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ON THE LOWEST ENERGY OF A 3D-MAGNETIC LAPLACIAN WITH AXISYMMETRICAL POTENTIAL

NICOLAS POPOFF

ABSTRACT. We study the bottom of the spectrum of a magnetic hamiltonian with axisymmetrical potential in \mathbb{R}^3 . The associated magnetic field is planar, unitary and non-constant. The problem reduces to a 1D-family of singular Sturm-Liouville operators on the half-line. We study to associated band functions and we compare it to the "de Gennes" operators arising in the study of a 2D-hamiltonian with monodimensional, odd and discontinuous magnetic field. We show in particular that the lowest energy is higher in dimension 3.

1. INTRODUCTION

1.1. **Problematic.** The action of a spatially inhomogeneous magnetic field on a two-dimensional electron gas has been the focus of several researches in the past decades (see [25] and [23] for example). Indeed a perpendicular magnetic field (modeled be a 2D-scalar vector field) modifies the transport properties of the electron gas (see [24] and also [13] for a more mathematical approach). In [29], the authors study among others the case of the magnetic field B^{ϵ} defined on \mathbb{R}^2 by $B^{\epsilon}(x, y) = \operatorname{sign}(x)$, this magnetic field follow the Iwatsuka model (see [20]): it is unidimensional and non-decreasing. Let $\mathbf{A}^{\epsilon}(x, y) := |x|$ be a magnetic potential satisfying curl $\mathbf{A}^{\epsilon} = B^{\epsilon}$ and

(1.1)
$$H_{\mathbf{A}^{\epsilon}} := (-i\nabla - \mathbf{A}^{\epsilon})^2 = D_x^2 + (D_y - |x|)^2$$

the associated hamiltonian with $D = -i\partial$. The discontinuity of the magnetic field can induce a quantum transport along the singularity called "edge current" and whose classical trajectory corresponds to the so-called *snake orbits* (see [29] for more references). Mathematical properties of the hamiltonian $H_{\mathbf{A}^{\epsilon}}$ for small electric perturbations are studied in [18] (see also [8] for a related hamiltonian on a half-plane). The bottom of the spectrum of the operator $H_{\mathbf{A}^{\epsilon}}$ is denoted by Θ_0 . This spectral quantity has been introduced in [30] for a problem coming from the modeling of the phenomenon of "surface superconductivity" (see also [2] or [14] for more references). The study of the spectrum of $H_{\mathbf{A}^{\epsilon}}$ leads to the 1D-parameter family of operators pencil

$$\mathbf{\mathfrak{h}}_{\tau} := -\partial_x^2 + (|x| - \tau)^2, \quad x \in \mathbb{R}$$

called the *de Gennes* operators (see Subsection 2.1 for references and former results). The bottom of the spectrum of such an operator family is called a "band function".

The aim of this article is to study the bottom of the spectrum of a hamiltonian associated to a planar inhomogeneous magnetic field of \mathbb{R}^3 whose associated magnetic potential is axisymmetrical. Let us denote by (r, θ, z) the cylindrical coordinates of \mathbb{R}^3 . If the magnetic

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potential has the shape $\mathbf{A}(r, \theta, z) = (0, 0, A(r))$ with A convenient, the classical trajectories of a particle in the associated magnetic field are described in [31, Section 3]. The spectrum and the scattering properties of such hamiltonians are also studied in [32]. The particular case of a magnetic potential created by an infinite rectilinear current in the z direction is studied in [31]: the spectrum of $P_{\mathbf{A},\mathbb{R}^3_+}$ is the half-line \mathbb{R}_+ and the band functions are increasing from 0 to $+\infty$. In this article we are interested to another 3D-hamiltonian with axisymmetrical potential and we show that its spectrum has very different properties that the one studied in [31].

