**) and that $dz=\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}dy$, we obtain

$$\sum_{j=1}^{N}\Big\langle e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j,\Pi_1(h,b_{m,l};\xi,\tau)e^{i\phi_{m,l}/h}\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l}\breve{f}_j\Big\rangle_{L^2(\widetilde{Q}^{m,l}_{(1+a)\varsigma})}$$
$$\leq(1+C_4\varsigma)\sum_{j=1}^{N}\langle f_j,H'(m,l,k,h,b_{m,l};\xi,\tau)f_j\rangle_{L^2(\Omega)}. \quad (6.1.46)$$

Here $H'(m,l,k,h,b_{m,l};\xi,\tau)$ is the positive operator given by,

$$H'(m,l,h,b_{m,l};\xi,\tau):=\psi_1\chi_l\varphi_{m,l}U_{\Phi_l}V_{z\to y}e^{-i\phi_{m,l}}\Pi_1(\xi,\tau;h,b_{m,l})e^{i\phi_{m,l}}V_{z\to y}^{-1}U_{\Phi_l}^{-1}\psi_1\chi_l\varphi_{m,l}$$

where U_{Φ_l} and $V_{z\to y}$ are the same as defined in (**??**) and (**??**) respectively. Since $\{f_j\}_{j=1}^N$ is an orthonormal family in $L^2(\Omega)$, we deduce that

$$\sum_{j=1}^{N}\langle f_j,H'(m,l,k,h,b_{m,l};\xi,\tau)f_j\rangle_{L^2(\Omega)}\leq\mathrm{Tr}\big(H'(m,l,k,h,b_{m,l};\xi,\tau)\big). \quad (6.1.47)$$

Inserting (**??**) and (**??**) into (**??**) yields

$$I_2\geq -h(1-C_5\varepsilon)(2\pi)^{-1}\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}} b_{m,l}\times$$
$$\int_{\mathbb{R}^2}\big(\mu_1(\xi)+\tau^2-h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\big)_-\mathrm{Tr}(H'(m,l,h,b_{m,l};\xi,\tau))d\xi d\tau. \quad (6.1.48)$$

It is easy to see that

$$\mathrm{Tr}(H'(m,l,h,b_{m,l};\xi,\tau))$$
$$=b_{m,l}^{3/2}h^{-3/2}\int_{\mathbb{R}^3_+}|g_l(y)|^{1/2}\widetilde{\psi}_1^2(y)\widetilde{\chi}_l^2(y)\widetilde{\varphi}_{m,l}^2(y_1,y_2,0)|V_{z\to y}(v_1(h^{-1/2}b_{m,l}^{1/2}z;\xi,\tau))|^2dy, \quad (6.1.49)$$

where the function v_1 is defined in (**??**). Using (**??**), (**??**), and that $|\psi_1(x)|\leq 1$ for all $x\in\Omega$, it follows that

$$\mathrm{Tr}(H'(m,l,h,b_{m,l};\xi,\tau))\leq(2\pi)^{-1}(1+c\varsigma)(\widetilde{\chi}^2(y_{m,l})+c_5\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}h^{-3/2}b_{m,l}^{3/2}\times$$
$$\int_{\mathbb{R}^3_+}\widetilde{\varphi}_{m,l}^2(y_1,y_2,0)|u_1(h^{-1/2}b_{m,l}^{1/2}y_3,\xi)|^2dy, \quad (6.1.50)$$

Using that the function $u_1(\cdot;\xi)$ (from (**??**)) is normalized in $L^2(\mathbb{R}_+)$, we get

$$\operatorname{Tr}(H'(m,l,h,b_{m,l};\xi,\tau)) \leq (2\pi)^{-1}h^{-1}b_{m,l}\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}(\chi_l^2(y_{m,l})+c_5\varsigma)(1+c\varsigma)(1+a)^2\varsigma^2. \quad (6.1.51)$$

Inserting (**??**) in (**??**) yields

$$I_2 \geq -h(1-C_6\varepsilon)(4\pi^2)^{-1}\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}} b_{m,l}^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}(\widetilde{\chi}_l^2(y_{m,l})+C\varsigma)(1+a)^2\varsigma^2\times$$
$$\int_{\mathbb{R}^2}\Big(\mu_1(\xi)+\tau^2-h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\Big)_-d\xi d\tau. \quad (6.1.52)$$

Using (**??**), it follows that

$$I_2 \geq -(1-C_6\varepsilon)(1+a)^2\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}} E\Big(0,\Lambda_1(h,a,\varsigma,\varepsilon)\Big)b_{m,l}^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}\big(\chi_l^2(y_{m,l})+c_5\varsigma\big)\varsigma^2. \quad (6.1.53)$$

Inserting (**??**) and (**??**) into (**??**), we obtain

$$\sum_{j=1}^{N}\big(\mathcal{Q}_h(f_j)-\Lambda h\big) \geq -(1-C_6\varepsilon)(1+a)^2\times$$
$$\sum_{l\in J}\sum_{m\in\mathcal{I}_l} b_{m,l}^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}\big(\chi_l^2(y_{m,l})+c_5\varsigma\big)E\Big(\theta_{m,l},h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\Big)\varsigma^2. \quad (6.1.54)$$

Using the fact that for all $\lambda_0\in(0,1)$ the function $(0,\lambda_0]\times[0,\pi/2]\mapsto E(\theta,\lambda)$ is bounded by Lemma **??**, we see that the term

$$C\varsigma(1+a)^2\sum_{l\in J}\sum_{m\in\mathcal{I}_l} b_{m,l}^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}E\Big(\theta_{m,l},h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\Big)\varsigma^2$$

is bounded by $C\varsigma\sum_{l\in J}\sum_{m\in\mathcal{I}_l}\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}\varsigma^2\sim C\varsigma|\partial\Omega|$. This leads to

$$\sum_{j=1}^{N}\big(\mathcal{Q}_h(f_j)-\Lambda h\big) \geq -(1-C_6\varepsilon)(1+a)^2\times$$
$$\sum_{l\in J}\sum_{m\in\mathcal{I}_l}\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}\widetilde{\chi}_l^2(y_{m,l})b_{m,l}^2E\Big(\theta_{m,l},h^{-1}b_{m,l}^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\Big)\varsigma^2+O(\varsigma). \quad (6.1.55)$$

