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Discrete spectrum of a model Schrödinger operator on the half-plane with Neumann conditions

Virginie BONNAILLIE-NOËL*, Monique DAUGE, Nicolas POPOFF, Nicolas RAYMOND

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Abstract

We study the eigenpairs of a model Schrödinger operator with a quadratic potential and Neumann boundary conditions on a half-plane. The potential is degenerate in the sense that it reaches its minimum all along a line which makes the angle θ with the boundary of the half-plane. We show that the first eigenfunctions satisfy localization properties related to the distance to the minimum line of the potential. We investigate the densification of the eigenvalues below the essential spectrum in the limit $\theta \to 0$ and we prove a two term asymptotics for these eigenvalues and their associated eigenvectors. We conclude the paper by numerical experiments obtained by a finite element method. The numerical results confirm and enlighten the theoretical approach.

1 Introduction and main results

The aim of this paper is to study the eigenpairs of a Schrödinger operator with a degenerate electric potential of the form $(t\cos\theta-s\sin\theta)^2$ on the half-plane t>0. This problem is motivated by the asymptotics of the lowest eigenvalues of Schrödinger operators with magnetic fields $(ih\nabla+\mathbf{A})^2$ and Neumann boundary conditions on smooth domains Ω in \mathbb{R}^3 . Indeed, near the boundary of Ω , the magnetic field can be approximated by a constant field which makes an angle $\theta\in\left[0,\frac{\pi}{2}\right]$ with the boundary (approximated by the tangent plane). Thus, after a choice of gauge, we are led to investigate the operator with Neumann conditions on the half-space $\mathbb{R}^3_+=\{(r,s,t)\in\mathbb{R}^3:t>0\}$:

$$h^2 D_s^2 + h^2 D_t^2 + (h D_r + t \cos \theta - s \sin \theta)^2$$
,

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where D_x denotes $-i\partial_x$ for any variable x. The first step in the study of this operator is a Fourier transform in r. If $\theta=0$, we are led to the so-called de Gennes operator on an half-line (see [7]). If $\theta\neq 0$, after a translation in s we are reduced to a Schrödinger operator with an electric potential on the half-plane $\mathbb{R}^2_+=\{(s,t)\in\mathbb{R}^2:t>0\}$:

$$h^2 D_s^2 + h^2 D_t^2 + (t\cos\theta - s\sin\theta)^2.$$

After a rescaling, we can reduce to the case h = 1.

Thus, this is a natural question to wonder how the eigenpairs of this operator behave when θ goes to 0 (the form domain does not depend continuously on θ).

In this paper, we investigate this question and study the exponential concentration of eigenvectors.

1.1 Discrete and essential spectrum of model operators

We denote by x=(s,t) the coordinates in \mathbb{R}^2 and by Ω the half-plane:

$$\Omega = \mathbb{R}^2_+ = \{ x = (s, t) \in \mathbb{R}^2, \ t > 0 \}.$$

We study the self-adjoint Neumann realization on the half-plane Ω of the Schrödinger operator \mathcal{L}_{θ} with potential V_{θ} :

$$\mathcal{L}_{\theta} = -\Delta + V_{\theta} = D_s^2 + D_t^2 + V_{\theta},$$

where V_{θ} is defined for any $\theta \in (0, \frac{\pi}{2})$ by

$$V_{\theta} \colon x = (s, t) \in \Omega \longmapsto (t \cos \theta - s \sin \theta)^2.$$

We can notice that V_{θ} reaches its minimum 0 all along the line $t \cos \theta = s \sin \theta$, which makes the angle θ with $\partial \Omega$. We denote by $D_N(\mathcal{L}_{\theta})$ the domain of \mathcal{L}_{θ} and we consider the associated quadratic form q_{θ} defined by:

$$q_{\theta}(u) = \int_{\Omega} (|\nabla u|^2 + V_{\theta}|u|^2) dx,$$

whose domain $D(q_{\theta})$ is:

$$D(q_{\theta}) = \{ u \in L^2(\Omega), \ \nabla u \in L^2(\Omega), \ \sqrt{V_{\theta}} \ u \in L^2(\Omega) \}.$$

The operator \mathcal{L}_{θ} is positive. We now recall the min-max principle which allows us to define the *n*-th eigenvalue using Rayleigh quotients (see [20, Theorem XIII.1], [21, p. 75]):

Proposition 1.1 (min-max principle) Let A be a self-adjoint operator that is bounded from below, q_A its quadratic form and $D(q_A)$ its form domain. Let us define

$$\mu_n = \sup_{\Psi_1, \dots, \Psi_{n-1} \in D(q_A)} \inf_{\substack{\Psi \in [\Psi_1, \dots, \Psi_{n-1}]^{\perp} \\ \Psi \in D(q_A), \ \|\Psi\| = 1}} q_A(\Psi) = \inf_{\Psi_1, \dots, \Psi_n \in D(q_A)} \sup_{\substack{\Psi \in [\Psi_1, \dots, \Psi_n] \\ \|\Psi\| = 1}} q_A(\Psi) . \quad (1.1)$$

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

Let $\sigma_n(\theta)$ be the *n*-th eigenvalue of \mathcal{L}_{θ} defined by the min-max principle and we denote by $\mathrm{sp}_{\mathrm{ess}}(\mathcal{L}_{\theta})$ its essential spectrum. Let us recall some fundamental spectral properties of \mathcal{L}_{θ} when $\theta \in \left(0, \frac{\pi}{2}\right)$.

It is proved in [10] that $\operatorname{sp}_{\operatorname{ess}}(\mathcal{L}_{\theta}) = [1, +\infty)$ and that $\theta \mapsto \sigma_n(\theta)$ is non decreasing. Moreover, the function $(0, \frac{\pi}{2}) \ni \theta \mapsto \sigma_1(\theta)$ is increasing, and corresponds to a simple eigenvalue < 1 associated with a positive eigenfunction (see [13, Lemma 3.6]). As a consequence $\theta \mapsto \sigma_1(\theta)$ is analytic (see for example [12, Chapter 7]).

Remark 1.2 By an even reflexion through the boundary, our problem is equivalent to a problem set on the whole plane \mathbb{R}^2 with a potential which reaches its minimum on the union of two half-lines: \mathcal{L}_{θ} has eingenvalues under its essential spectrum if and only if the half-lines are not colinear. It is interesting to note the analogy with quantum wave guides which have eigenvalues below their essential spectrum as soon as their middle fiber has a non zero curvature, [8, 5].

In all our investigations, of fundamental importance is the family of one-dimensional self-adjoint operators H_{ζ} , $\zeta \in \mathbb{R}$ defined by:

$$H_{\zeta} = H_{\zeta}(t; D_t) = D_t^2 + (t - \zeta)^2,$$
 (1.2)

on their common Neumann domain on the half-line:

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

The spectral properties of this family of operators have been studied in [7]. Let us recall some of these. We denote by $\mu(\zeta)$ the lowest eigenvalue of H_{ζ} , and by v_{ζ} a normalized associated eigenfunction. We have the following limits (see [7, §3]):

$$\lim_{\zeta \to +\infty} \mu(\zeta) = 1 \quad \text{ and } \quad \lim_{\zeta \to -\infty} \mu(\zeta) = +\infty.$$

Let us also mention that

$$\mu(\zeta) = \mathcal{O}(\zeta^2). \tag{1.3}$$

In addition, the function μ reaches (non degenerately) its minimum denoted by Θ_0 for a unique value ζ_0 (as proved in [7, Theorem 4.3]). There holds (see [4] for refined numerical computations):

$$\zeta_0^2 = \Theta_0$$
 and $\Theta_0 \simeq 0.590106125$.

1.2 Main results of the paper

Our results concern exponential decay estimates for eigenvectors of \mathcal{L}_{θ} and the asymptotic behavior of its eigenvalues in the small angle limit $\theta \to 0$. All along this paper, $(\sigma(\theta), u_{\theta})$ will denote an eigenpair of \mathcal{L}_{θ} with $\sigma(\theta) < 1$. We prove the exponential decay estimates for u_{θ} stated in the following two theorems, improving the results of [19]. Our first result gives an isotropic exponential decay with a weight of the type $e^{\alpha|x|}$:

Theorem 1.3 Let $(\sigma(\theta), u_{\theta})$ be an eigenpair of \mathcal{L}_{θ} with $\sigma(\theta) < 1$. We have:

$$\forall \alpha \in \left(0, \sqrt{1 - \sigma(\theta)}\right), \ \exists C_{\alpha, \theta} > 0, \quad q_{\theta}(e^{\alpha|x|}u_{\theta}) \le C_{\alpha, \theta} \|u_{\theta}\|_{L^{2}(\Omega)}^{2}. \tag{1.4}$$

Our second result is an anisotropic decay estimate in the orthogonal direction of the zero set of V_{θ} :

Theorem 1.4 Let $0 < \beta < \frac{1}{2}$. Let $(\sigma(\theta), u_{\theta})$ be an eigenpair of \mathcal{L}_{θ} with $\sigma(\theta) < 1$. Then there exists a constant $K(\beta)$ such that

$$q_{\theta}(e^{\beta V_{\theta}}u_{\theta}) \le K(\beta) \|u_{\theta}\|_{L^{2}(\Omega)}^{2}. \tag{1.5}$$

Estimates (1.4) and (1.5) have different performances in different directions: For $\gamma \in [0, \pi]$, let us consider the points

$$x = r(\cos \gamma, \sin \gamma), \quad r > 0,$$

on the half-line of angle γ with $\partial\Omega$. Then

$$|x| = r$$
 and $V_{\theta}(x) = r^2 \sin^2(\gamma - \theta)$.

Thus estimate (1.4) is stronger than (1.5) if $\gamma = \theta$, but weaker as soon as $\gamma \neq \theta$.

Then, we want to analyze the behavior of the eigenvalues below the essential spectrum when θ goes to zero. In a first step, we prove that the number of such eigenvalues tends to infinity:

Theorem 1.5 We have the following upper bound for the n-th eigenvalue $\sigma_n(\theta)$ of \mathcal{L}_{θ} :

$$\sigma_n(\theta) \le \Theta_0 \cos \theta + (2n - 1)\sin \theta, \quad \forall n \ge 1.$$
 (1.6)

Therefore, if we denote by $n(\theta)$ the number of eigenvalues of \mathcal{L}_{θ} below the essential spectrum, we have:

$$n(\theta) \ge \frac{1 - \Theta_0 \cos \theta}{2 \sin \theta} + \frac{1}{2}.\tag{1.7}$$

In a second step, we use semi-classical techniques to get a two term asymptotics for those eigenvalues:

Theorem 1.6 For all $M_0 \ge 1$, there exist $h_0 > 0$ and $C(M_0) > 0$ such that for all $0 < \theta \le h_0$ and $1 \le n \le M_0$:

$$\left| \sigma_n(\theta) - \left(\Theta_0 + \theta \sqrt{\frac{\mu''(\zeta_0)}{2}} \left(2n - 1 \right) \right) \right| \le C(M_0) \, \theta^{3/2}. \tag{1.8}$$

Moreover, the gap between successive eigenvalues provides information on the associated eigenfunctions: We will see that they are close to some quasimodes we are going to construct, see section 4.3.

1.3 Organization of the paper

After the present introduction, we prove in Section 2 the isotropic and anisotropic decay estimate of Theorems 1.3 and 1.4. In Section 3, we prove Theorem 1.5, which shows that the number of eigenvalues below 1 tends to infinity as the angle θ tends to 0. We also prove that eigenvalues densify on the whole interval $[\Theta_0, 1]$ when $\theta \to 0$. Section 4 is devoted to the proof of Theorem 4.1 which immediately implies Theorem 1.6.

In Section 5 we present a series of computations of eigenpairs performed with the finite element library MÉLINA [14]. They illustrate the anisotropic exponential decay of eigenvectors, and also clearly display an asymptotic expansion for the n-th eigenvalue of \mathcal{L}_{θ} as $\theta \to 0$ in the form:

$$\sigma_n(\theta) = \Theta_0 + (2n - 1)a_1\theta - a_{2,n}\theta^2 - a_{3,n}\theta^3 + \mathcal{O}(\theta^3),$$

where $a_1 \simeq 0.7651882$ and $a_{2,n}$, $a_{3,n}$ are some coefficients. This expansion is coherent with (1.8), all the more since a_1 coincides with the 7-digit numerical approximation of $\sqrt{\mu''(\zeta_0)/2}$ according to the 1D computations presented in [4]. In addition, for small angles θ , the eigenvectors show their resemblance with the quasimodes constructed in tensor product form, cf. section 4.3 and Figures 8-10.