We define in \mathbb{R}^3 the magnetic potential

$$\mathcal{A}(x, y, z) := (0, 0, \sqrt{x^2 + y^2})$$

The associated magnetic field $\mathcal{B} := \operatorname{curl} \mathcal{A}$ satisfies $\mathcal{B}(x, y, z) = (\sin \theta, -\cos \theta, 0)$. This magnetic field is unitary and non-constant and its field lines are circles centered at the origin. The restriction of the magnetic field \mathcal{B} to a plane of the form $\{y = ax\}$ with $a \in \mathbb{R}$ has the shape of the magnetic field B^{ϵ} associated to the hamiltonian (1.1). Let

$$H_{\mathcal{A}} := (-i\nabla - \mathcal{A})^2 = D_x^2 + D_y^2 + (D_z - \sqrt{x^2 + y^2})^2$$

be the hamiltonian associated to the magnetic field \mathcal{B} acting on $L^2(\mathbb{R}^3)$ and

(1.2)
$$\Xi_0 := \inf \mathfrak{S}(H_{\mathcal{A}})$$

its lowest energy, where $\mathfrak{S}(\mathcal{L})$ denotes the spectrum of a self-adjoint operator \mathcal{L} . One of our goals is to compare Ξ_0 with the lowest energy Θ_0 of the hamiltonian $H_{\mathbf{A}^{\epsilon}}$ defined in (1.1). Let \mathcal{F}_z be the partial Fourier transform in the z-variable. We have the direct integral decomposition (see [28]):

(1.3)
$$\mathcal{F}_{z}^{*}H_{\mathcal{A}}\mathcal{F}_{z} = \int_{\tau\in\mathbb{R}}^{\oplus} \mathfrak{h}_{\tau}^{2\mathrm{d}} \,\mathrm{d}\tau$$

with

$$\label{eq:basic_states} \mathbf{\mathfrak{h}}_{\tau}^{\rm 2d} := -\Delta + (\|x\| - \tau)^2, \quad x \in \mathbb{R}^2$$

where ||x|| denotes the euclidean norm of \mathbb{R}^2 . The operator \mathfrak{h}_{τ}^{2d} has compact resolvent and we denote by $\lambda_1(\tau)$ its first eigenvalue. This operator can be seen as a 2D-version of the operator \mathfrak{h}_{τ} arising in the study of $H_{\mathbf{A}^{\epsilon}}$. Using (1.3) we have the fundamental relation

$$\Xi_0 = \inf_{\tau \in \mathbb{R}} \lambda_1(\tau)$$

The restriction of \mathfrak{h}_{τ}^{2d} to axisymmetrical functions reduces the problem to the singular 1Doperator \mathfrak{g}_{τ} introduced in Subsection 2.2. We denote by $(\zeta_n(\tau))_{n\in\mathbb{N}^*}$ the spectrum of this operator and we have $\zeta_1(\tau) = \lambda_1(\tau)$. We are interested in the description of the first "band function" ζ_1 and of its infimum Ξ_0 . We are also interested in comparisons with the spectral quantities associated to the operator \mathfrak{h}_{τ} coming from the study of the hamiltonian $H_{\mathbf{A}^{\epsilon}}$ defined in (1.1).

Let us notice that the family of operators $(\mathfrak{h}_{\tau}^{2d})_{\tau \in \mathbb{R}}$ appears also in the asymptotic analysis of the Neumann magnetic Laplacian with constant magnetic on an infinite wedge of small opening, provided that the magnetic field is not tangent to the plane of symmetry of the wedge (see [26, Section 6.1] and [27]).

1.2. Contents and main results. In Section 2 we reduce the problem to a family of singular 1D-Sturm-Liouville operators $(\mathbf{g}_{\tau})_{\tau \in \mathbb{R}}$ on the half-line. We study the eigenvalues of this 1D-operators: we show that the first eigenvalue reaches its infimum Ξ_0 and we provide an upper bound. In Section 3 we give a formula for the derivative of the eigenvalues of \mathbf{g}_{τ} with respect to τ and we use it to show that $\Theta_0 < \Xi_0$. In Annex A we give numerical computations.