By (**??**), we have $\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}=|g_l(y_{m,l})|^{1/2}$. Recall that $b_{m,l}=|\widetilde{\mathbf{B}}(y_{m,l})|$ and $\theta_{m,l}=\widetilde{\theta}(y_{m,l})$. For $y=(y^\perp,0)\in F_\varsigma^{m,l}\times\{0\}$, we define the function

$$G(y):=|g_l(y)|^{1/2}\widetilde{\chi}_l^2(y)|\widetilde{\mathbf{B}}(y)|^2E\Big(\widetilde{\theta}(y),h^{-1}|\widetilde{\mathbf{B}}(y)|^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\Big). \quad (6.1.56)$$

We pick $y_{m,l}\in F_\varsigma^{m,l}\times\{0\}$ so that

$$\min_{y\in F_\varsigma^{m,l}\times\{0\}} G(y)=G(y_{m,l}).$$

Then the right-hand side of (**??**) is a lower Riemann sum. Hence, we find

$$\sum_{m\in\mathcal{I}_l} |g_l(y_{m,l})|^{1/2}\widetilde{\chi}_l^2(y_{m,l})b_{m,l}^2 E\big(\theta_{m,l}, h^{-1}b_{m,l}\Lambda_1(h,a,\varsigma,\varepsilon,\eta)\big)\varsigma^2 = \sum_{m\in\mathcal{I}_l} G(y_{m,l})\varsigma^2 \leq$$
$$\int_{(-\delta_l,\delta_l)^2} G(y_1,y_2,0)dy_1dy_2 = \int_{\partial\Omega} \chi_l^2(x)|\mathbf{B}(x)|^2 E\big(\theta(x), h^{-1}|\mathbf{B}(x)|^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\big)d\sigma(x). \tag{6.1.57}$$

Plugging this into (**??**), and using that $\sum_{l\in J}\chi_l^2(x) = 1$, we obtain

$$\sum_{j=1}^N \big(\mathcal{Q}_h(f_j) - \Lambda h\big)$$
$$\geq -(1-C_6\varepsilon)(1+a)^2 \int_{\partial\Omega} |\mathbf{B}(x)|^2 E\big(\theta(x), h^{-1}|\mathbf{B}(x)|^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)\big)d\sigma(x) + O(\varsigma). \tag{6.1.58}$$

We make the following choice of ε, a and ς,

$$\varepsilon = h^{1/4}, \qquad a = h^{1/16} \qquad \varsigma = h^{3/8}. \tag{6.1.59}$$

This choice yields that for some constant $C_7 > 0$, one has

$$h^{-1}\Lambda_1(h,a,\varsigma,\varepsilon,\eta) \sim \frac{\Lambda + C_7 h^{1/8}}{1-\widetilde{C}h^{1/4}} \qquad \text{as} \quad h\to 0.$$

The function $[0,1)\times[0,\pi/2] \mapsto E(\theta,\lambda)$ is Lipschitz according to Lemma **??**. This gives

$$\Big|E\big(\theta(x), h^{-1}\Lambda_1(h,a,\varsigma,\varepsilon)|\mathbf{B}(x)|^{-1}\big) - E(\theta(x),\Lambda|\mathbf{B}(x)|^{-1})\Big| \leq C_8 h^{1/8}b^{-1}, \tag{6.1.60}$$

for some constant $C_8 > 0$ and b is the same as in (**??**). It follows that for some constant $C_9 > 0$, we have

$$\sum_{j=1}^N \big(\mathcal{Q}_h(f_j) - \Lambda h\big) \geq -(1+C_9h^{1/8}) \int_{\partial\Omega} |\mathbf{B}(x)|^2 E\Big(\theta(x), \Lambda|\mathbf{B}(x)|^{-1}\big)\Big)dx + O(h^{1/8}), \tag{6.1.61}$$

uniformly with respect to N and the orthonormal family $\{f_j\}_j$. Finally, Lemma **??** yields the desired lower bound.

6.2 Upper bound

Let $\varsigma > 0$ be as in (**??**) and $F_\varsigma^{m,l}$ be the set defined in (**??**) with $l \in J$ and $m \in \mathcal{I}_l$ being the indices corresponding to the partitions $\{\chi_l\}_{l\in J}$ and $\{\widetilde{\varphi}_{m,l}\}_{m\in\mathcal{I}_l}$ introduced in (**??**) and (**??**) respectively. Let $\{y_{m,l}\}$ be a finite family of points in $F_\varsigma^{m,l}\times\{0\}$ to be specified later at the end of this section. To each point $y_{m,l}$ we associate $b_{m,l} = |\widetilde{\mathbf{B}}(y_{m,l})|$ and $\theta_{m,l} = \widetilde{\theta}(y_{m,l})$ defined in (**??**) and (**??**) respectively (with y_0 replaced by $y_{m,l}$). Let $y \in Q_{(1+a)\varsigma}^{m,l}$ (see the definition of the set in (**??**)) and $\lambda_{m,l,1}, \lambda_{m,l,2}$ be the diagonal components of the matrix $g_l(y_{m,l})$ from (**??**). We put $z = (\lambda_{m,l,1}^{1/2}y_1, \lambda_{m,l,2}^{1/2}y_2, y_3)$. Let $(\xi,\tau)\in\mathbb{R}^2$. Recall the notation from (**??**) and define the functions