2 Exponential decay of eigenvectors

The aim of this section is to prove Theorems 1.3 and 1.4. For that purpose, we need to recall some ingredients in order to implement the so-called "Agmon's estimates".

2.1 Preliminaries

Here we recall a few classical identities due to Agmon. There are consequences of the "IMS" formula and can be found in [2] (see also [6] and [18] for the same kind of applications).

Lemma 2.1 Let $u \in D_N(\mathcal{L}_\theta)$ and Φ be a bounded and uniform Lipschitz function defined on Ω . Then we have

$$\langle \mathcal{L}_{\theta} u, e^{2\Phi} u \rangle = q_{\theta}(e^{\Phi} u) - \||\nabla \Phi|e^{\Phi} u\|_{L^{2}(\Omega)}^{2}. \tag{2.1}$$

Taking $u = u_{\theta}$ in Lemma 2.1, we get the obvious corollary:

Corollary 2.2 Let $(\sigma(\theta), u_{\theta})$ be an eigenpair for \mathcal{L}_{θ} and Φ be a bounded and uniform Lipschitz function defined on Ω . We have the following identities:

$$\int_{\Omega} (\sigma(\theta) + |\nabla \Phi|^2) e^{2\Phi} |u_{\theta}|^2 = q_{\theta}(e^{\Phi}u_{\theta}), \tag{2.2}$$

$$\int_{\Omega} |\nabla (e^{\Phi} u_{\theta})|^2 + \int_{\Omega} (V_{\theta} - \sigma(\theta) - |\nabla \Phi|^2) e^{2\Phi} |u_{\theta}|^2 = 0.$$
 (2.3)

Let (Ω^+, Ω^-) be a partition of Ω : $\Omega = \Omega^+ \cup \Omega^-$ with $\Omega^+ \cap \Omega^- = \emptyset$, then we have

$$\int_{\Omega^{+}} (V_{\theta} - \sigma(\theta) - |\nabla \Phi|^{2}) e^{2\Phi} |u_{\theta}|^{2} \le \sup_{\Omega^{-}} |V_{\theta} - \sigma(\theta) - |\nabla \Phi|^{2} |\int_{\Omega^{-}} e^{2\Phi} |u_{\theta}|^{2}.$$
 (2.4)

In order to satisfy the hypotheses of this corollary, we will need to perform a partition of unity. This is the aim of the following two lemmas to explain how to deal with such a partition.

Lemma 2.3 Let $\chi \in C_0^{\infty}(\overline{\Omega})$ and $u \in D(q_{\theta})$, then

$$q_{\theta}(\chi u) = \int_{\Omega} |\chi|^2 (|\nabla u|^2 + V_{\theta}|u|^2) + \frac{1}{2} \int_{\Omega} \nabla |\chi|^2 \nabla |u|^2 + \int_{\Omega} |\nabla \chi|^2 |u|^2. \tag{2.5}$$

If we suppose moreover that $u \in D_N(\mathcal{L}_{\theta})$ *, we have:*

$$q_{\theta}(\chi u) = \langle \chi^2 \mathcal{L}_{\theta} u, u \rangle + \||\nabla \chi|u||_{L^2(\Omega)}^2.$$
(2.6)

Lemma 2.4 Let $(\chi_i)_i$ be a finite regular partition of unity with $\sum_i \chi_i^2 = 1$. Then for all $u \in D(q_\theta)$,

$$\sum_{i} q_{\theta}(\chi_{i}u) = q_{\theta}(u) + \int_{\Omega} \sum_{i} |\nabla \chi_{i}|^{2} |u|^{2}. \tag{2.7}$$

2.2 Isotropic decay of the eigenvectors

This subsection is devoted to the proof of Theorem 1.3.

PRELIMINARIES. Let (χ_1, χ_2) be a partition of unity on \mathbb{R}^+ with $\chi_1^2 + \chi_2^2 = 1$ and:

$$\begin{cases} 0 \le \chi_1 \le 1, & \chi_1(r) = 1 \text{ if } r \le 1, \text{ and } 0 \text{ if } r \ge 2, \\ 0 \le \chi_2 \le 1, & \chi_2(r) = 0 \text{ if } r \le 1, \text{ and } 1 \text{ if } r \ge 2. \end{cases}$$

We define

$$\chi_1^R(x) = \chi_1(\frac{|x|}{R}) \quad \text{and} \quad \chi_2^R(x) = \chi_2(\frac{|x|}{R}).$$
(2.8)

We have $\nabla \chi_j^R(x) = \frac{1}{R} \nabla \chi_j(\frac{x}{R})$. Thus we deduce:

$$\exists C > 0, \ \forall j = 1, 2, \ \forall x \in \Omega, \quad |\nabla \chi_j^R(x)| \le \frac{C}{R}.$$
 (2.9)

Let us fix $\alpha > 0$. As Agmon's distance, we choose the function:

$$\Phi(s,t) = \alpha \sqrt{s^2 + t^2} = \alpha |x|. \tag{2.10}$$

It clearly satisfies $|\nabla \Phi|^2 = \alpha^2$. We do not know yet that $e^{\Phi}u_{\theta} \in D(q_{\theta})$. This is the reason why we use a cut-off function in order to use the Corollary 2.2. We define for $k \in \mathbb{N}$:

$$\begin{cases} \Phi_k(x) = \alpha |x| & \text{if } |x| \le k, \\ \Phi_k(x) = \alpha (2k - |x|) & \text{if } k \le |x| \le 2k, \\ \Phi_k(x) = 0 & \text{if } |x| \ge 2k. \end{cases}$$

We have:

$$\begin{cases} |\nabla \Phi_k|^2 = |\nabla \Phi|^2 = \alpha^2 & \text{if } |x| \le 2k, \\ |\nabla \Phi_k|^2 = 0 & \text{if } |x| > 2k. \end{cases}$$

FIRST STEP. Using (2.2) and (2.7) we have:

$$\int_{\Omega} (\sigma(\theta) + |\nabla \Phi_k|^2) e^{2\Phi_k} |u_{\theta}|^2 = \sum_{j=1}^2 q_{\theta}(\chi_j^R e^{\Phi_k} u_{\theta}) - \sum_{j=1}^2 \int_{\Omega} |\nabla \chi_j^R|^2 e^{2\Phi_k} |u_{\theta}|^2.$$
 (2.11)

Let us choose $\varepsilon \in (0, 1 - \sigma(\theta))$ and

$$\alpha = \sqrt{1 - \varepsilon - \sigma(\theta)}. (2.12)$$

Thus, we have:

$$\sigma(\theta) + |\nabla \Phi|^2 = 1 - \varepsilon. \tag{2.13}$$

It follows that:

$$\int_{\Omega} (\sigma(\theta) + |\nabla \Phi_k|^2) e^{2\Phi_k} |u_{\theta}|^2 = (1 - \varepsilon) \|e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2 + (\sigma(\theta) - 1 + \varepsilon) \int_{|x| > 2k} |u_{\theta}|^2 dx. \quad (2.14)$$

We choose R > 0 such that

$$\frac{C^2}{R^2} \le \frac{\varepsilon}{4},\tag{2.15}$$

where C is the constant appearing in (2.9). Hence we get:

$$\sum_{j=1}^{2} \int_{\Omega} |\nabla \chi_{j}^{R}|^{2} |e^{\Phi_{k}} u_{\theta}|^{2} \leq \frac{\varepsilon}{2} ||e^{\Phi_{k}} u_{\theta}||_{L^{2}(\Omega)}^{2}.$$
 (2.16)

Relations (2.11), (2.14) and (2.16) provide:

$$\frac{\varepsilon}{2} \|e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2 \le \|e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2 - \sum_{j=1}^2 q_{\theta} (\chi_j^R e^{\Phi_k} u_{\theta}) + (\sigma(\theta) - 1 + \varepsilon) \int_{|x| > 2k} |u_{\theta}|^2 dx
\le \|e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2 - q_{\theta} (\chi_2^R e^{\Phi_k} u_{\theta}).$$
(2.17)

SECOND STEP. In order to bound from below the energy "far from the origin" $q_{\theta}(\chi_2^R e^{\Phi_k} u_{\theta})$, we introduce a classical notation attached to Persson's lemma:

$$\Sigma(\mathcal{L}_{\theta}, r) = \inf \Big\{ q_{\theta}(u), \ \|u\|_{L^{2}(\Omega)} = 1, \ u \in C_{0}^{\infty}(\overline{\Omega} \cap \complement B_{r}) \Big\},\,$$

where B_r denotes the ball of radius r centered at 0, and $\complement B_r$ its complement. It results from Persson's lemma (see [17]) that the limit of $\Sigma(\mathcal{L}_{\theta}, r)$ as $r \to +\infty$ equals the bottom of the essential spectrum of \mathcal{L}_{θ} , thus 1:

$$\lim_{r \to +\infty} \Sigma(\mathcal{L}_{\theta}, r) = 1. \tag{2.18}$$

We have:

$$\frac{q_{\theta}(\chi_2^R e^{\Phi_k} u_{\theta})}{\|\chi_2^R e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2} \ge \Sigma(\mathcal{L}_{\theta}, R), \tag{2.19}$$

and so:

$$q_{\theta}(\chi_2^R e^{\Phi_k} u_{\theta}) \ge \Sigma(\mathcal{L}_{\theta}, R) \int_{|x| > 2R} e^{2\Phi_k} |u_{\theta}|^2 \mathrm{d}x. \tag{2.20}$$

Using (2.17), we get:

$$\frac{\varepsilon}{2} \|e^{\Phi_k} u_{\theta}\|_{L^2(\Omega)}^2 \le \int_{|x|<2R} e^{2\Phi_k} |u_{\theta}|^2 dx + (1 - \Sigma(\mathcal{L}_{\theta}, R)) \int_{|x|>2R} e^{2\Phi_k} |u_{\theta}|^2 dx.$$

Using (2.18), we can choose R large enough such that, besides (2.15):

$$1 - \Sigma(\mathcal{L}_{\theta}, R) < \frac{\varepsilon}{4}$$
.

We deduce:

$$\frac{\varepsilon}{4} \int_{\Omega} e^{2\Phi_k} |u_{\theta}|^2 \le \int_{|x| < 2R} e^{2\Phi_k} |u_{\theta}|^2 dx.$$

We finally get:

$$\forall k \in \mathbb{N}, \quad \|e^{\Phi_k} u_\theta\|_{L^2(\Omega)}^2 \le \frac{4}{\varepsilon} e^{4\alpha R} \|u_\theta\|_{L^2(\Omega)}^2. \tag{2.21}$$

CONCLUSION. However, $|e^{\Phi_k}u_{\theta}|$ converges pointwise to $|e^{\Phi}u_{\theta}|$ as k goes to infinity. It follows from Fatou's lemma that $e^{\Phi}u_{\theta} \in L^2(\Omega)$. The conclusion comes from:

$$\|\nabla(e^{\Phi}u_{\theta})\|_{L^{2}(\Omega)}^{2} + \|V_{\theta}e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)}^{2} = (1 - \varepsilon)\|e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)}^{2},$$

as a direct consequence of (2.3) and (2.13).

Remark 2.5 This proof is the key point in order to prove that u_{θ} is in the Schwartz's class, see [19].

Examining the arguments of this proof, we can see that α and the constant $C_{\alpha,\theta}$ can be chosen uniformly in any closed interval $[\theta_0,\theta_1]$ with $\theta_0>0$ and $\theta_1<\frac{\pi}{2}$. Since $\sigma(\theta)\to 1$ as $\theta\to\frac{\pi}{2}$, it is impossible to obtain uniform estimates as $\theta\to\frac{\pi}{2}$. When $\theta\to 0$, there is no valid uniform estimates in the tangential variable s. However, considering only a dependence with respect to t, we get a uniform control in θ :

Proposition 2.6 Let $\eta < 1$. There exist C > 0 and $\gamma > 0$ such that for any eigenpair $(\sigma(\theta), u_{\theta})$ of \mathcal{L}_{θ} with $\sigma(\theta) \leq \eta$ there holds

$$\int_{\Omega} e^{2\gamma t} |u_{\theta}|^2 ds dt \le C ||u_{\theta}||_{L^2(\Omega)}^2.$$
 (2.22)

Proof: The proof is similar as for Theorem 1.3. We choose $\Phi = \gamma t$ and instead (2.8) we use the partition of unity (χ_i^R) with respect to t:

$$\chi_1^R(x) = \chi_1(\frac{t}{R})$$
 and $\chi_2^R(x) = \chi_2(\frac{t}{R})$. (2.23)

The first step of the proof goes the same way with

$$\varepsilon \in (0, 1 - \eta),$$

and the key point of the second point is then the lower bound, — which replaces (2.20):

$$q_{\theta}(\chi_{2}^{R}e^{\Phi}u_{\theta}) \ge \|\chi_{2}^{R}e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)}^{2}.$$
 (2.24)

This inequality is a consequence of the fact that the support of χ_2^R is now far from the boundary of Ω , — since the bottom of the spectrum of the self-adjoint realization on \mathbb{R}^2 of $D_t^2 + D_s^2 + V_\theta$ is 1. Thus, as ε is set and the size of R does not depend anymore on θ for this choice of Φ , we get that the upper bound in (2.21) is independent from θ .