2. DESCRIPTION OF THE 1D OPERATORS

2.1. The de Gennes operator. We first recall known results about the de Gennes operator arising in the study of the hamiltonian H_A defined in (1.1). Let \mathcal{F}_y be the partial Fourier transform in the y-variable. We have the following direct integral decomposition

(2.1)
$$\mathcal{F}_{y}^{*}H_{\mathbf{A}^{\epsilon}}\mathcal{F}_{y} := \int_{\tau \in \mathbb{R}}^{\bigoplus} \mathfrak{h}_{\tau} \,\mathrm{d}\tau$$

where

$$\mathbf{\mathfrak{h}}_{\tau} := -\partial_x^2 + (|x| - \tau)^2, \quad x \in \mathbb{R}$$

This operator has compact resolvent and we denote by $\mu_n(\tau)$ its *n*-th eigenvalue. Let $\mathfrak{h}_{\tau}^{\mathrm{N}}$ (resp. $\mathfrak{h}_{\tau}^{\mathrm{D}}$) be the operator $\partial_x^2 + (x - \tau)^2$ acting on $L^2(\mathbb{R}_+)$ with Neumann (resp. Dirichlet) boundary condition in x = 0. We denote by $\mu_n^{\mathrm{N}}(\tau)$ (resp. $\mu_n^{\mathrm{D}}(\tau)$) its *n*-eigenvalue. We have (see [14]) for all $n \ge 1$ that $\mu_{2n-1}(\tau) = \mu_n^{\mathrm{N}}(\tau)$ and $\mu_{2n}(\tau) = \mu_n^{\mathrm{D}}(\tau)$. When τ goes to $+\infty$, $\mu_n^{\mathrm{N}}(\tau)$ is exponentially close to the Landau level (see [15]):

(2.2)
$$\forall n \ge 1, \exists C > 0, \exists \tau_0, \forall \tau \ge \tau_0, \quad |\mu_n^{\mathsf{N}}(\tau) - (2n-1)| \le C e^{-\tau^2/2}$$

Let $u_{n,\tau}$ be a normalized eigenfunction of \mathfrak{h}_{τ}^{N} associated to $\mu_{n}^{N}(\tau)$. Using the technics from [10] and [4], it is known that

(2.3)
$$(\mu_n^N)'(\tau) = (\tau^2 - \mu_n^N(\tau))u_{n,\tau}^2(0)$$

and that there exists $\xi_0^n \in \mathbb{R}$ such that $\tau \mapsto \mu_n^N(\tau)$ is decreasing on $(-\infty, \xi_0^n)$ and increasing on $(\xi_0^n, +\infty)$. Moreover the unique minimum of μ_n^N is non-degenerate, and if we denote by $\xi_0 := \xi_0^1$ and $\Theta_0 := \inf_{\tau} \mu_1^N(\tau)$, (2.3) provides $\xi_0^2 = \Theta_0$. Using (2.1) we get $\inf_{\tau} \mathfrak{S}(H_{\mathbf{A}^{\epsilon}}) = \Theta_0$. Numerical computations (see [30], [9] or [6] for more rigorous analysis) show that $(\xi_0, \Theta_0) \approx$ (0.7682, 0.5901).