$$\widetilde{f}_{j,l,m}(y,\xi;h) := h^{-3/4}b_{m,l}^{3/4}v_{j,\theta_{m,l}}\big(h^{-1/2}b_{m,l}^{1/2}z;\xi\big)\big(\widetilde{\varphi}_{m,l}\widetilde{\chi}_l\widetilde{\psi}_1\big)(y) \qquad \text{if} \quad \theta_{m,l}\in(0,\pi/2]$$
$$\widetilde{g}_{l,m}(y;\xi,\tau,h) := (2\pi)^{-1/2}h^{-3/4}b_{m,l}^{3/4}v_1\big(h^{-1/2}b_{m,l}^{1/2}z;\xi,\tau\big)\big(\widetilde{\varphi}_{m,l}\widetilde{\chi}_l\widetilde{\psi}_1\big)(y) \qquad \text{if} \quad \theta_{m,l} = 0.$$

where $v_{j,\theta}(\cdot;\xi)$, $v_1(\cdot;\xi,\tau)$ and $\widetilde{\psi}_1$ are the functions in (**??**), (**??**) and (**??**) respectively.

Recall the coordinate transformation Φ_l valid near a neighborhood of the point x_l (see Subsection **??**). Let $x = \Phi_l^{-1}(y)$. We define $f_{j,l,m}(x,\xi;h) := \widetilde{f}_{j,l,m}(y,\xi;h)$ and $g_{l,m}(x,\xi,\tau;h) := \widetilde{g}_{l,m}(y,\xi,\tau;h)$. With $\Lambda \in [0,b)$, we put

$$M_{j,m,l} = \mathbf{1}_{\left\{(j,m,l)\in\mathbb{N}\times I_l\times J\,:\,\zeta_j(\theta_{m,l})-b_{m,l}^{-1}\Lambda\leq 0\right\}}$$

and

$$M'_{m,l,\xi,\tau} = \mathbf{1}_{\left\{(j,m,l,\xi,\tau)\in\mathbb{N}\times I_l\times J\times\mathbb{R}^2\,:\quad \mu_1(\xi)+\tau^2-b_{m,l}^{-1}\Lambda\leq 0\right\}}.$$

Note that $b_{m,l}^{-1}\Lambda \leq b^{-1}\Lambda < 1$. Hence the condition $\mu_1(\xi)+\tau^2-b_{m,l}^{-1}\Lambda \leq 0$ implies, in view of Proposition **??** , that there exists a constant $K>0$ (independent of m,l) such that

$$(\xi,\tau)\in I_{\xi,\tau} := (0,K)\times(-1,1). \tag{6.2.1}$$

Define, for $f\in L^2(\Omega)$,

$$(\gamma_1 f)(x) = \sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j M_{j,m,l}\int_{\mathbb{R}}\big\langle f, f_{j,l,m}(\cdot,\xi;h)\big\rangle f_{j,l,m}(x,\xi;h)d\xi,$$

and

$$(\gamma_2 f)(x) = \sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}}\int_{\mathbb{R}^2} M'_{m,l,\xi,\tau}\big\langle f, g_{l,m}(\cdot,\xi,\tau;h)\big\rangle g_{l,m}(x,\xi,\tau;h)d\xi d\tau.$$

We have the following lemma.

Lemma 6.2.1. *Let $f\in L^2(\Omega)$ and define the operator γ by*

$$\gamma f = \gamma_1 f + \gamma_2 f.$$

There exists a constant $C_{10}>0$ such that the quadratic form associated to γ satisfies

$$0\leq \langle \gamma f, f\rangle_{L^2(\Omega)} \leq (1+C_{10}\varsigma)\,\|f\|^2_{L^2(\Omega)}\,. \tag{6.2.2}$$

Proof. Consider $f\in L^2(\Omega)$. It is easy to see that $\langle\gamma f,f\rangle\geq 0$. Next, using that $M_{j,m,l}\leq 1$, we see that

$$\big\langle f,\gamma_1 f\big\rangle_{L^2(\Omega)} \leq \sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j\int_{\mathbb{R}}\Big|\big\langle f, f_{j,l,m}(x,\xi;h)\big\rangle_{L^2(\Omega)}\Big|^2 d\xi. \tag{6.2.3}$$

By (**??**), we have

$$\Big|\big\langle f, f_{j,l,m}(x,\xi;h)\big\rangle_{L^2(\Omega)}\Big|^2 = \Big|\int_{\mathbb{R}^3_+}\widetilde{f}\ \overline{\widetilde{f}_{j,l,m}(y,\xi;h)}|g_l|^{1/2}\,dy\Big|^2. \tag{6.2.4}$$

Approximating $|g_l|^{1/2}$ using (**??**), it follows that there exists a constant $C_{11}>0$ such that

$$\begin{aligned}\Big|\big\langle f, f_{j,l,m}(x,\xi;h)\big\rangle_{L^2(\Omega)}\Big|^2 &\leq (1+C_{11}\varsigma)\lambda_{m,l,1}\lambda_{m,l,2}\Big|\int_{\mathbb{R}^3_+}\widetilde{f}\ \overline{\widetilde{\chi}_l\widetilde{\psi}_1\widetilde{\varphi}_{m,l}\big(U_{h,b_{m,l}}v_{j,\theta_{m,l}}(z;\xi)\big)}dy\Big|^2\\ &= (1+C_{11}\varsigma)\Big|\int_{\mathbb{R}^3_+}\breve{f}\ \overline{\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}\big(U_{h,b_{m,l}}v_{j,\theta_{m,l}}(z;\xi)\big)}dz\Big|^2.\end{aligned} \tag{6.2.5}$$

Here, the transformation $U_{h,b_{m,l}}$ is defined in (**??**) and for a function u, $\breve{u}$ is associated to u using (**??**) and (**??**).