2.3 Anisotropic decay from the minimum of the potential

In this section we prove the decay of u_{θ} away from the minimum of V_{θ} stated in Theorem 1.4. Let $\delta \in (0,1)$. Following [1], we introduce the function associated with Agmon's geodesics:

$$\Phi(x) = (1 - \delta) \int_{\sqrt{\sigma(\theta)}}^{\sqrt{V_{\theta}(x)}} \sqrt{\left(l^2 - \sigma(\theta)\right)_+} dl, \qquad (2.25)$$

where f_+ denotes the positive part of a function f. Let's notice that if we define the function

$$g(d) = \int_{\sqrt{\sigma(\theta)}}^{d} \sqrt{(l^2 - \sigma(\theta))_{+}} \, \mathrm{d}l,$$

we have

$$\Phi(x) = (1 - \delta)g(\sqrt{V_{\theta}(x)}).$$

It is an elementary computation to check that we have (uniformly in θ):

$$g(d) \underset{d \to +\infty}{=} \frac{d^2}{2} + \mathcal{O}(\ln d) \quad \text{and} \quad g'(d) \underset{d \to +\infty}{=} d + \mathcal{O}(d^{-1}). \tag{2.26}$$

So Theorem 1.4 holds if and only if $q_{\theta}(e^{\Phi}u_{\theta})$ is bounded uniformly in θ for all $\delta \in (0,1)$. Let us prove this. We choose $\delta \in (0,1)$. By construction of Φ , we have:

$$|\nabla \Phi|^2 = (1 - \delta)^2 (V_\theta - \sigma(\theta))_+. \tag{2.27}$$

Let $\eta > 0$, we define a partition of unity for Ω :

$$A_{\eta}^+ = \{(s,t) \in \Omega, V_{\theta}(s,t) - \sigma(\theta) > \eta\} \quad \text{ and } \quad A_{\eta}^- = \{(s,t) \in \Omega, V_{\theta}(s,t) - \sigma(\theta) \leq \eta\}.$$

On A_n^+ , we have:

$$V_{\theta} - \sigma(\theta) - |\nabla \Phi|^2 = (V_{\theta} - \sigma(\theta))(2\delta - \delta^2) > \eta(2\delta - \delta^2). \tag{2.28}$$

Similarly, we have on A_n^- :

$$|V_{\theta} - \sigma(\theta) - |\nabla \Phi|^2| = \begin{cases} \sigma(\theta) - V_{\theta} & \text{if } V_{\theta} < \sigma(\theta), \\ (V_{\theta} - \sigma(\theta))(2\delta - \delta^2) & \text{if not.} \end{cases}$$

Let us assume that

$$0 < \eta(2\delta - \delta^2) \le \Theta_0 < \sigma(\theta). \tag{2.29}$$

Then, we have the following upper bound:

$$\sup_{A_n^-} \left| V_{\theta} - \sigma(\theta) - |\nabla \Phi|^2 \right| \le \sigma(\theta). \tag{2.30}$$

We now combine (2.4), (2.28) and (2.30) in order to get:

$$\eta(2\delta - \delta^2) \int_{A_{\eta}^+} e^{2\Phi} |u_{\theta}|^2 \le \int_{A_{\eta}^+} (V_{\theta} - \sigma(\theta) - |\nabla \Phi|^2) e^{2\Phi} |u_{\theta}|^2 \le \sigma(\theta) \int_{A_{\eta}^-} e^{2\Phi} |u_{\theta}|^2. \tag{2.31}$$

Since $||u_{\theta}||_{L^{2}(\Omega)} = 1$ and that Φ is maximal on the boundary of A_{η}^{-} , we get:

$$||e^{\Phi}u_{\theta}||_{L^{2}(\Omega)} \leq \left(\frac{\sigma(\theta)}{\eta(2\delta - \delta^{2})} + 1\right) \exp \int_{\sqrt{\sigma(\theta)}}^{\sqrt{\sigma(\theta) + \eta}} (1 - \delta)\sqrt{l^{2} - \sigma(\theta)} \, \mathrm{d}l. \tag{2.32}$$

We denote by $K(\eta, \delta, \sigma(\theta))$ the right hand side of the last inequality. If we fix $\delta > 0$, the function

$$\mathbb{R}_{+} \times [\Theta_{0}, 1] \to \mathbb{R}$$
$$(\eta, \sigma) \to K(\eta, \delta, \sigma)$$

is clearly positive and continuous. We notice that:

$$\lim_{\eta \to 0} K(\eta, \delta, \sigma) = +\infty.$$

Recall that we assume the condition on η given by (2.29). We introduce the interval $I(\delta) = \left(0, \frac{\Theta_0}{2\delta - \delta^2}\right]$. This allows us to define the positive constant

$$K_0(\delta) = \max_{\sigma \in [\Theta_0, 1]} \min_{\eta \in I(\delta)} K(\eta, \delta, \sigma).$$

The minimum is achieved for a $\eta_0 \in I(\delta)$. Choosing this η_0 , we deduce from (2.32):

$$\|e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)} \le K_{0}(\delta).$$
 (2.33)

If we define

$$\tilde{\Phi}(x) = \left(1 - \frac{\delta}{2}\right) \int_{\sqrt{\sigma(\theta)}}^{\sqrt{V_{\theta}(x)}} \sqrt{(l^2 - \sigma(\theta))_+} \, \mathrm{d}l,$$

we have

$$\|e^{\tilde{\Phi}}u_{\theta}\|_{L^2(\Omega)} \le K_0\left(\frac{\delta}{2}\right).$$

Because of (2.26), we have easily

$$\exists K_1(\delta) > 0, \ \forall d > 0, \ |d e^{-\frac{\delta}{2}g(d)}| < K_1(\delta).$$
 (2.34)

We notice that $\sqrt{V_{\theta}} e^{\Phi - \tilde{\Phi}} = \sqrt{V_{\theta}} e^{-\frac{\delta}{2}g(\sqrt{V_{\theta}})}$ and with (2.34), we deduce:

$$\exists K_1(\delta) > 0, \quad \|\sqrt{V_{\theta}} e^{\Phi - \tilde{\Phi}}\|_{L^{\infty}(\Omega)} \le K_1(\delta). \tag{2.35}$$

Therefore, we have:

$$\|\sqrt{V_{\theta}} e^{\Phi} u_{\theta}\|_{L^{2}(\Omega)} \leq \|\sqrt{V_{\theta}} e^{\Phi-\tilde{\Phi}}\|_{L^{\infty}(\Omega)} \|e^{\tilde{\Phi}} u_{\theta}\|_{L^{2}(\Omega)},$$

and finally, with a new constant $K_2(\delta)$:

$$\|\sqrt{V_{\theta}} e^{\Phi} u_{\theta}\|_{L^{2}(\Omega)} \le K_{2}(\delta). \tag{2.36}$$

With the definition of Φ , we also get:

$$\||\nabla \Phi| e^{\Phi} u_{\theta}\|_{L^{2}(\Omega)} \le K_{3}(\delta). \tag{2.37}$$

Using (2.1), we finally obtain

$$q_{\theta}(e^{\Phi}u_{\theta}) = \||\nabla\Phi|e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)}^{2} + \sigma(\theta)\|e^{\Phi}u_{\theta}\|_{L^{2}(\Omega)}^{2} \le K(\delta).$$

3 Densification of the spectrum for small angles

In this section, we investigate the behavior of the eigenvalues below 1.

3.1 An upper bound

In this section, we give the proof of Theorem 1.5. In order to get the announced upper bound, we will construct a family of quasimodes and use the min-max principle.

Let us introduce first some tools from spectral theory of self-adjoint operators (see for example [20]). We denote by $b_{\theta}(u)$ the Rayleigh quotient associated with a function u for \mathcal{L}_{θ} :

$$\forall u \in D(q_{\theta}) \setminus \{0\}, \quad b_{\theta}(u) = \frac{q_{\theta}(u)}{\|u\|_{L^{2}(\Omega)}^{2}}.$$

The bilinear form associated with q_{θ} is defined on the form domain by:

$$a_{\theta}(u,v) = \int_{\Omega} \left(D_t u D_t v + D_s u D_s v + V_{\theta} u v \right) dx.$$

Lemma 3.1 Let v_{ζ_0} be a normalized eigenvector associated with the first eigenvalue Θ_0 of the operator H_{ζ_0} (cf. (1.2) and the properties recalled there), and let ψ_n be the n-th Hermite function with the "physicists" convention. We recall that:

$$\forall n \geq 0, \ \forall x \in \mathbb{R}, \quad -\psi_n''(x) + x^2 \psi_n(x) = (2n+1)\psi_n(x).$$

We define the normalized function $\widetilde{u}_{n,\theta}$ by:

$$\widetilde{u}_{n,\theta}(s,t) = (\cos\theta \sin\theta)^{\frac{1}{4}} v_{\zeta_0}(t\sqrt{\cos\theta}) \psi_n \left(s\sqrt{\sin\theta} - \frac{\zeta_0}{\sqrt{\tan\theta}}\right). \tag{3.1}$$

Then we have:

$$\forall n \in \mathbb{N}, \ \forall \theta \in \left(0, \frac{\pi}{2}\right), \quad b_{\theta}(\widetilde{u}_{n,\theta}) = \Theta_0 \cos \theta + (2n+1)\sin \theta.$$
 (3.2)

Proof: The function $\widetilde{u}_{n,\theta}$ is clearly in the form domain $D(q_{\theta})$. We are going to estimate $q_{\theta}(\widetilde{u}_{n,\theta})$. Let us make the following rescaling and translation:

$$\begin{cases} y = s\sqrt{\sin\theta} - \frac{\zeta_0}{\sqrt{\tan\theta}}, \\ z = t\sqrt{\cos\theta}. \end{cases}$$
 (3.3)

Then

$$q_{\theta}(\widetilde{u}_{n,\theta}) = \int_{\Omega} \left(\cos \theta |v'_{\zeta_0}(z)\psi_n(y)|^2 + \sin \theta |v_{\zeta_0}(z)\psi'_n(y)|^2 + (z\sqrt{\cos \theta} - y\sqrt{\sin \theta} - \zeta_0\sqrt{\cos \theta})^2 |v_{\zeta_0}(z)\psi_n(y)|^2 \right) dy dz$$

$$= \cos \theta \int_{\Omega} \left(|v'_{\zeta_0}(z)\psi_n(y)|^2 + (z - \zeta_0)^2 |v_{\zeta_0}(z)\psi_n(y)|^2 \right) dy dz$$

$$+ \sin \theta \int_{\Omega} \left(|v_{\zeta_0}(z)\psi'_n(y)|^2 + y^2 |v_{\zeta_0}(z)\psi_n(y)|^2 \right) dy dz$$

$$- 2\sqrt{\sin \theta} \sqrt{\cos \theta} \int_{\Omega} y(z - \zeta_0) |v_{\zeta_0}(z)\psi_n(y)|^2 dy dz.$$

We have the following relations:

$$\int_{\mathbb{R}_{+}} |v'_{\zeta_{0}}(z)|^{2} + (z - \zeta_{0})^{2} |v_{\zeta_{0}}(z)|^{2} dz = \Theta_{0},$$
(3.4)

$$\int_{\mathbb{R}_{+}} (z - \zeta_{0}) |v_{\zeta_{0}}(z)|^{2} dz = 0,$$
 (3.5)

$$\int_{\mathbb{R}} |\psi'_n(y)|^2 + y^2 |\psi_n(y)|^2 \, \mathrm{d}y = 2n + 1, \tag{3.6}$$

where (3.5) is a direct consequence of the Feynman-Hellman formula (see [11] and also Section 4.1). Thus we have

$$q_{\theta}(\widetilde{u}_{n,\theta}) = \Theta_0 \cos \theta \|\psi_n\|_{L^2(\mathbb{R})}^2 + (2n+1)\sin \theta \|v_{\zeta_0}\|_{L^2(\mathbb{R}_+)}^2. \tag{3.7}$$

Since v_{ζ_0} and ψ_n are normalized, and $\|\widetilde{u}_{n,\theta}\|_{L^2(\Omega)}^2 = 1$, we deduce (3.2).