2.2. Reduction to a 1D-problem. We reduce the study of the first eigenvalue of \mathfrak{h}_{τ}^{2d} to a 1D-singular Sturm-Liouville operator on a weighted space. In the polar coordinate (r, ϕ) the operator \mathfrak{h}_{τ}^{2d} writes

$$-\partial_r^2 - \frac{1}{r}\partial_r - \frac{1}{r^2}\partial_\phi^2 + (r-\tau)^2 , \quad (r,\phi) \in \mathbb{R}_+ \times (-\pi,\pi)$$

The eigenfunctions associated to the first eigenvalue are axisymmetric therefore we restrict the operator to the functions that does not depend on the variable ϕ . Let $L_r^2(\mathbb{R}_+)$ be the space of the functions squared integrable on the half axis \mathbb{R}_+ for the weight $r \, dr$. We denote by

$$\langle u, v \rangle_{L^2_r(\mathbb{R}_+)} := \int_{\mathbb{R}_+} u(r) v(r) r \, \mathrm{d}r$$

the associated scalar product. Let $B_r^1(\mathbb{R}_+) := \{ u \in L^2_r, u' \in L^2_r(\mathbb{R}_+), ru \in L^2_r(\mathbb{R}_+) \}$. We define the operator

$$\mathbf{g}_{\tau} = -\partial_r^2 - \frac{1}{r}\partial_r + (r - \tau)^2$$

on the domain

$$Dom(\mathbf{g}_{\tau}) = \{ u \in B_r^1(\mathbb{R}_+), u'' \in L_r^2(\mathbb{R}_+), \frac{1}{\sqrt{r}} u \in L_r^2(\mathbb{R}_+), r^2 u \in L_r^2(\mathbb{R}_+), (ru'(r))|_{r=0} = 0 \}.$$

The operator \mathbf{g}_{τ} is unitary equivalent to the restriction of \mathbf{h}_{τ}^{2d} to axisymmetric functions of \mathbb{R}^2 . The form domain of \mathbf{g}_{τ} is $B_r^1(\mathbb{R}_+)$ and the associated quadratic form is

$$\mathbf{q}_{\tau}(u) := \int_{\mathbb{R}_{+}} \left(|u'(r)|^2 + r^2 |u(r)|^2 \right) r \, \mathrm{d}r$$

Using the results from [5] we get that the operator \mathbf{g}_{τ} has compact resolvent and we denote by $\zeta_n(\tau)$ its *n*-th eigenvalue. We have $\zeta_1(\tau) = \lambda_1(\tau)$ and

(2.4)
$$\Xi_0 = \inf_{\tau \in \mathbb{R}} \zeta_1(\tau)$$

moreover the $\zeta_n(\tau)$ corresponds to the eigenvalues of \mathfrak{h}_{τ}^{2d} which have axisymmetric eigenfunctions.

2.3. Elementary results about the spectrum of the 1D-operator. The boundary value problem associated to the eigenvalue $\zeta_n(\tau)$ is the following:

(2.5a)
$$\begin{cases} -ru''(r) - u'(r) + r(r-\tau)^2 u(r) = r\zeta_n(\tau)u(r), \quad r > 0, \end{cases}$$

(2.5b)
$$(ru'(r))_{|r=0} = 0$$

The EDO (2.5a) is singular and the point r = 0 is regular singular, therefore using Fuchs theory for EDO's (see [3] for example) and the boundary condition (2.5b) we get (see [26, Proposition 6.4] for more details):

Proposition 2.1. For all $\tau \in \mathbb{R}$ and for all $n \ge 1$, $\zeta_n(\tau)$ is a simple eigenvalue of \mathfrak{g}_{τ} . We denote by $z_{n,\tau}$ an associated eigenfunction. The function $z_{n,\tau}$ is the restriction on \mathbb{R}_+ of an analytic function on \mathbb{R} , moreover it satisfies the Neumann boundary condition

(2.6)
$$z'_{n,\tau}(0) = 0$$
.

Since the form domain of \mathbf{g}_{τ} does not depend on τ , we deduce from Kato's theory (see [21]) that all the $\zeta_n(\tau)$ are analytic with respect to τ . Moreover the Feynman-Hellmann ([19]) formula provides

(2.7)
$$\forall n \ge 1, \forall \tau \in \mathbb{R}, \quad \zeta'_n(\tau) = -2 \int_{\mathbb{R}_+} (r-\tau)^2 z_{n,\tau}(r) r \, \mathrm{d}r \; ,$$

and we deduce that for all $n \ge 1$, the function $\tau \mapsto \zeta_n(\tau)$ is decreasing on $(-\infty, 0)$.