Substituting (**??**) into (**??**), we find

$$\big\langle f, \gamma_1 f\big\rangle_{L^2(\Omega)} \le (1+C_{11}\varsigma)\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j\Big|\int_{\mathbb{R}^3_+}\breve{f}\,\overline{\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}U_{h,b_{m,l}}v_{j,\theta_{m,l}}(z;\xi)\big)}dz\Big|^2 d\xi. \quad (6.2.6)$$

In a similar fashion, one can show that

$$\big\langle f, \gamma_2 f\big\rangle_{L^2(\Omega)} \le (1+C_{11}\varsigma)\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}}\sum_j\int_{\mathbb{R}}\Big|\int_{\mathbb{R}^3_+}\breve{f}\,\overline{\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}(2\pi)^{-1/2}(U_{h,b_{m,l}}v_j(z;\xi,\tau)\big)}dz\Big|^2 d\xi d\tau.$$

Next, we recall the definition of $v_{j,\theta}(\cdot;\xi)$ from (**??**) (resp. v_j from (**??**)) and use the fact that $\{v_{j,\theta_{m,l}}\}_j$ (resp. $u_j(\cdot,\xi)$ for all $\xi\in\mathbb{R}$) is an orthonormal set of eigenfunctions, we thus find

$$\big\langle f, \gamma f\big\rangle_{L^2(\Omega)} \le (1+C_{11}\varsigma)\sum_{l\in J}\sum_{m\in\mathcal{I}_l}\int_{\mathbb{R}^3_+}\big|\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}\breve{f}(z)\big|^2 dz. \quad (6.2.7)$$

By the change of variables $z=(\lambda_{m,l,1}^{1/2}y_1,\lambda_{m,l,2}^{1/2}y_2,y_3)$ and implementing $1=|g_l(y)|^{1/2}|g_l(y)|^{-1/2}$, we see that

$$\int_{\mathbb{R}^3_+}\big|\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}\breve{f}(z)\big|^2 dz = \lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}\int_{\mathbb{R}^3_+}|g_l|^{-1/2}(y)|g_l|^{1/2}(y)\big|\widetilde{\chi}_l\widetilde{\psi}_1\widetilde{\varphi}_{m,l}\widetilde{f}(y)\big|^2 dy.$$

We approximate $|g_l|^{-1/2}(y)$ using (**??**), we obtain that for some constant $C_{12}>0$

$$\begin{aligned}\int_{\mathbb{R}^3_+}\big|\breve{\chi}_l\breve{\psi}_1\breve{\varphi}_{m,l}\breve{f}(z)\big|^2 dz &\le (1+C_{12}\varsigma)\int_{\mathbb{R}^3_+}|g_l|^{1/2}\big|\widetilde{\chi}_l\widetilde{\psi}_1\widetilde{\varphi}_{m,l}\widetilde{f}(y)\big|^2 dy\\ &= (1+C_{12}\varsigma)\int_{\Omega}\big|\chi_l\varphi_{m,l}\psi_1 f(x)\big|^2 dx.\end{aligned} \quad (6.2.8)$$

Here we have used (**??**) in the last step.

Implementing (**??**) into (**??**), and using (**??**) and (**??**), we get the claim of the lemma. □

By the variational principle in Lemma **??**, an upper bound of the sum of eigenvalues of $\mathcal{P}_h$ below Λh follows if we can prove an upper bound on

$$(1+C_{12}\varsigma)^{-1}\mathrm{Tr}\big[(\mathcal{P}_h-\Lambda h)\gamma\big] = (1+C_{12}\varsigma)^{-1}\Big(\mathrm{Tr}\big[(\mathcal{P}_h-\Lambda h)\gamma_1\big]+\mathrm{Tr}\big[(\mathcal{P}_h-\Lambda h)\gamma_2\big]\Big)$$

We start by estimating

$$\mathrm{Tr}\big[(\mathcal{P}_h-\Lambda h)\gamma_1\big] := \sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j M_{j,m,l}\int_{\mathbb{R}}\big(\mathcal{Q}_h(f_{j,l,m}(x,\xi;h)) - \Lambda h\,\|f_{j,l,m}(x,\xi;h)\|^2\big)d\xi. \quad (6.2.9)$$

Here we recall the quadratic form $\mathcal{Q}_h$ defined in (**??**).

By (**??**), we have

$$\int_{\Omega}|f_{j,l,m}(x,\xi;h)|^2 dx = \int_{\mathbb{R}^3_+}|g_l|^{1/2}(y)|\widetilde{f}_{j,l,m}(y,\xi;h)|^2 dy \quad (6.2.10)$$

Recall the transformation $V_{z\to y}$ introduced in (??). It follows from (??) and (??) that there exists a constant $C_{13} > 0$ such that

$$\begin{aligned}&\int_\Omega |f_{j,l,m}(x,\xi;h)|^2 dx \\ &\qquad \geq (\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^{3/2}h^{-3/2}\int_{\mathbb{R}^3_+}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)\widetilde{\varphi}_{m,l}\widetilde{\psi}_1(y)|^2dy,\end{aligned} \tag{6.2.11}$$

Let us write the last integral as

$$\begin{aligned}\int_{Q^{m,l}_{(1+a)\varsigma}}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)\widetilde{\varphi}_{m,l}\widetilde{\psi}_1|^2dy &= \int_{Q^{m,l}_{(1+a)\varsigma}}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)|^2dy \\ &+\int_{Q^{m,l}_{(1+a)\varsigma}}\big[-1+\widetilde{\varphi}_{m,l}^2\widetilde{\psi}_1^2\big]|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)|^2dy.\end{aligned} \tag{6.2.12}$$

As we shall work on the support of $M_{j,m,l}$ in view of (??), we may restrict ourselves to the indices (j,m,l) satisfying $\zeta_j(\theta_{m,l}) \leq \Lambda b_{m,l}^{-1} < \Lambda b^{-1}$. Using Lemma ??, it follows that for all $\alpha \in \sqrt{1-\Lambda b^{-1}}$, there exists a constant $C_{14} > 0$ such that

$$\begin{aligned}&\int_{Q^{m,l}_{(1+a)\varsigma}}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)\big(\widetilde{\varphi}_{m,l}\widetilde{\psi}_1\big)(y)|^2dz \\ &\qquad\qquad \geq (1-e^{-C_{14}\alpha\varsigma h^{-1/2}})\int_{Q^{m,l}_{(1+a)\varsigma}}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)|^2dy,\end{aligned} \tag{6.2.13}$$

where we have used (??) and (??).