Lemma 3.2 The functions $\widetilde{u}_{n,\theta}$, $n \geq 0$, are orthogonal for the bilinear form a_{θ} .

Proof: Let $n \neq m$ be two integers. We recall that $\int_{\mathbb{R}} \psi_n \psi_m = 0$. As in the proof of Lemma 3.1, we have:

$$a_{\theta}(\widetilde{u}_{n,\theta}, \widetilde{u}_{m,\theta}) = \Theta_{0} \cos \theta \int_{\mathbb{R}} \psi_{n}(y) \psi_{m}(y) \, \mathrm{d}y$$

$$+ \sin \theta \int_{\mathbb{R}} \psi'_{n}(y) \psi'_{m}(y) + y^{2} \psi_{n}(y) \psi_{m}(y) \, \mathrm{d}y$$

$$- 2\sqrt{\sin \theta} \sqrt{\cos \theta} \int_{\Omega} y(z - \zeta_{0}) \psi_{n}(y) \psi_{m}(y) |v_{\zeta_{0}}(z)|^{2} \, \mathrm{d}y \, \mathrm{d}z.$$

For the second term, we make an integration by parts:

$$\int_{\mathbb{R}} \psi'_n(y)\psi'_m(y) \, \mathrm{d}y = \int_{\mathbb{R}} -\psi''_n(y)\psi_m(y) \, \mathrm{d}y$$

$$= \int_{\mathbb{R}} (2n+1-y^2)\psi_n(y)\psi_m(y) \, \mathrm{d}y$$

$$= -\int_{\mathbb{R}} y^2 \psi_n(y)\psi_m(y) \, \mathrm{d}y.$$

Since the other terms are clearly equal to 0, we have $a_{\theta}(\widetilde{u}_{n,\theta},\widetilde{u}_{m,\theta})=0$.

Combining Lemmas 3.1 and 3.2, we deduce Theorem 1.5: Indeed, we only have to apply the min-max principle with the functions $(\tilde{u}_{n,\theta})_{n\in\mathbb{N}}$ which are orthogonal for the bilinear form associated with \mathcal{L}_{θ} .

Remark 3.3 We have just proved that the number of eigenvalues below the essential spectrum gets large as θ tends to 0. In [16, Theorem 4.3], the authors prove an asymptotic expansion of this number.

We now show that the eigenvalues get dense in $[\Theta_0, 1]$.

3.2 Spectrum density

Proposition 3.4 Let $\zeta > 0$ and n be an integer such that

$$\mu(\zeta)\cos\theta + (2n+1)\sin\theta < 1.$$

Then, there exist an eigenvalue λ of \mathcal{L}_{θ} and a constant $C_{\zeta} > 0$ such that:

$$|\mu(\zeta)\cos\theta + (2n+1)\sin\theta - \lambda| \le C_{\zeta}\sqrt{2\cos\theta\sin\theta}\sqrt{n^2 + 1}.$$
 (3.8)

Proof: In the same way as previously, we define the functions:

$$\widetilde{u}_{n,\theta;\zeta}(s,t) = (\cos\theta\sin\theta)^{\frac{1}{4}}v_{\zeta}(t\sqrt{\cos\theta})\psi_{n}\left(s\sqrt{\sin\theta} - \frac{\zeta}{\sqrt{\tan\theta}}\right). \tag{3.9}$$

where v_{ζ} is the normalized eigenfunction associated with the first eigenvalue $\mu(\zeta)$ of H_{ζ} (cf. § 1.1). These functions are clearly in the form domain of \mathcal{L}_{θ} . We have:

$$D_t^2 \widetilde{u}_{n,\theta;\zeta}(s,t) = \cos\theta \Big(\mu(\zeta) - (t\sqrt{\cos\theta} - \zeta)^2 \Big) \widetilde{u}_{n,\theta;\zeta}(s,t),$$

$$D_s^2 \widetilde{u}_{n,\theta;\zeta}(s,t) = \sin\theta \left(2n + 1 - \left(s\sqrt{\sin\theta} - \frac{\zeta}{\sqrt{\tan\theta}} \right)^2 \right) \widetilde{u}_{n,\theta;\zeta}(s,t).$$

We deduce

$$\mathcal{L}_{\theta}\widetilde{u}_{n,\theta;\zeta} - (\mu(\zeta)\cos\theta + (2n+1)\sin\theta)\widetilde{u}_{n,\theta;\zeta} = 2(\cos\theta\sin\theta)^{\frac{1}{2}} \Big(\frac{\zeta}{\sqrt{\tan\theta}} - s\sqrt{\sin\theta}\Big) (t\sqrt{\cos\theta} - \zeta)\widetilde{u}_{n,\theta;\zeta}. \quad (3.10)$$

Thus, noticing that $\|\widetilde{u}_{n,\theta;\zeta}\|_{L^2(\Omega)} = 1$, we get:

$$\|\mathcal{L}_{\theta}\widetilde{u}_{n,\theta;\zeta} - (\mu(\zeta)\cos\theta + (2n+1)\sin\theta)\widetilde{u}_{n,\theta;\zeta}\|_{L^{2}(\Omega)} = 2(\cos\theta\sin\theta)^{\frac{1}{2}} \|(t-\zeta)v_{\zeta}(t)\|_{L^{2}(\mathbb{R}_{+})} \|s\psi_{n}(s)\|_{L^{2}(\mathbb{R})}.$$
(3.11)

It is well known that

$$\int_{\mathbb{R}} s^2 \psi_n^2(s) \, \mathrm{d}s = \frac{n^2 + 1}{2},$$

and if we define $C_{\zeta}=\|(t-\zeta)v_{\zeta}\|_{L^{2}(\mathbb{R}_{+})}$, we can conclude with the spectral theorem. \qed

We can notice that the right part of (3.8) goes to infinity as n gets large, so the previous proposition is useless if θ is fixed and n goes to infinity. However we have the following proposition:

Proposition 3.5 *We have the densification result:*

$$\forall \lambda_0 \in (\Theta_0, 1), \ \forall \varepsilon > 0, \ \exists \theta_0 \in \left(0, \frac{\pi}{2}\right), \ \forall \theta \in (0, \theta_0], \ \exists \lambda \in \operatorname{sp}(\mathcal{L}_\theta), \ |\lambda_0 - \lambda| < \varepsilon.$$
 (3.12)

Proof: We only consider the case $\varepsilon < 1$. In the previous lemma we choose n = 0 and ζ such that $\mu(\zeta) = \lambda_0$, which is possible since $\Theta_0 < \lambda_0 < 1$ and $\mu(\zeta)$ takes all values of $[\Theta_0, 1)$ when ζ lays in \mathbb{R}_+^* . Thus we get (3.12).

In the next section, we improve the estimate of Theorem 1.5 for each fixed rank n when θ goes to zero.

4 Asymptotics of eigenvalues in the small angle limit

As it has been proved in Theorem 1.5, when θ goes to zero, the number of eigenvalues $n(\theta)$ below the essential spectrum tends to infinity. Thus, for any arbitrary integer M_0 , we can find a value of θ small enough such that $\sigma_{M_0}(\theta) < 1$. In this section, we investigate the asymptotics of those eigenvalues and prove Theorem 1.6. We use again the scaling (3.3):

$$\begin{cases} y = s\sqrt{\sin\theta} - \frac{\zeta_0}{\sqrt{\tan\theta}}, \\ z = t\sqrt{\cos\theta}. \end{cases}$$

In the new variables, the operator \mathcal{L}_{θ} rewrites

$$\sin \theta D_y^2 + \cos \theta D_z^2 + \cos \theta (z - \zeta_0 - y\sqrt{\tan \theta})^2 = \cos \theta (\mathfrak{L}_h + \Theta_0),$$

where we have set $h = \tan \theta$ and

$$\mathfrak{L}_h = hD_y^2 + D_z^2 + (z - \zeta_0 - yh^{1/2})^2 - \Theta_0. \tag{4.1}$$

We denote by $\mathfrak{s}_n(h)$ the *n*-th eigenvalue of \mathfrak{L}_h . Due to the change of variables, we have

$$\sigma_n(\theta) = \cos\theta (\Theta_0 + \mathfrak{s}_n(\tan\theta)).$$

Thus, in order to prove Theorem 1.6, we are going to establish the following asymptotics for $\mathfrak{s}_n(h)$:

Theorem 4.1 For all $M_0 \ge 1$, there exist $C(M_0) > 0$ and $h_0 > 0$ such that for all $1 \le n \le M_0$ and $0 < h < h_0$:

$$\left| \mathbf{s}_n(h) - h \sqrt{\frac{\mu''(\zeta_0)}{2}} (2n - 1) \right| \le C(M_0) h^{3/2}.$$

Remark 4.2 It follows from Theorem 4.1 that for h small enough the eigenvalues $\mathfrak{s}_n(h)$, $1 \le n \le M_0$, are simple.

The proof of Theorem 4.1 is organized in two main steps. Using the one-dimensional operators H_{ζ} (1.2), we can rewrite (4.1) as

$$\mathfrak{L}_h = hD_y^2 + H_{\zeta_0 + y\sqrt{h}}(z; D_z) - \Theta_0.$$

In a first step we construct quasimodes by an expansion in powers of $h^{1/2}$, and using the spectral theorem, we get a family of approximate eigenvalues and a rough upper bound for $\mathfrak{s}_n(h)$. In a second step, we establish a lower bound. The basic idea to get such a lower bound is to use a Born-Oppenheimer technique which consists of replacing $H_{\zeta_0+y\sqrt{h}}$ by its ground energy $\mu(\zeta_0+y\sqrt{h})$ and to implement the standard harmonic approximation in the semi-classical limit for the one-dimensional operator $\mathfrak{L}_{h,\mathrm{BO}}$ defined as:

$$\mathfrak{L}_{h,\mathrm{BO}} = hD_y^2 + \mu(\zeta_0 + y\sqrt{h}) - \Theta_0.$$

However $\mathfrak{L}_{h,\mathrm{BO}}$, seen as an operator acting on the domain of \mathfrak{L}_h – i.e. as two-dimensional operator, has eigenvalues of infinite multiplicity, and we cannot use directly the min-max principle to compare its spectrum with the eigenvalues of \mathfrak{L}_h . Thus, we have to justify, through Agmon estimates and a Grushin type argument, that the eigenvalues of \mathfrak{L}_h are bounded from below by those of $\mathfrak{L}_{h,\mathrm{BO}}$ seen as one-dimensional operator. Such a procedure was described in [15] for degenerate potentials in \mathbb{R}^n . Nevertheless, we cannot apply directly the techniques of [15] because the minimal line of the potential V_{θ} goes to infinity and we work in a domain with boundary.