In the special case $\tau = 0$, the operator \mathbf{g}_{τ} is also known as the Laguerre operator (see [1]) whose eigenvalues are known:

$$\forall n \ge 1, \quad \zeta_n(0) = 4n - 2.$$

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Remark 2.2. The eigenvalues of the 2D harmonic oscillator $-\Delta + |x|^2$ with $x \in \mathbb{R}^2$ are the even positive integers. Only the eigenspaces associated to eigenvalues of the form 4n - 2 have axisymmetric eigenfunctions.

• *Limit for large parameters.* Using the lower bound $(r - \tau)^2 \ge \tau^2$ for $\tau \le 0$ we deduce from the min-max principle that for all $\tau \le 0$ we have $\zeta_n(\tau) \ge \tau^2$ and therefore

(2.8)
$$\lim_{\tau \to -\infty} \zeta_n(\tau) = +\infty \; .$$

When τ goes to $+\infty$, as in the case of the de Gennes operator we expect that the eigenfunctions concentrate in the wells of the potential $(r - \tau)^2$ and therefore that the $\zeta_n(\tau)$ converge toward the Landau level (2n - 1) (see (2.2)). However we work in a weighted space and the harmonic approximation that consist in using the Hermite's functions as quasi-modes is not as good as in the case of the de Gennes operator:

Proposition 2.3. We have

$$\forall n \ge 1, \quad \lim_{\tau \to +\infty} \zeta_n(\tau) = 2n - 1 \quad and \quad \zeta_1(\tau) \stackrel{=}{\underset{\tau \to +\infty}{=}} 1 - \frac{1}{4\tau^2} + O\left(\frac{1}{\tau^3}\right)$$

Proof. The proof is elementary and we give the main lines. The details can be found in [26, Subsection 6.2.1]. First we take for quasi-modes the Hermite's functions centered in the wells $\{r = \tau\}$ and the min-max principle provides a rough upper bound. To get the lower bound, we use the technics of the semi-classical analysis (see [12, Theorem 4.23] for example): partition of the unity near and far the wells of the potential, IMS formula, comparison to the harmonic oscillator using Agmon estimates for the eigenfunctions. This gives $\zeta_n(\tau) \rightarrow 2n-1$ for large τ (see [26, Proposition 6.10]). The asymptotic expansion for $\zeta_1(\tau)$ needs a better quasi-mode construction: we first perform a change of variable $t = \frac{r^2}{2}$ in order to work in a unweighted space, then we construct suitable test-functions using the Hermite's functions (see [26, Proposition 6.11]) and we conclude with the spectral theorem.

Remark 2.4. In the case of a 2D-electron gas submitted to the magnetic field B^{ϵ} , the group velocity of the electron associated to the frequence τ is given by $-(\mu_1^N)'(\tau)$ (see [29, Section II]). Let us notice that unlike for the eigenvalues of the de Gennes operator (see (2.2)), the convergence of $\zeta_1(\tau)$ toward 1 is not exponential. Therefore we should expect different transport properties associated to a 3D-electron gas submitted to the magnetic field \mathcal{B} .

• *Existence of the minimum.* We can deduce that the function $\tau \mapsto \zeta_1(\tau)$ reaches its infimum. We provide an upper bound:

Proposition 2.5. We have

 $(2.9) \qquad \qquad \Xi_0 \leqslant \sqrt{4-\pi}$

and there exists $\tau^* \in \mathbb{R}$ such that $\Xi_0 = \zeta_1(\tau^*)$.