Implementing (??) in (??), we obtain

$$\begin{aligned}&\int_\Omega |f_{j,l,m}(x,\xi;h)|^2dx \\ &\qquad\geq (1-e^{-C_{14}\alpha\varsigma h^{-1/2}})(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^{3/2}h^{-3/2}\times \\ &\qquad\qquad \int_{Q^{m,l}_{(1+a)\varsigma}}|V_{z\to y}\big(v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)|^2dy.\end{aligned} \tag{6.2.14}$$

As in (??), we find

$$\int_{\mathbb{R}}\int_{Q^{m,l}_{(1+a)\varsigma}}|v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)|^2dyd\xi = (2\pi)^{-1}(1+a)^2\varsigma^2\sin(\theta_{m,l}). \tag{6.2.15}$$

Substituting this in (??), we deduce that

$$\begin{aligned}&\int_{\mathbb{R}}\int_\Omega |f_{j,l,m}(x,\xi;h)|^2dxd\xi \\ &\geq (1-e^{-C_{14}\alpha\varsigma h^{-1/2}})(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)(1+a)^2\varsigma^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}h^{-1}b_{m,l}(2\pi)^{-1}\sin(\theta_{m,l}).\end{aligned} \tag{6.2.16}$$

Let us estimate $\mathcal{Q}_h(f_{j,l,m})$. Applying Lemma **??** with $u = f_{j,l,m}$, we find, for all $\varepsilon \gg \varsigma$,

$$
\begin{aligned}
&\mathcal{Q}_h(f_{j,l,m}) \\
&\quad \leq (1+C\varepsilon)\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} \big|(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})e^{i\phi_{m,l}/h}\,\breve{f}_{j,l,m}\big|^2\,dz + C\varsigma^4\varepsilon^{-1}\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |\breve{f}_{j,l,m}|^2\,dz \\
&\quad \leq (1+C\varepsilon)h^{-3/2}b_{m,l}^{3/2}\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} (\breve{\varphi}_{m,l}\breve{\psi}_1\breve{\chi}_l)^2\big|(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big|^2\,dz \\
&\quad + h^{-3/2}b_{m,l}^{3/2}\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}}\Big(|\nabla(\breve{\psi}_1\breve{\chi}_l\breve{\varphi}_{m,l})|^2 + C\varsigma^4\varepsilon^{-1}\breve{\varphi}_{m,l}^2\breve{\psi}_1^2\breve{\chi}_l^2\Big)\big|v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big|^2dz, \quad (6.2.17)
\end{aligned}
$$

where C is the constant from Lemma **??** and the set $\widetilde{Q}^{m,l}_{(1+a)\varsigma}$ is defined in (**??**).

By (**??**), (**??**), (**??**), and approximating $\widetilde{\chi}_l^2$ using (**??**), it follows that for some constant $C_{15} > 0$,

$$
\begin{aligned}
&\mathcal{Q}_h(f_{j,l,m}) \\
&\quad \leq h^{-3/2}b_{m,l}^{3/2}(\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon)\int_{Q^{m,l}_{(1+a)\varsigma}} |(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})\,v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)|^2\,dz \\
&\qquad\qquad + C_{15}h^{-3/2}b_{m,l}^{3/2}(\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2})\int_{\widetilde{Q}^{m,l}_{(1+a)\varsigma}} |v_{j,\theta_{m,l}}(h^{-1/2}b_{m,l}^{1/2}z;\xi)|^2\,dz. \quad (6.2.18)
\end{aligned}
$$

Performing the integration over $\xi \in \mathbb{R}$, we get

$$
\begin{aligned}
\int_{\mathbb{R}} \mathcal{Q}_h(f_{j,l,m})d\xi \leq \lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^2(2\pi)^{-1}(1+a)^2\varsigma^2\sin(\theta_{m,l})\times& \\
\big\{(\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon)\zeta_j(\theta_{m,l}) + C_{15}h^{-1}b_{m,l}^{-1}(\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2})\big\}.& \quad (6.2.19)
\end{aligned}
$$

This combined with (**??**) yields, in view of (**??**),

$$
\begin{aligned}
&\mathrm{Tr}\big[(\mathcal{P}_h - \Lambda h)\gamma_1\big] \\
&\quad \leq \sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j M_{j,m,l}\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^2\varsigma^2(2\pi)^{-1}\sin(\theta_{m,l})(1+a)^2\times \\
&\qquad \Big\{(\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon)\zeta_j(\theta_{m,l}) + C_{15}h^{-1}b_{m,l}^{-1}(\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2}) \\
&\qquad\qquad - \Lambda b_{m,l}^{-1}(1 - e^{-C_{14}\alpha\varsigma h^{-1/2}})(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\Big\} \\
&= -(1+a)^2\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}} \widetilde{\chi}_l^2(y_{m,l})\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^2\varsigma^2\Big\{\sum_j(2\pi)^{-1}\sin(\theta_{m,l})\big(\zeta_j(\theta_{m,l}) - \Lambda b_{m,l}^{-1}\big)_-\Big\} \\
&\qquad + I^{(1)}_{\mathrm{rest}},
\end{aligned}
$$

where

$$
\begin{aligned}
&I^{(1)}_{\mathrm{rest}} = (1+a)^2\sum_{l\in J}\sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}}\sum_j M_{j,m,l}\varsigma^2\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2}b_{m,l}^2(2\pi)^{-1}\sin(\theta_{m,l})\times \\
&\Big\{C_{15}\big(\varepsilon\zeta_j(\theta_{m,l}) + h^{-1}b_{m,l}^{-1}(\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2}\big) + \Lambda b_{m,l}^{-1}\big(e^{-C_{14}\alpha\varsigma h^{-1/2}}(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma) + C_{13}\varsigma\big)\Big\}. \quad (6.2.20)
\end{aligned}
$$