4.1 Construction of quasimodes

We can write \mathfrak{L}_h as:

$$\mathfrak{L}_h = P_0 + h^{1/2} P_1 + h P_2,$$

with:

$$P_0 = D_z^2 + (z - \zeta_0)^2 - \Theta_0 = H_{\zeta_0} - \Theta_0,$$

$$P_1 = -2(z - \zeta_0)y,$$

$$P_2 = D_y^2 + y^2.$$

We look for a quasimode in the form:

$$u_h = \varphi_0 + h^{1/2}\varphi_1 + h\varphi_2,$$

attached to an eigenvalue expressed as:

$$\gamma_h = \gamma_0 + h^{1/2} \gamma_1 + h \gamma_2.$$

We are led to the system:

$$h^0: (P_0 - \gamma_0)\varphi_0 = 0, (4.2)$$

$$h^{1/2}: (P_0 - \gamma_0)\varphi_1 = \gamma_1\varphi_0 - P_1\varphi_0,$$
 (4.3)

$$h: (P_0 - \gamma_0)\varphi_2 = \gamma_2\varphi_0 + \gamma_1 u_1 - P_2\varphi_0 - P_1\varphi_1. \tag{4.4}$$

Considering (4.2), we are led to choose $\gamma_0 = 0$ and

$$\varphi_0(y,z) = v_{\zeta_0}(z)f(y),$$

for some f to determine. Then, we want to solve (4.3). In order to solve this equation, we recall an easy computation. Let us take the derivative with respect to ζ of:

$$(H_{\zeta} - \mu(\zeta))v_{\zeta} = 0.$$

Let us take $\zeta = \zeta_0$, we get:

$$(H_{\zeta_0} - \Theta_0)(\partial_{\zeta} v_{\zeta})_{|\zeta = \zeta_0} = 2(z - \zeta_0)v_{\zeta_0}.$$
(4.5)

We deduce:

$$\int_{\mathbb{R}_{+}} (z - \zeta_0) v_{\zeta_0}^2(z) \, \mathrm{d}z = 0. \tag{4.6}$$

We recall now that (4.3) admits a solution if and only if:

$$\langle \gamma_1 \varphi_0 - P_1 \varphi_0, v_{\zeta_0} \rangle_{L^2(\mathbb{R}_{+,z})} = 0,$$

where $\langle \cdot, \cdot \rangle_{L^2(\mathbb{R}_{+,z})}$ denotes the standard L^2 scalar product on \mathbb{R}_+ with respect to z. By (4.5), we get: $\gamma_1 = 0$ and, with (4.6), we can take:

$$\varphi_1(y,z) = w_{\zeta_0}(z)yf(y), \quad \text{with } w_{\zeta_0}(z) = (\partial_{\zeta}v_{\zeta})_{|\zeta=\zeta_0}.$$

Finally, we consider (4.4) and, in the same way, we want:

$$\langle \gamma_2 \varphi_0 - P_2 \varphi_0 - P_1 \varphi_1, v_{\zeta_0} \rangle_{L^2(\mathbb{R}_+, z)} = 0.$$

This leads to the equation:

$$\left(D_y^2 + \left(1 - 2\int_{\mathbb{R}_+} (z - \zeta_0) w_{\zeta_0}(z) v_{\zeta_0}(z) dz\right) y^2\right) f = \gamma_2 f.$$

This is well-known that (see [3, p. 1283-1284] and also [9]):

$$\frac{\mu''(\zeta_0)}{2} = 1 - 2 \int_{\mathbb{R}_+} (z - \zeta_0) w_{\zeta_0}(z) v_{\zeta_0}(z) \, \mathrm{d}z,$$

thus, we infer:

$$H_{\text{harm}}f = \gamma_2 f, \quad \text{with} \quad H_{\text{harm}} = D_y^2 + \frac{\mu''(\zeta_0)}{2} y^2.$$
 (4.7)

Thus, for f we take an eigenfunction f_n of H_{harm} , associated with the eigenvalue

$$\lambda_{n,\text{harm}} = \sqrt{\frac{\mu''(\zeta_0)}{2}}(2n-1). \tag{4.8}$$

In this way, we have determined the coefficients γ_i and the functions φ_i (which are in the Schwartz class) for i = 0, 1, 2. This analysis provides a quasimode for \mathfrak{L}_h :

$$\| (\mathfrak{L}_h - h\lambda_{n,\text{harm}}) u_h(y,z) \|_{L^2(\Omega)} \le C(n) h^{3/2} \| u_h(y,z) \|_{L^2(\Omega)}. \tag{4.9}$$

Using the spectral theorem, we immediately deduce that:

Proposition 4.3 For all $M_0 \ge 1$, there exist $C(M_0) > 0$ and $h_0 > 0$ such that for all $1 \le n \le M_0$ and $0 < h < h_0$, there exists an eigenvalue $\mathfrak{s}_{k(n)}(h)$ of \mathfrak{L}_h such that:

$$|\mathfrak{s}_{k(n)}(h) - h\lambda_{n,\text{harm}}| \le C(M_0) h^{3/2}.$$

Remark 4.4 In particular, we observe that, for $1 \le n \le M_0$ and $h \in (0, h_0)$:

$$0 \le \mathfrak{s}_n(h) \le \mathfrak{s}_{k(n)}(h) \le h\lambda_{n,\text{harm}} + C(M_0) h^{3/2} \le \tilde{C}(M_0) h.$$
 (4.10)

4.2 Lower bound

To get a suitable lower bound of $\mathfrak{s}_n(h)$, we will use the so-called Born-Oppenheimer approximation $\mathfrak{L}_{h,\mathrm{BO}}$ with

$$\mathfrak{L}_{h,BO} := hD_y^2 + W_h(y), \text{ with } W_h(y) = \mu(\zeta_0 + yh^{1/2}) - \Theta_0 \ge 0.$$

Thus, we have

$$\forall v \in D_N(\mathfrak{L}_h), \quad \langle \mathfrak{L}_h v, v \rangle \ge \langle \mathfrak{L}_{h,BO} v, v \rangle.$$
 (4.11)

4.2.1 Localization estimates of Agmon type

Let us take N_0 such that $1 \leq N_0 \leq M_0$. We are going to prove some localization of the eigenfunctions of \mathfrak{L}_h associated with $(\mathfrak{s}_n(h))_{1\leq n\leq N_0}$. For all $1\leq n\leq N_0$, we will consider a normalized eigenfunction $\mathfrak{u}_n(h)$ associated with $\mathfrak{s}_n(h)$ so that the distinct $\mathfrak{u}_n(h)$ are orthogonal. It is convenient to introduce the sum of the first eigenspaces of \mathfrak{L}_h :

$$\mathfrak{E}_{N_0}(h) = \operatorname{span}(\mathfrak{u}_1(h), \dots, \mathfrak{u}_{N_0}(h)). \tag{4.12}$$

Combining Proposition 2.6 and the scaling (3.3), we have the following localization with respect to the normal variable z:

Proposition 4.5 There exist C > 0, $\gamma > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$ and $v \in \mathfrak{E}_{N_0}(h)$:

$$\int_{\Omega} e^{2\gamma z} |v|^2 dy dz \le C ||v||_{L^2(\Omega)}^2.$$
 (4.13)

In this subsection, we improve the result of Theorem 1.3 by proving an optimal localization with respect to y when h goes to 0:

Proposition 4.6 There exists C > 0 and $h_0 > 0$ such that for all $h \in (0, h_0)$ and $v \in \mathfrak{E}_{N_0}(h)$:

$$\int_{\Omega} e^{2|y|} |v|^2 dy dz \le C ||v||_{L^2(\Omega)}^2.$$
(4.14)

Proof: For $v = \mathbf{u}_n(h)$, we can write:

$$\mathbf{q}_{h}(e^{\Phi}v) - \int_{\Omega} (|D_{z}\Phi|^{2} + h|D_{y}\Phi|^{2} + \mathbf{s}_{n}(h))|e^{\Phi}v|^{2} \,\mathrm{d}y \,\mathrm{d}z = 0, \tag{4.15}$$

where \mathbf{q}_h is the quadratic form associated to (4.1). Let us choose $\Phi(y) = |y|$. With (4.11), we deduce:

$$\int_{\Omega} (W_h - h - \mathfrak{s}_n(h)) |e^{\Phi}v|^2 \, \mathrm{d}y \, \mathrm{d}z \le 0 \tag{4.16}$$

Let us consider the positivity of:

$$W_h - h - \mathfrak{s}_n(h)$$

in a region of the type $|y| \ge C_0$ with $C_0 > 0$.

(i) Using the non-degeneracy of the minimum, we know that it exists ε_0 such that:

$$W_h(y) \ge \frac{\mu''(\zeta_0)}{4} |y|^2 h, \quad \text{for } |y| \le \varepsilon_0 h^{-1/2}.$$
 (4.17)

(ii) With $\eta_0 := \min\{\mu(\zeta_0 \pm \varepsilon_0)\} - \Theta_0$, we have $W_h(y) \ge \eta_0 > 0$ for $|y| \ge \varepsilon_0 h^{-1/2}$. We deduce from (i) and (ii) that

$$W_h(y) \ge \min \left\{ \eta_0, \ \frac{\mu''(\zeta_0)}{4} C_0^2 h \right\} \quad \text{if} \quad |y| \ge C_0.$$

Therefore, using Remark 4.4 and choosing C_0 large enough, and h small enough we get the existence of c > 0 such that, for $|y| \ge C_0$:

$$W_h(y) - h - \mathfrak{s}_n(h) \ge ch. \tag{4.18}$$

Combining this with (4.16), we obtain:

$$ch \int_{|y| \ge C_0} |e^{\Phi}v|^2 dy dz \le \int_{|y| \le C_0} |W_h - h - \mathfrak{s}_n(h)| |e^{\Phi}v|^2 dy dz.$$

Then we take advantage of Remark 4.4 and bound $W_h(y)$ for $|y| \le C_0$ by C'_0h for a suitable constant C'_0 to deduce finally

$$ch \int_{|y|>C_0} |e^{\Phi}v|^2 dy dz \le Ch ||v||_{L^2(\Omega)}^2.$$

Thus we have proved (4.14) for $v = \mathbf{u}_n(h)$, $1 \le n \le N_0$. Using the orthogonality of the eigenvectors $\mathbf{u}_n(h)$, we obtain (4.14) for $v \in \mathfrak{E}_{N_0}(h)$.

Combining Propositions 4.5 and 4.6, we get the following two corollaries:

Corollary 4.7 There exist C > 0, $\delta > 0$ and $h_0 > 0$ such that for all $h \in (0, h_0)$ and $v \in \mathfrak{E}_{N_0}(h)$:

$$\int_{\Omega} e^{\delta(|y|+z)} |v|^2 dy dz \le C ||v||_{L^2(\Omega)}^2,$$

and in particular:

$$\int_{\Omega} (1+z|y|^3+y^6)|v|^2 dy dz \le C||v||_{L^2(\Omega)}^2.$$
(4.19)

Corollary 4.8 For all $\varepsilon_0 > 0$, there exist $h_0 > 0$, $\gamma > 0$ and C > 0 such that, for all $h \in (0, h_0)$ and $v \in \mathfrak{E}_{N_0}(h)$:

$$\int_{|y| > \varepsilon_0 h^{-1/2}} (1 + |y|^4) |v|^2 \, \mathrm{d}y \, \mathrm{d}z \le C e^{-\gamma h^{-1/2}} ||v||_{L^2(\Omega)}^2.$$

4.2.2 Approximation of eigenvectors

We will consider the projection $\Pi_0: L^2(\Omega) \to L^2(\mathbb{R}_y) \otimes \operatorname{span}\{v_{\zeta_0}\}$ defined by

$$w \longmapsto \langle w, v_{\zeta_0} \rangle_{L^2(\mathbb{R}_{+,z})} v_{\zeta_0}$$
.

The aim of the following proposition is to approximate $u_n(h)$ by a tensor product:

Proposition 4.9 There exists C > 0 and $h_0 > 0$ such that for all $h \in (0, h_0)$:

$$Q(\mathbf{u}_{n}(h) - \Pi_{0}\mathbf{u}_{n}(h)) \leq Ch^{1/2}\|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2},$$

$$Q(D_{y}\mathbf{u}_{n}(h) - \Pi_{0}D_{y}\mathbf{u}_{n}(h)) \leq Ch^{1/4}\|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2},$$

$$Q(y\mathbf{u}_{n}(h) - \Pi_{0}y\mathbf{u}_{n}(h)) \leq Ch^{1/2}\|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2},$$

where Q is the quadratic form of $Id_{L^2(\mathbb{R}_y)} \otimes (H_{\zeta_0} - \Theta_0)$.

Proof: 1) We first notice that, since Θ_0 is the first eigenvalue of H_{ζ_0} , the quadratic form Q is non-negative: $Q(w) \geq 0$ for all $w \in L^2(\mathbb{R}_y) \otimes B^1(\mathbb{R}_+)$.

2) We also notice that, since v_{ζ_0} generates the kernel of $H_{\zeta_0} - \Theta_0$, there holds

$$Q(w) = Q(w - \Pi_0 w), \quad \forall w \in L^2(\mathbb{R}_y) \otimes B^1(\mathbb{R}_+).$$

Hence we only have to bound $Q(\mathbf{u}_n(h))$, $Q(D_y\mathbf{u}_n(h))$, and $Q(y\mathbf{u}_n(h))$.