Proof. In order to get an upper bound we use gaussian quasi-modes: for $\rho > 0$ we define $u_{\rho}(r) := e^{-\rho r^2}$. Elementary computations show that

1 /0

$$\frac{\mathbf{q}_{\tau}(u_{\rho})}{\|u_{\rho}\|_{L^{2}_{\tau}(\mathbb{R}_{+})}} = 2\rho + \frac{1}{2\rho} + \tau^{2} - \tau \left(\frac{\pi}{2\rho}\right)^{1/2} \,.$$

We minimize the right hand side by choosing $\rho = \frac{\pi}{8\tau^2}$ and we deduce from the min-max principle:

$$\zeta_1(\tau) \leqslant \frac{\pi}{4} \frac{1}{\tau^2} + \frac{4-\pi}{\pi} \tau^2$$

This upper bound is minimal for $\tau = (\frac{\pi^2}{4(4-\pi)})^{1/4}$ and provides (2.9) by using (2.4). Since ζ_1 is analytic, we deduce from (2.8), Proposition 2.3 and (2.9) that $\tau \mapsto \zeta_1(\tau)$ reaches its infimum on \mathbb{R} .

3. CHARACTERIZATION OF THE MINIMUM

In this section we give a new expression of the derivative of the function ζ_n . We use it to get a comparison between Θ_0 and Ξ_0 .

In order to have a parameter-independent potential, we perform the translation $\rho = r - \tau$ and we get that \mathbf{g}_{τ} is unitary equivalent to the operator

$$\hat{\mathbf{g}}_{\tau} := -\partial_{\rho}^2 - \frac{1}{\rho + \tau}\partial_{\rho} + \rho^2$$

acting on $L^2_{\rho+\tau}(I_{\tau})$ with $I_{\tau} := (-\tau, +\infty)$. The domain of the operator $\hat{\mathbf{g}}_{\tau}$ is deduced from $\text{Dom}(\mathbf{g}_{\tau})$ using the translation $\rho = r - \tau$. The interval I_{τ} depends now on the parameter. Usually the technics from [10] and [11] give a trace formula for the derivative with respect to the boundary of the eigenvalues of such an operator (see the formula (2.3) for example). However the results of [11] specific to weighted spaces cannot be applied, indeed the weight $\rho + \tau$ depends on the parameter τ . We prove à la "Bolley-Dauge-Helffer" a formula for the derivative that is of a different kind from (2.3) and [11, Theorem 1.8] and is independent from the Feynman-Hellmann formula (2.7):

Proposition 3.1. Let $n \ge 1$ and let $z_{n,\tau}$ be a normalized eigenfunction associated to $\zeta_n(\tau)$ for the operator \mathfrak{g}_{τ} . We have

(3.1)
$$\zeta'_n(\tau) = \langle (\mathbf{\mathfrak{h}}^{\mathrm{N}}_\tau - \zeta_n(\tau)) z_{n,\tau}, z_{n,\tau} \rangle_{L^2(\mathbb{R}_+)} .$$

Proof. We denote by $\hat{z}_{n,\tau}(\rho) := z_{n,\tau}(\rho + \tau)$ a normalized eigenfunction of $\hat{\mathbf{g}}_{\tau}$ associated to $\zeta_n(\tau)$. It satisfies

(3.2)
$$-\hat{z}_{n,\tau}'(\rho) - \frac{\hat{z}_{n,\tau}'(\rho)}{\rho + \tau} + \rho^2 \hat{z}_{n,\tau}(\rho) = \zeta_n(\tau) \hat{z}_{n,\tau}(\rho) .$$

For h > 0 we introduce the quantity

$$d_{n,\tau}(h) := \left(\zeta_n(\tau+h) - \zeta_n(\tau)\right) \langle \hat{z}_{n,\tau+h}, \hat{z}_{n,\tau} \rangle_{L^2_{\rho+\tau}(I_{\tau})}$$

The analyticity of the eigenpairs $(\zeta_n(\tau), \hat{z}_{n,\tau})_{n \in \mathbb{N}}$ is a direct consequence of the simplicity of the eigenvalues (see proposition 2.1) and of Kato's theory. Since the $\hat{z}_{n,\tau}$ are normalized in $L^2_{\rho+\tau}(I_{\tau})$ we deduce that