By virtue of Lemma **??**, (**??**) reads

$$\mathrm{Tr}\big[(\mathcal{P}_h - \Lambda h)\gamma_1\big] \le -(1+a)^2 \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}\in(0,\pi/2]}} \widetilde{\chi}_l^2(y_{m,l})\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2} b_{m,l}^2 \varsigma^2 E(\theta_{m,l}, \Lambda b_{m,l}^{-1}) + I_{\mathrm{rest}}^{(1)}. \tag{6.2.21}$$

It remains to estimate

$$\mathrm{Tr}\big[(\mathcal{P}_h - \Lambda h)\gamma_2\big] := \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l\\ \theta_{m,l}=0}} M'_{m,l,\xi,\tau} \int_{\mathbb{R}} \big(\mathcal{Q}_h(g_{l,m}(x,\xi,\tau;h)) - \Lambda h\, \|g_{l,m}(x,\xi,\tau;h)\|^2\big) d\xi. \tag{6.2.22}$$

We start by estimating $\|g_{l,m}(x,\xi,\tau;h)\|^2$. It follows from (**??**) (**??**) and (**??**) that there exists a constant $C_{13} > 0$ such that

$$\begin{aligned}
&\int_\Omega |g_{l,m}(x,\xi,\tau;h)|^2 dx \\
&\quad \ge (2\pi)^{-1}(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2} b_{m,l}^{3/2} h^{-3/2} \int_{\mathbb{R}^3_+} |V_{z\to y}\big(v_1(h^{-1/2}b_{m,l}^{1/2}z;\xi)\big)\widetilde{\varphi}_{m,l}\widetilde{\psi}_1(y)|^2 dy \\
&\quad = (2\pi)^{-2}(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2} b_{m,l}^{3/2} h^{-3/2} \int_{\mathbb{R}^3_+} |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)\widetilde{\varphi}_{m,l}\widetilde{\psi}_1(y)|^2 dy,
\end{aligned} \tag{6.2.23}$$

where the function $u_1(\cdot,\xi)$ is introduced in (**??**). Let us write the last integral as

$$\begin{aligned}
\int_{Q^{m,l}_{(1+a)\varsigma}} |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)\widetilde{\varphi}_{m,l}\widetilde{\psi}_1|^2 dy &= \int_{Q^{m,l}_{(1+a)\varsigma}} |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)|^2 dy \\
&\quad + \int_{Q^{m,l}_{(1+a)\varsigma}} \big[-1 + \widetilde{\varphi}_{m,l}^2\widetilde{\psi}_1^2\big] |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)|^2 dy.
\end{aligned} \tag{6.2.24}$$

Due to the support of $\widetilde{\psi}_1$, we note that the integral on the right hand side is restricted to the set where $y_3 \ge \varsigma/2$. Recalling (**??**) and selecting ς as in (**??**), one has for h sufficiently small,

$$(b^{1/2}h^{-1/2}\varsigma - \xi)^2 \ge (b^{1/2}h^{-1/2}\frac{\varsigma}{2} - \xi)^2 \gg \frac{1}{16} b h^{-1}\varsigma^2 \gg 1. \tag{6.2.25}$$

Using this and Lemma **??**, we obtain for some constant $C_{16} > 0$

$$\begin{aligned}
&\int_{Q^{m,l}_{(1+a)\varsigma}} |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)\big(\widetilde{\varphi}_{m,l}\widetilde{\psi}_1\big)(y)|^2 dy \\
&\qquad \ge (1 - e^{-C_{16}\varsigma^2 h^{-1}}) \int_{Q^{m,l}_{(1+a)\varsigma}} |u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)|^2 dy,
\end{aligned} \tag{6.2.26}$$

where we have used (**??**) and (**??**).

Implementing (**??**) in (**??**), we obtain

$$\begin{aligned}
&\int_\Omega |g_{l,m}(x,\xi,\tau;h)|^2 dx \\
&\ge (2\pi)^{-2}(1 - e^{-C_{16}\varsigma^2 h^{-1}})(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma)\lambda_{m,l,1}^{1/2}\lambda_{m,l,2}^{1/2} b_{m,l}^{3/2} h^{-3/2} \int_{Q^{m,l}_{(1+a)\varsigma}} \Big|u_1(h^{-1/2}b_{m,l}^{1/2}y_3;\xi)\Big|^2 dy.
\end{aligned} \tag{6.2.27}$$

Using the same arguments that have led to (**??**), one can show that

$$
\begin{aligned}
\mathcal{Q}_h(g_{l,m}) &\le h^{-3/2} b_{m,l}^{3/2} (2\pi)^{-1} \big(\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon\big) \int_{Q^{m,l}_{(1+a)\varsigma}} |(-ih\nabla_z + b_{m,l}\mathbf{F}_{\theta_{m,l}})\, v_1(h^{-1/2} b_{m,l}^{1/2} z;\xi)|^2\, dz \\
&\quad + C_{15} h^{-3/2} b_{m,l}^{3/2} (2\pi)^{-1} \big(\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2}\big) \int_{Q^{m,l}_{(1+a)\varsigma}} |v_1(h^{-1/2} b_{m,l}^{1/2} z;\xi)|^2\, dz \\
&\le \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 (1+a)^2 \varsigma^2 (2\pi)^{-2} \times \\
&\qquad \Big\{ (\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon)(\mu_1(\xi) + \tau^2) + C_{15} h^{-1} b_{m,l}^{-1} (\varsigma^4\varepsilon^{-1} + h^2(a\varsigma)^{-2}) \Big\}.
\end{aligned} \tag{6.2.28}
$$