3) Using the equation satisfied by $\mathbf{u}_n(h)$:

$$\mathfrak{L}_h \mathfrak{u}_n(h) = \mathfrak{s}_n(h)\mathfrak{u}_n(h), \tag{4.20}$$

and taking the scalar product with $\mathbf{u}_n(h)$ we find the identity

$$h\|D_{y}\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2} + Q(\mathbf{u}_{n}(h))$$
$$-2h^{1/2}\langle (z-\zeta_{0})y\mathbf{u}_{n}(h),\mathbf{u}_{n}(h)\rangle + h\|y\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2} = \mathbf{s}_{n}(h)\|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2}.$$

With (4.10) and (4.19), we deduce

$$Q(\mathbf{u}_n(h)) \le Ch^{1/2} \|\mathbf{u}_n(h)\|_{L^2(\Omega)}^2.$$

4) Considering again the scalar product of identity (4.20) with $u_n(h)$, we observe that, using (4.10) and (4.11):

$$||D_y \mathbf{u}_n(h)||_{L^2(\Omega)}^2 \le C ||\mathbf{u}_n(h)||_{L^2(\Omega)}^2. \tag{4.21}$$

Moreover, calculating the derivative with respect to y of (4.20), we obtain:

$$\mathfrak{L}_h D_y \mathfrak{u}_n(h) + 2ih^{1/2} (z - \zeta_0 - yh^{1/2}) \mathfrak{u}_n(h) = \mathfrak{s}_n(h) D_y \mathfrak{u}_n(h)$$

$$\tag{4.22}$$

and taking the scalar product with $D_y \mathbf{u}_n(h)$, we get:

$$||D_y^2 \mathbf{u}_n(h)||_{L^2(\Omega)}^2 \le Ch^{-1/2} ||\mathbf{u}_n(h)||_{L^2(\Omega)}^2, \tag{4.23}$$

where we have used (4.19) to control the commutator term.

Considering once more the scalar product of (4.22) with $D_y \mathbf{u}_n(h)$, we infer:

$$h\|D_{y}^{2}\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2} + Q(D_{y}\mathbf{u}_{n}(h)) + 2ih^{1/2}\langle(z - \zeta_{0} - yh^{1/2})\mathbf{u}_{n}(h), D_{y}\mathbf{u}_{n}(h)\rangle$$
$$-2h^{1/2}\langle(z - \zeta_{0})yD_{y}\mathbf{u}_{n}(h), D_{y}\mathbf{u}_{n}(h)\rangle + h\|yD_{y}\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2} = \mathbf{s}_{n}(h)\|D_{y}\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2}.$$

With the help of (4.19), (4.21), (4.23) and integration by parts, we find

$$Q(D_y \mathbf{u}_n(h)) \le Ch^{1/4} \|\mathbf{u}_n(h)\|_{L^2(\Omega)}^2$$
.

5) Similarly, we multiply (4.20) by y and find the identity

$$\mathfrak{L}_h(y\mathfrak{u}_n(h)) + 2h\partial_y\mathfrak{u}_n(h) = \mathfrak{s}_n(h)y\mathfrak{u}_n(h), \tag{4.24}$$

from which we deduce

$$\begin{split} h\|D_{y}(y\mathbf{u}_{n}(h))\|_{L^{2}(\Omega)}^{2} + Q(y\mathbf{u}_{n}(h)) + 2h\langle\partial_{y}\mathbf{u}_{n}(h), y\mathbf{u}_{n}(h)\rangle \\ - 2h^{1/2}\langle(z - \zeta_{0})y^{2}\mathbf{u}_{n}(h), y\mathbf{u}_{n}(h)\rangle + h\|y^{2}\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2} = \mathbf{s}_{n}(h)\|y\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}^{2}. \end{split}$$

We obtain finally

$$Q(y\mathbf{u}_n(h)) \le Ch^{1/2} \|\mathbf{u}_n(h)\|_{L^2(\Omega)}^2,$$

which concludes the proof.

Corollary 4.10 There exist C > 0 and $h_0 > 0$ such that for all $h \in (0, h_0)$ and $v \in \mathfrak{E}_{N_0}(h)$:

$$||v - \Pi_0 v||_{H^1(\Omega)} + ||yv - \Pi_0 yv||_{L^2(\Omega)} \le Ch^{1/8} ||v||_{L^2(\Omega)}.$$
(4.25)

Proof: Let us assume that $w \in L^2(\mathbb{R}_y) \otimes B^1(\mathbb{R}_+)$ is such that: $\langle w, v_{\zeta_0} \rangle_{L^2(\mathbb{R}_+,z)} = 0$. Then, we get:

$$Q(w) \ge (\mu_2(\zeta_0) - \Theta_0) \|w\|_{L^2(\Omega)}^2,$$

where $\mu_2(\zeta_0)$ denotes the second eigenvalue of H_{ζ_0} . Therefore the left-hand side of (4.25) is bounded by $(\mu_2(\zeta_0) - \Theta_0)^{-1} \{Q(w) + Q(D_y w) + Q(yw)\}$. Then, the conclusion follows from Proposition 4.9.

Corollary 4.11 There exists $h_0 > 0$ such that for $h \in (0, h_0)$, the projection Π_0 is an isomorphism from $\mathfrak{E}_{N_0}(h)$ onto its range.

4.2.3 Conclusion

For all $v \in \mathfrak{E}_{N_0}(h)$, we have

$$\langle (hD_y^2 + \mu(\zeta_0 + yh^{1/2}) - \Theta_0)v, v \rangle \leq \mathfrak{s}_{N_0}(h) ||v||_{L^2(\Omega)}^2.$$

We recall (1.3) and we have, with Corollary 4.8:

$$\int_{|y| \ge \varepsilon_0 h^{-1/2}} \left| \left(\mu(yh^{1/2} + \zeta_0) - \Theta_0 - h \frac{\mu''(\zeta_0)}{2} y^2 \right) v \right|^2 dy dz = \mathcal{O}(h^\infty) \|v\|_{L^2(\Omega)}^2,$$

and, by a Taylor approximation (using that μ is smooth):

$$\int_{|y| \le \varepsilon_0 h^{-1/2}} \left| \left(\mu(yh^{1/2} + \zeta_0) - \Theta_0 - h \frac{\mu''(\zeta_0)}{2} y^2 \right) v \right|^2 dy dz \le C(\varepsilon_0) \|y^3 h^{3/2} v\|_{L^2(\Omega)}^2
\le \tilde{C}(\varepsilon_0) h^3 \|v\|_{L^2(\Omega)}^2,$$

the last inequality coming from (4.19). We get:

$$h\left\langle \left(D_y^2 + \frac{\mu''(\zeta_0)}{2}y^2\right)v, v\right\rangle - Ch^{3/2}\|v\|_{L^2(\Omega)}^2 \le \mathfrak{s}_{N_0}(h)\|v\|_{L^2(\Omega)}^2.$$

Applying Corollary 4.10, we obtain for all $v \in \mathfrak{E}_{N_0}(h)$:

$$h\left\langle \left(D_y^2 + \frac{\mu''(\zeta_0)}{2}y^2\right)\Pi_0v, \Pi_0v\right\rangle - Ch^{9/8}\|\Pi_0v\|_{L^2(\Omega)}^2 \le \mathfrak{s}_{N_0}(h)\|\Pi_0v\|_{L^2(\Omega)}^2.$$

With Corollary 4.11 and the min-max principle, we infer that:

$$h(2N_0 - 1)\sqrt{\frac{\mu''(\zeta_0)}{2}} - Ch^{9/8} \le \mathfrak{s}_{N_0}(h)$$

and thus k(n) = n in Proposition 4.3. This ends the proof of Theorem 4.1.

4.3 Eigenvector asymptotics

From Theorem 4.1, we obtain that the gap between the eigenvalues is of order h. Thus, combining the construction of section 4.1 with the spectral theorem (see [22, Lemmas 12-13, Section 9]), we can deduce approximation results for the eigenfunctions $\mathbf{u}_n(h)$ of \mathfrak{L}_h . Let us denote by $\tilde{\mathbf{u}}_n^{\flat}(h)$ and $\tilde{\mathbf{u}}_n^{\sharp}(h)$ the n-th quasimode with one and two terms, respectively, constructed in section 4.1: We recall

$$\tilde{\mathbf{u}}_{n}^{\flat}(h)(y,z) = f_{n}(y) \, v_{\zeta_{0}}(z),
\tilde{\mathbf{u}}_{n}^{\sharp}(h)(y,z) = f_{n}(y) \, v_{\zeta_{0}}(z) + h^{1/2} y f_{n}(y) \, \partial_{\zeta} v_{\zeta} \big|_{\zeta = \zeta_{0}}(z).$$
(4.26)

Here f_n is the *n*-th eigenfunction of the harmonic oscillator H_{harm} cf. (4.7). It is straightforward that we can take

$$f_n(y) = \psi_{n-1} \left(\left[\frac{\mu''(\zeta_0)}{2} \right]^{1/4} y \right), \quad n \ge 1,$$
 (4.27)

with ψ_m the Hermite function of rank m. Then there exists an eigenmode $\mathfrak{u}_n(h)$ such that

$$\|\mathbf{u}_{n}(h) - \tilde{\mathbf{u}}_{n}^{\flat}(h)\|_{L^{2}(\Omega)} \leq C h^{1/2} \|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)},$$
and
$$\|\mathbf{u}_{n}(h) - \tilde{\mathbf{u}}_{n}^{\sharp}(h)\|_{L^{2}(\Omega)} \leq C h \|\mathbf{u}_{n}(h)\|_{L^{2}(\Omega)}.$$
(4.28)

Setting

$$\tilde{u}_{n,\theta}^{\flat}(s,t) = \tilde{\mathbf{u}}_{n}^{\flat}(h)(y,z) \quad \text{and} \quad \tilde{u}_{n,\theta}^{\sharp}(s,t) = \tilde{\mathbf{u}}_{n}^{\sharp}(h)(y,z),$$
 (4.29)

with $h = \tan \theta$ and (s, t) given by the change of variables (3.3), we obtain quasimodes for \mathcal{L}_{θ} which satisfy, for suitable eigenvectors $u_{n,\theta}$ of \mathcal{L}_{θ}

$$\|u_{n,\theta} - \tilde{u}_{n,\theta}^{\flat}\|_{L^{2}(\Omega)} \le C \,\theta^{1/2} \|u_{n,\theta}\|_{L^{2}(\Omega)} \quad \text{and} \quad \|u_{n,\theta} - \tilde{u}_{n,\theta}^{\sharp}\|_{L^{2}(\Omega)} \le C \,\theta \|u_{n,\theta}\|_{L^{2}(\Omega)}. \tag{4.30}$$

5 Finite element computation of eigenpairs

In this section, we illustrate theoretical results given by Theorems 1.3, 1.4 on isotropic and anisotropic decay of the eigenvectors of \mathcal{L}_{θ} . We also show computations of the eigenvalues which enhance the eigenvalue asymptotics given by Theorem 1.6.

The simulations have been realized with the Finite Element Library MÉLINA, see [14].

5.1 Eigenvalues

We illustrate here the behavior of the first eigenvalues of \mathcal{L}_{θ} . The operator \mathcal{L}_{θ} is defined on an infinite domain Ω . We have to bound this infinite domain by a large box $R_{a,b,c} := (-a,b) \times (0,c)$ to make numerical approximations possible. The eigenvalues

of the problem set in the bounded domain have to be close to those of the original problem; the convergence is expected as a,b,c tend to infinity. Numerically, we compute the eigenvalues denoted by $\sigma_n(\theta;a,b,c)$ of the operator $\mathcal{L}_{\theta}(a,b,c) = -\Delta + V_{\theta}$ on $R_{a,b,c}$ with Neumann condition on t=0 and Dirichlet conditions on the artificial boundary $\{s=-a\} \cup \{s=b\} \cup \{t=c\}$. Using the inclusion of the form domain of $\mathcal{L}_{\theta}(a,b,c)$ in that of \mathcal{L}_{θ} , we prove

$$\sigma_n(\theta) \leq \sigma_n(\theta; a, b, c).$$

Furthermore, by similar arguments, we obtain the monotonicity of $\sigma_n(\theta; a, b, c)$ according to each variable a, b or c.

Figure 1 gives an approximation of the first 12 eigenvalues of \mathcal{L}_{θ} below 1. For this, we compute the first 12 eigenvalues of $\mathcal{L}_{\theta}(a,a,a)$ with $\theta \in \{\vartheta\pi/2, \vartheta = k/100, 1 \leq k \leq 99\}$ and $a \in \{10n, n = 1, \ldots, 10\}$ by using a finite element method with square elements of degree \mathbb{Q}_{10} in each direction. We have performed computations with 10 or 15 elements in each direction.