Integrating in ξ and τ and taking into account (**??**), it follows that (recall (**??**))

$$
\begin{aligned}
\operatorname{Tr}\big[(\mathcal{P}_h - \Lambda h)\gamma_2\big] &\le \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} M_{1,m,l,\xi,\tau} \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 (2\pi)^{-2} \varsigma^2 (1+a)^2 \times \\
&\quad \int_{\mathbb{R}^2} \Big((\widetilde{\chi}_l^2(y_{m,l}) + C_{15}\varepsilon)(\mu_1(\xi) + \tau^2) + C_{15} h^{-1} b_{m,l}^{-1} (\varsigma^4\varepsilon^{-1} + h^2 a^{-2}\varsigma^{-2}) \\
&\qquad - \Lambda b_{m,l}^{-1} (1 - e^{-C_{16}\varsigma^2 h^{-1}})(\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma) \Big) d\xi d\tau \\
&= -(1+a)^2 \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} \widetilde{\chi}_l^2(y_{m,l}) \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 \varsigma^2 (2\pi)^{-2} \int_{\mathbb{R}^2} \big(\mu_1(\xi) + \tau^2 - \Lambda b_{m,l}^{-1}\big)_- d\xi d\tau \\
&\qquad + I^{(2)}_{\mathrm{rest}},
\end{aligned} \tag{6.2.29}
$$

where

$$
\begin{aligned}
I^{(2)}_{\mathrm{rest}} &= \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} M'_{m,l,\xi,\tau} \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 (2\pi)^{-2} \varsigma^2 (1+a)^2 \int_{\mathbb{R}^2} \Big(C_{15}\varepsilon(\mu_1(\xi) + \tau^2) \\
&\quad + C_{15} h^{-1} b_{m,l}^{-1} (\varsigma^4\varepsilon^{-1} + h^2 a^{-2}\varsigma^{-2}) - \Lambda b_{m,l}^{-1} \big(e^{-C_{16}\varsigma^2 h^{-1}} (\widetilde{\chi}_l^2(y_{m,l}) - C_{13}\varsigma) + C_{13}\varsigma \big) \Big) d\xi d\tau.
\end{aligned} \tag{6.2.30}
$$

In view of Lemma **??**, the estimate (**??**) reads

$$
\operatorname{Tr}\big[(\mathcal{P}_h - \Lambda h)\gamma_2\big] \le -(1+a)^2 \sum_{l\in J} \sum_{\substack{m\in\mathcal{I}_l \\ \theta_{m,l}=0}} \widetilde{\chi}_l^2(y_{m,l}) \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 \varsigma^2 (2\pi)^{-2} E(0, \Lambda b_{m,l}^{-1}) + I^{(2)}_{\mathrm{rest}}. \tag{6.2.31}
$$

Combining (**??**) and (**??**), and recalling (**??**), we obtain

$$
\begin{aligned}
&\operatorname{Tr}\Big[(\mathcal{P}_h - \Lambda h)\frac{\gamma}{1 + C_{10}\varsigma}\Big] \\
&\quad \le -(1 + C_{10}\varsigma)^{-1} \Big\{ (1+a)^2 \sum_{l\in J} \sum_{m\in\mathcal{I}_l} \widetilde{\chi}_l^2(y_{m,l}) \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} b_{m,l}^2 E(\theta_{m,l}, \Lambda b_{m,l}^{-1}) + I^{(1)}_{\mathrm{rest}} + I^{(2)}_{\mathrm{rest}} \Big\}.
\end{aligned} \tag{6.2.32}
$$

By (**??**), we have $\lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} = |g_l(y_{m,l})|^{1/2}$. For $y = (y_1, y_2, 0) \in F_\varsigma^{m,l} \times \{0\}$, we define the function

$$
v(y) := |g_l(y)|^{1/2} \widetilde{\chi}_l^2(y) |\widetilde{\mathbf{B}}(y)|^2 E\big(\widetilde{\theta}(y), |\widetilde{\mathbf{B}}(y)|^{-1}\Lambda\big) \tag{6.2.33}
$$

We choose the points $y_{m,l} \in F_\varsigma^{m,l} \times \{0\}$ so that

$$\max_{y \in F_\varsigma^{m,l} \times \{0\}} v(y) = v(y_{m,l}).$$

Then the right-hand side of (**??**) is an upper Riemann sum. We thus get

$$\sum_{m \in \mathcal{I}_l} |g_l(y_{m,l})|^{1/2} \widetilde{\chi}_l^2(y_{m,l}) b_{m,l}^2 E\big(\theta_{m,l}, b_{m,l}^{-1}\Lambda\big)\varsigma^2 = \sum_{m \in \mathcal{I}_l} v(y_{m,l})\varsigma^2 \geq$$

$$\int_{(-\delta_l,\delta_l)^2} v(y_1, y_2, 0) dy_1 dy_2 = \int_{\partial\Omega} \chi_l^2(x) |\mathbf{B}(x)|^2 E\big(\theta(x), |\mathbf{B}(x)|^{-1}\Lambda\big) d\sigma(x). \quad (6.2.34)$$

Using the upper bound estimate in Lemma **??**, together with the fact that $|B|$ is bounded on $\partial\Omega$ and that $\sum_{l \in J} \sum_{m \in \mathcal{I}_l} \varsigma^2 \lambda_{m,l,1}^{1/2} \lambda_{m,l,2}^{1/2} \sim |\partial\Omega|$, we find

$$|I_{\rm rest}^{(1)}| + |I_{\rm rest}^{(2)}| = \mathcal{O}(\varepsilon + h^{-1}\varsigma^4\varepsilon^{-1} + h(a\varsigma)^{-2}). \quad (6.2.35)$$