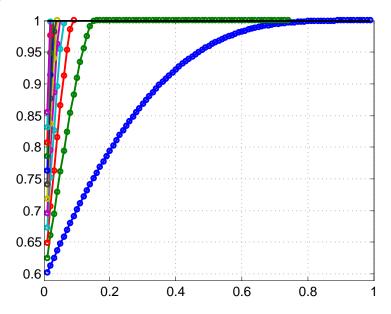


Figure 1: Approximation of $\sigma_n(\theta)$ for $\theta = \vartheta \pi/2$ with $\vartheta \in \{k/100, 1 \le k \le 99\}$.

By looking at Figure 1, we can conjecture that the derivative of $\sigma_1(\theta)$ tends to zero when θ goes to $\frac{\pi}{2}$. This is true indeed, as we prove in the following proposition:

Proposition 5.1 For all $\theta \in (0, \frac{\pi}{2})$, we have:

$$\sigma_1(\theta)\cos\theta - \sigma_1'(\theta)\sin\theta > 0.$$

Moreover, we have:

$$\lim_{\substack{\theta \to \frac{\pi}{2} \\ \theta < \frac{\pi}{2}}} \sigma'_1(\theta) = 0.$$

Proof: For $\gamma \geq 0$, we introduce the operator:

$$\mathcal{L}(\theta, \gamma) = D_s^2 + D_t^2 + (t(\cos \theta + \gamma) - s\sin \theta)^2$$

and we denote by $\sigma_1(\theta,\gamma)$ the bottom of its spectrum. Let $\rho>0$ and $\alpha\in(0,\frac{\pi}{2})$ satisfy

$$\cos \theta + \gamma = \rho \cos \alpha$$
 and $\sin \theta = \rho \sin \alpha$.

We perform the rescaling $t=\rho^{-1/2}\hat{t},\ s=\rho^{-1/2}\hat{s}$ and obtain that $\mathcal{L}(\theta,\gamma)$ is unitarily equivalent to:

$$\rho(D_{\hat{s}}^2 + D_{\hat{t}}^2 + (\hat{t}\cos\alpha - \hat{s}\sin\alpha)^2) = \rho\mathcal{L}_{\alpha}.$$

In particular, we observe that $\sigma_1(\theta, \gamma) = \rho \sigma_1(\alpha)$ is a simple eigenvalue: there holds

$$\sigma_1(\theta, \gamma) = \sqrt{(\cos \theta + \gamma)^2 + \sin^2 \theta} \ \sigma_1 \left(\arctan\left(\frac{\sin \theta}{\cos \theta + \gamma}\right)\right).$$
 (5.1)

Performing the rescaling $\tilde{t} = (\cos \theta + \gamma)t$, we get the operator $\tilde{\mathcal{L}}(\theta, \gamma)$ which is unitarily equivalent to $\mathcal{L}(\theta, \gamma)$:

$$\tilde{\mathcal{L}}(\theta, \gamma) = D_s^2 + (\cos \theta + \gamma)^2 D_{\tilde{t}}^2 + (\tilde{t} - s \sin \theta)^2.$$

We observe that the domain of $\tilde{\mathcal{L}}(\theta, \gamma)$ does not depend on $\gamma \geq 0$. Denoting by $\tilde{u}_{\theta, \gamma}$ the L^2 -normalized and positive eigenfunction of $\tilde{\mathcal{L}}(\theta, \gamma)$ associated with $\sigma_1(\theta, \gamma)$, we write:

$$\tilde{\mathcal{L}}(\theta, \gamma)\tilde{u}_{\theta, \gamma} = \sigma_1(\theta, \gamma)\tilde{u}_{\theta, \gamma}.$$

Taking the derivative with respect to γ , multiplying by $\tilde{u}_{\theta,\gamma}$ and integrating, we get the Feynman-Hellman formula:

$$\partial_{\gamma}\sigma_1(\theta,\gamma) = 2(\cos\theta + \gamma) \int_{\Omega} |D_t \tilde{u}_{\theta,\gamma}|^2 ds dt \ge 0.$$

We deduce that, if $\partial_{\gamma}\sigma_1(\theta,\gamma)=0$, then $D_t\tilde{u}_{\theta,\gamma}=0$ and $\tilde{u}_{\theta,\gamma}$ only depends on s, which is a contradiction with $\tilde{u}_{\theta,\gamma}\in L^2(\Omega)$. Consequently, we have $\partial_{\gamma}\sigma_1(\theta,\gamma)>0$ for any $\gamma\geq 0$. An easy computation using formula (5.1) provides:

$$\partial_{\gamma}\sigma_1(\theta,0) = \sigma_1(\theta)\cos\theta - \sigma_1'(\theta)\sin\theta.$$

As recalled in Subsection 1.1, the function σ_1 is analytic and increasing. Thus we deduce:

$$\forall \theta \in \left(0, \frac{\pi}{2}\right), \qquad 0 \le \sigma_1'(\theta) < \frac{\cos \theta}{\sin \theta} \sigma_1(\theta).$$

We get:

$$0 \le \liminf_{\substack{\theta \to \frac{\pi}{2} \\ \theta < \frac{\pi}{2}}} \sigma'_1(\theta) \le \limsup_{\substack{\theta \to \frac{\pi}{2} \\ \theta < \frac{\pi}{2}}} \sigma'_1(\theta) \le 0,$$

which ends the proof.

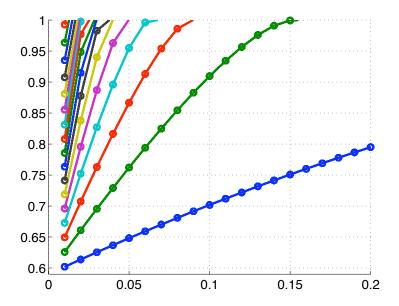


Figure 2: Approximations of $\sigma_n(\theta)$ for $\theta = \vartheta \pi/2$ with $\vartheta \in \{k/100, 1 \le k \le 20\}$.

Figure 2 gives an approximation of the first eigenvalues of \mathcal{L}_{θ} for small θ . For this, we compute the eigenvalues of $\mathcal{L}_{\theta}(a,a,c)$ with square 20×20 elements and degree \mathbb{Q}_{10} . Figure 2 shows the computations on the rectangle $[-100,100]\times[0,50]$ when $\theta=\vartheta\pi/2,\vartheta\in\{k/100,1\leq k\leq 10\}$ and on $[-100,100]\times[0,100]$ when $\theta=\vartheta\pi/2,\vartheta\in\{k/100,10\leq k\leq 20\}$. The figure corroborates the densification of the spectrum in $[\Theta_0,1]$ described in Section 3.

We now illustrate formula (1.8). According to this formula, we have the convergence:

$$\frac{\sigma_n(\theta) - \Theta_0}{a_1 \theta} \to 2n - 1 \quad \text{as} \quad \theta \to 0, \quad \text{with} \quad a_1 = \sqrt{\frac{\mu''(\zeta_0)}{2}}, \tag{5.2}$$

for all $n \ge 1$. Using numerical computations for H_{ζ} , we find good approximations of Θ_0 and a_1 , cf. Tables 1-2 in [4]:

$$\label{eq:tildeG0} \breve{\Theta}_0 = 0.590106125 \quad \text{and} \quad \breve{a}_1 \simeq 0.7651881.$$

Let us denote by $\check{\sigma}_n(\theta)$ the *n*-th computed eigenvalue of \mathcal{L}_{θ} , with a convenient choice of the computational domain $(-a,b)\times(0,c)$. On Figure 3 we represent the functions

$$\log 10(\vartheta) \longmapsto \rho_{n,1}(\theta) := \frac{\breve{\sigma}_n(\theta) - \breve{\Theta}_0}{\breve{a}_1 \theta}$$
 (5.3)

where we recall that $\vartheta = 2\theta/\pi$.

We can see that the ratio $\rho_{n,1}(\theta)$ converges to 2n-1, corroborating formula (5.2).

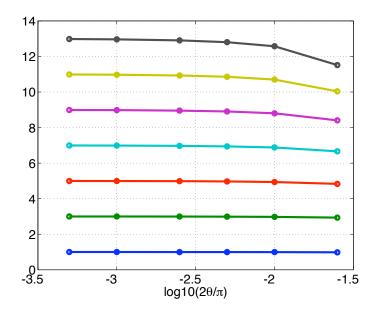


Figure 3: Convergence of the ratio $\rho_{n,1}(\theta)$ as $\theta \to 0$, $n = 1, \dots, 7$ (bottom to top).

Computations displayed in Figures 4 and 5 allow to conjecture the next terms of the asymptotic expansion for $\sigma_n(\theta)$. Indeed on Figure 4 we represent the functions

$$\log 10(\vartheta) \longmapsto \rho_{n,2}(\theta) := \frac{\breve{\Theta}_0 + \breve{a}_1(2n-1)\theta - \breve{\sigma}_n(\theta)}{\theta^2} . \tag{5.4}$$

We observe that the ratio $\rho_{n,2}(\theta)$ converges to a numerical limit $\check{a}_{n,2}$ as $\theta \to 0$ for any $n=1,\ldots,7$, see Table 1.

n	1	2	3	4	5	6	7
$\breve{a}_{n,2}$	0.32616	1.1577	2.8206	5.3148	8.6402	12.797	17.784

Table 1: Numerical limits $\breve{a}_{n,2}$.

Thus we are lead to conjecture that $\sigma_n(\theta)$ admits an expansion of the form:

$$\sigma_n(\theta) = \Theta_0 + a_1(2n-1)\theta - a_{n,2}\theta^2 + o(\theta^2).$$

We can still determine numerically the next term of the expansion. On Figure 5 we represent the functions

$$\log 10(\theta) \longmapsto \rho_{n,3}(\theta) := \frac{\check{\Theta}_0 + \check{a}_1(2n-1)\theta - \check{a}_{n,2}\theta^2 - \check{\sigma}_n(\theta)}{\theta^3} . \tag{5.5}$$

Figure 5 encourages to conjecture the following asymptotic expansion:

$$\sigma_n(\theta) = \Theta_0 + a_1(2n-1)\theta - a_{n,2}\theta^2 - a_{n,3}\theta^3 + o(\theta^3).$$

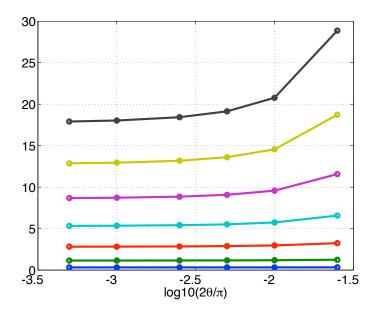


Figure 4: Convergence of $\rho_{n,2}(\theta)$ as $\theta \to 0$, $n=1,\ldots,7$ (bottom to top).

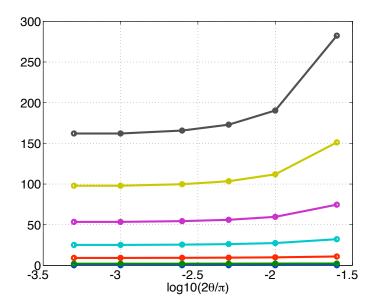


Figure 5: Convergence of $\rho_{n,3}(\theta)$ as $\theta \to 0$, $n=1,\ldots,7$ (bottom to top).

5.2 Eigenvectors

In this section, we highlight the isotropic exponential decay of the eigenvectors of \mathcal{L}_{θ} and the anisotropic one given respectively in Theorems 1.3 and 1.4. Figure 6 illustrates the anisotropic decay for θ close to $\pi/2$: we compute the first eigenpair of $\mathcal{L}_{\theta}(5,15,75)$ on $[-5,15]\times[0,75]$ for $\theta=\vartheta\pi/2$, $\vartheta=0.9,0.85,0.8,0.7$ with unit square elements of degree \mathbb{Q}_2 . The first eigenvector is localized along the line $V_{\theta}=0$ and we see the exponential decay far away from this line. When θ is close to $\pi/2$, the eigenvector spreads along the line $V_{\theta}=0$ and the exponential decay far away from the origin is not predominant.

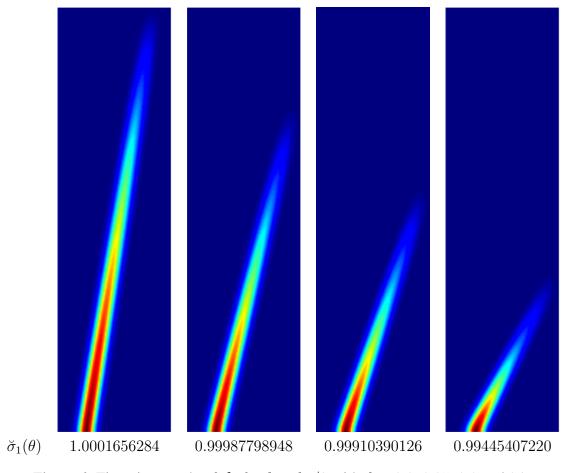


Figure 6: First eigenmode of \mathcal{L}_{θ} for $\theta = \vartheta \pi / 2$ with $\vartheta = 0.9, 0.85, 0.8$ and 0.7.

When $\theta = \vartheta \pi/2$ with $\vartheta \in \{0.1, \ldots, 0.6\}$, we observe equivalently the decay far away from the line $V_{\theta} = 0$ and the origin (see (1.4) and (1.5)). Figure 7 gives an approximation of the first eigenvector and eigenvalue of \mathcal{L}_{θ} on the computational domain $[-15, 25] \times [0, 15]$ with unit square elements of degree \mathbb{Q}_{6} . We observe also that the first eigenvector spreads less and less along the line $V_{\theta} = 0$ when θ is decreasing and the decay becomes essentially radial.

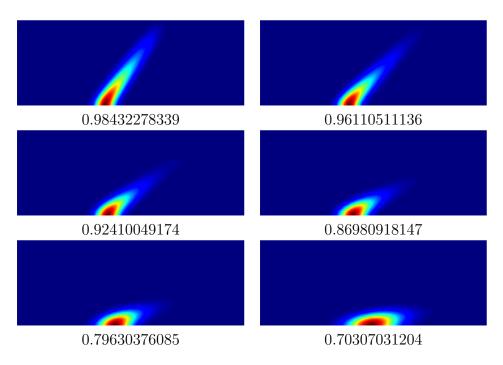


Figure 7: First eigenmode of \mathcal{L}_{θ} for $\theta = \vartheta \pi / 2$ with $\vartheta = 0.6, 0.5, 0.4, 0.3, 0.2$ and 0.1.

On Figure 8, 9, and 10 we consider the asymptotics $\theta \to 0$. Figure 8 gives an approximation of the first eight eigenmodes of \mathcal{L}_{θ} computed by a finite element method with rectangular 2×1 elements and degree \mathbb{Q}_{6} on the domain $[-20,80] \times [0,10]$. The oscillations with respect to the horizontal variable appear clearly. We can compare with Figures 9 and 10 where are represented the quasimodes $\tilde{u}_{n,\theta}^{\flat}$ and $\tilde{u}_{n,\theta}^{\sharp}$ introduced in (4.26)–(4.30). We observe an interesting correlation between the computed eigenvectors on Figure 8 and the quasimodes on Figures 9 and 10.

 $^{^1}$ To compute these quasimodes, we approximate the one-dimensional eigenvector v_{ζ_0} with a finite difference method for the operator $D_t^2+(t-\zeta_0)^2$ on [0,10] with Dirichlet condition on t=10, and $\zeta_0=0.76818365314$ according to computations of [4].

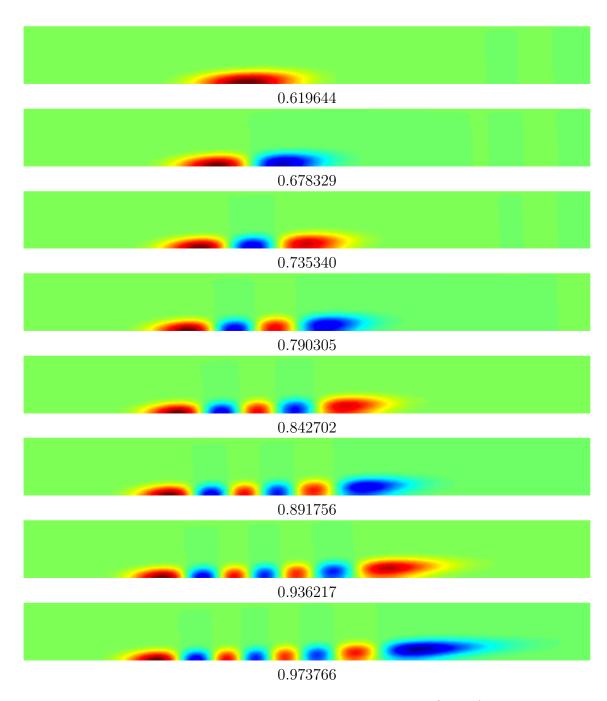


Figure 8: First 8 computed eigenvectors and eigenvalues of \mathcal{L}_{θ} for $\theta = 0.0125\pi$.

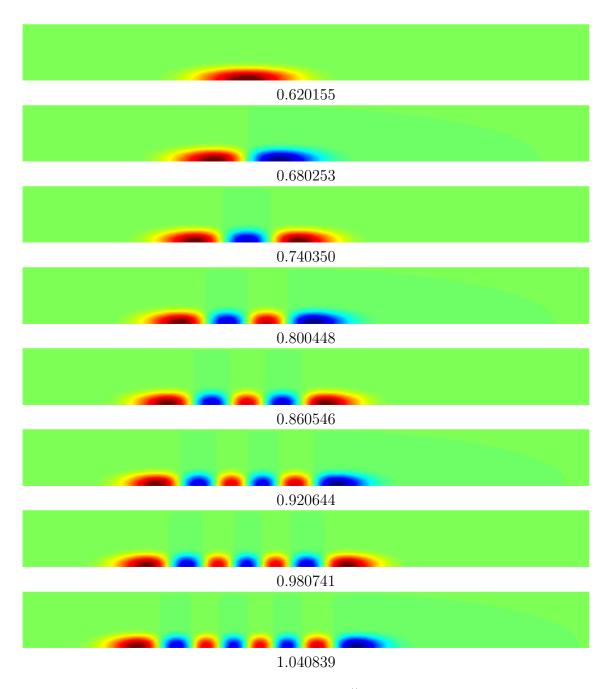


Figure 9: Quasimodes $\tilde{u}_{n,\theta}^{\flat}$ and quasieigenvalues $\Theta_0 + \breve{a}_1(2n-1)\theta$ for $\theta = 0.0125\pi$.

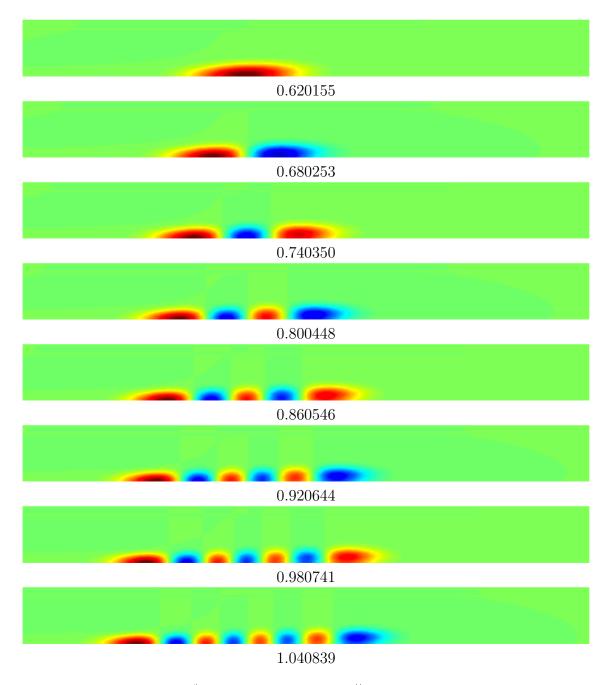


Figure 10: Quasimodes $\tilde{u}_{n,\theta}^{\sharp}$ and quasieigenvalues $\Theta_0 + \check{a}_1(2n-1)\theta$ for $\theta = 0.0125\pi$.

References

- [1] S. AGMON. Lectures on exponential decay of solutions of second-order elliptic equations: bounds on eigenfunctions of N-body Schrödinger operators, volume 29 of Mathematical Notes. Princeton University Press, Princeton, NJ 1982.
- [2] S. AGMON. Bounds on exponential decay of eigenfunctions of Schrödinger operators. In *Schrödinger operators (Como, 1984)*, volume 1159 of *Lecture Notes in Math.*, pages 1–38. Springer, Berlin 1985.
- [3] A. BERNOFF, P. STERNBERG. Onset of superconductivity in decreasing fields for general domains. *J. Math. Phys.* **39**(3) (1998) 1272–1284.
- [4] V. BONNAILLIE-NOËL. Harmonic oscillators with Neumann condition on the half-line. *In preparation* (2010).
- [5] B. CHENAUD, P. DUCLOS, P. FREITAS, D. KREJČIŘÍK. Geometrically induced discrete spectrum in curved tubes. *Differential Geom. Appl.* **23**(2) (2005) 95–105.
- [6] H. L. CYCON, R. G. FROESE, W. KIRSCH, B. SIMON. *Schrödinger operators with application to quantum mechanics and global geometry*. Texts and Monographs in Physics. Springer-Verlag, Berlin, study edition 1987.
- [7] M. DAUGE, B. HELFFER. Eigenvalues variation. I. Neumann problem for Sturm-Liouville operators. *J. Differential Equations* **104**(2) (1993) 243–262.
- [8] P. DUCLOS, P. EXNER. Curvature-induced bound states in quantum waveguides in two and three dimensions. *Rev. Math. Phys.* **7**(1) (1995) 73–102.
- [9] S. FOURNAIS, B. HELFFER. *Spectral methods in surface superconductivity*. Progress in Nonlinear Differential Equations and their Applications, 77. Birkhäuser Boston Inc., Boston, MA 2010.
- [10] B. HELFFER, A. MORAME. Magnetic bottles for the Neumann problem: the case of dimension 3. *Proc. Indian Acad. Sci. Math. Sci.* **112**(1) (2002) 71–84. Spectral and inverse spectral theory (Goa, 2000).
- [11] M. E. H. ISMAIL, R. ZHANG. On the Hellmann-Feynman theorem and the variation of zeros of certain special functions. *Adv. in Appl. Math.* **9**(4) (1988) 439–446.
- [12] T. KATO. *Perturbation theory for linear operators*. Classics in Mathematics. Springer-Verlag, Berlin 1995. Reprint of the 1980 edition.
- [13] K. Lu, X.-B. Pan. Surface nucleation of superconductivity in 3-dimensions. *J. Differential Equations* **168**(2) (2000) 386–452. Special issue in celebration of Jack K. Hale's 70th birthday, Part 2 (Atlanta, GA/Lisbon, 1998).

- [14] D. MARTIN. Mélina, bibliothèque de calculs éléments finis. http://anum-maths.univ-rennes1.fr/melina (2010).
- [15] A. MARTINEZ. Développements asymptotiques et effet tunnel dans l'approximation de Born-Oppenheimer. *Ann. Inst. H. Poincaré Phys. Théor.* **50**(3) (1989) 239–257.
- [16] A. MORAME, F. TRUC. Remarks on the spectrum of the Neumann problem with magnetic field in the half-space. *J. Math. Phys.* **46**(1) (2005) 012105, 13.
- [17] A. PERSSON. Bounds for the discrete part of the spectrum of a semi-bounded Schrödinger operator. *Math. Scand.* **8** (1960) 143–153.
- [18] N. RAYMOND. Sharp asymptotics for the Neumann Laplacian with variable magnetic field: case of dimension 2. *Ann. Henri Poincaré* **10**(1) (2009) 95–122.
- [19] N. RAYMOND. On the semi-classical 3D Neumann Laplacian with variable magnetic field. *Asymptotic Analysis* **68**(1-2) (2010) 1–40.
- [20] M. REED, B. SIMON. *Methods of modern mathematical physics. IV. Analysis of operators.* Academic Press [Harcourt Brace Jovanovich Publishers], New York 1978.
- [21] M. SCHATZMAN. *Analyse numérique*. InterEditions, Paris 1991. Cours et exercices pour la licence. [Course and exercises for the bachelor's degree].
- [22] M. I. VIŠIK, L. A. LJUSTERNIK. Regular degeneration and boundary layer for linear differential equations with small parameter. *Amer. Math. Soc. Transl.* (2) **20** (1962) 239–364.