The choice in (**??**) yields

$$|I_{\rm rest}^{(1)}| + |I_{\rm rest}^{(2)}| = \mathcal{O}(h^{1/8}).$$

Inserting this and (**??**) into (**??**), and using (**??**), we obtain

$$\begin{aligned}
&\mathrm{Tr}\Big[(\mathcal{P}_h - \Lambda h)\frac{\gamma}{1 + C_{10}\varsigma}\Big] \\
&\qquad \leq -(1 + C_{10}h^{3/8})^{-1}(1 + h^{1/8})^2 \int_{\partial\Omega} |\mathbf{B}(x)|^2 E\big(\theta(x), \Lambda|\mathbf{B}(x)|^{-1}\big) d\sigma(x) + \mathcal{O}(h^{1/8}).
\end{aligned}$$

The upper bound then follows from Lemmas **??** and **??**.

6.3 Proof of Corollary ??

Let us start by computing the left and right derivatives of the function $(0,1) \ni \lambda \to E(\theta, \lambda)$, since we shall need these quantities later in the proof. Using the formula of $E(\theta, \lambda)$ given in Theorem **??**, we find

$$\frac{\partial E}{\partial \lambda_+}(\theta, \lambda) = \begin{cases} \dfrac{1}{2\pi^2} \displaystyle\int_0^\infty (\mu_1(\xi) - \lambda)_-^{1/2} d\xi & \text{if} \quad \theta = 0, \\ \dfrac{\sin(\theta)}{2\pi} \mathrm{card}\{j \,:\, \zeta_j(\theta) \leq \lambda\} & \text{if} \quad \theta \in (0, \pi/2], \end{cases} \quad (6.3.1)$$

and

$$\frac{\partial E}{\partial \lambda_-}(\theta, \lambda) = \begin{cases} \dfrac{1}{2\pi^2} \displaystyle\int_0^\infty (\mu_1(\xi) - \lambda)_-^{1/2} d\xi & \text{if} \quad \theta = 0, \\ \dfrac{\sin(\theta)}{2\pi} \mathrm{card}\{j \,:\, \zeta_j(\theta) < \lambda\} & \text{if} \quad \theta \in (0, \pi/2]. \end{cases} \quad (6.3.2)$$

Let $\varepsilon > 0$. Using Corollary **??** and recall the notation from (**??**), we deduce that

$$\mathrm{Tr}\,(\mathcal{P}_h - (\Lambda + \varepsilon)h)_- - \mathrm{Tr}\,(\mathcal{P}_h - \Lambda h)_- \geq \varepsilon h \mathcal{N}(\Lambda h; \mathcal{P}_h, \Omega). \quad (6.3.3)$$

On the other hand, by the formula in (**??**), we have

$$\begin{aligned}
&\mathrm{Tr}\,(\mathcal{P}_h - (\Lambda + \varepsilon)h)_- - \mathrm{Tr}\,(\mathcal{P}_h - \Lambda h)_- \\
&\quad = \int_{\partial\Omega} |\mathbf{B}(x)|^2 \Big(E(\theta(x), (\Lambda + \varepsilon)|\mathbf{B}(x)|^{-1}) - E(\theta(x), \Lambda|\mathbf{B}(x)|^{-1})\Big) d\sigma(x) + o(1), \quad \text{as } h \to 0.
\end{aligned}$$

Implementing this into (**??**), then taking $\limsup_{h\to 0_+}$, we see that

$$\limsup_{h\to 0_+} h\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega) \le \int_{\partial\Omega} |\mathbf{B}(x)| \frac{E(\theta(x),(\Lambda+\varepsilon)|\mathbf{B}(x)|^{-1}) - E(\theta(x),\Lambda|\mathbf{B}(x)|^{-1})}{\varepsilon|\mathbf{B}(x)|^{-1}} d\sigma(x).$$

We recall here that $|\mathbf{B}(x)| > 0$ for all $x \in \partial\Omega$. Taking the limit $\varepsilon \to 0_+$, we deduce using (**??**), and Lebesgue's dominated convergence Theorem, that

$$\limsup_{h\to 0_+} h\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega) \le \int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_+}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x). \tag{6.3.4}$$

Replacing ε by $-\varepsilon$ in (**??**) and following the same arguments that led to (**??**), we find

$$\liminf_{h\to 0_+} h\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega) \ge \int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_-}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x). \tag{6.3.5}$$

It follows by the assumption (**??**) that

$$\int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_+}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x) = \int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_-}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x). \tag{6.3.6}$$

Combining (**??**) and (**??**) we obtain

$$\lim_{h\to 0_+} h\mathcal{N}(\Lambda h;\mathcal{P}_h,\Omega) = \int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_+}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x). \tag{6.3.7}$$

Denote $n(\theta,\lambda) := \dfrac{\partial E}{\partial \lambda_+}(\theta,\lambda)$. We have thus proven the statement of the corollary.

Remark 6.3.1. Notice that if Λ does not satisfy the condition in (**??**), the proof of Corollary **??** still gives us,

$$\begin{aligned}\int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_-}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big)\, d\sigma(x) &\le \liminf_{h\to 0_+} \mathcal{N}(\Lambda h,\mathcal{P}_h,\Omega) \\ &\le \limsup_{h\to 0_+} \mathcal{N}(\Lambda h,\mathcal{P}_h,\Omega) \le \int_{\partial\Omega} |\mathbf{B}(x)| \frac{\partial E}{\partial \lambda_+}\Big(\theta(x),\Lambda|\mathbf{B}(x)|^{-1}\Big) d\sigma(x). \end{aligned} \tag{6.3.8}$$

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