(3.3)
$$\lim_{h \to 0} \frac{d_{n,\tau}(h)}{h} = \zeta'_n(\tau) \; .$$

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On the other side using the eigenvalue equation (3.2) we get:

$$d_{n,\tau}(h) = \int_{-\tau}^{+\infty} \left(\zeta_n(\tau+h) \hat{z}_{n,\tau+h}(\rho) \hat{z}_{n,\tau}(\rho) - \zeta_n(\tau) \hat{z}_{n,\tau+h}(\rho) \hat{z}_{n,\tau}(\rho) \right) (\rho+\tau) \, \mathrm{d}\rho$$

=
$$\int_{-\tau}^{+\infty} \left(-\hat{z}_{n,\tau+h}''(\rho) - \frac{1}{\rho+\tau+h} \hat{z}_{n,\tau+h}'(\rho) + \rho^2 \hat{z}_{n,\tau+h}(\rho) \right) \hat{z}_{n,\tau}(\rho) (\rho+\tau) \, \mathrm{d}\rho$$

$$- \int_{-\tau}^{+\infty} \left(-\hat{z}_{\tau}''(\rho) - \frac{1}{\rho+\tau} \hat{z}_{n,\tau}'(\rho) + \rho^2 \hat{z}_{n,\tau}(\rho) \right) \hat{z}_{n,\tau+h}(\rho) (\rho+\tau) \, \mathrm{d}\rho \; .$$

We make integrations by part on the terms with second derivative:

$$d_{\tau}(h) = \int_{-\tau}^{+\infty} \hat{z}'_{n,\tau+h}(\rho) \left((\rho + \tau) \hat{z}'_{n,\tau}(\rho) + \hat{z}_{n,\tau}(\rho) \right) - \frac{\rho + \tau}{\rho + \tau + h} \hat{z}'_{n,\tau+h}(\rho) \hat{z}_{n,\tau}(\rho) \, \mathrm{d}\rho \\ + \int_{-\tau}^{+\infty} -\hat{z}'_{n,\tau}(\rho) \left((\rho + \tau) \hat{z}'_{n,\tau+h}(\rho) + \hat{z}_{n,\tau+h}(\rho) \right) + \hat{z}'_{n,\tau}(\rho) \hat{z}_{n,\tau+h}(\rho) \, \mathrm{d}\rho \\ = h \int_{-\tau}^{+\infty} \frac{1}{\rho + \tau + h} \hat{z}'_{n,\tau+h}(\rho) \hat{z}_{n,\tau}(\rho) \, \mathrm{d}\rho \; .$$

Thanks to (3.3) and to the analyticity of the eigenpairs with respect to the parameter we have

$$\zeta_n'(\tau) = \int_{-\tau}^{+\infty} \frac{1}{\rho + \tau} \hat{z}_{n,\tau}'(\rho) \hat{z}_{n,\tau}(\rho) \,\mathrm{d}\rho \,.$$

Using (3.2) we deduce

$$\zeta'_{n}(\tau) = \int_{-\tau}^{+\infty} \left(-\hat{z}''_{n,\tau}(\rho) + \rho^{2} \hat{z}_{n,\tau}(\rho) - \zeta_{n}(\tau) \hat{z}_{n,\tau}(\rho) \right) \hat{z}_{n,\tau}(\rho) \,\mathrm{d}\rho \,.$$

We make the translation $\rho = r - \tau$:

$$\zeta_n'(\tau) = \int_{\mathbb{R}_+} \left(-z_{n,\tau}''(r) + \left((r-\tau)^2 z_{n,\tau}(r) - \zeta_n(\tau) z_{n,\tau}(r) \right) \right) z_{n,\tau}(r) \, \mathrm{d}r \; .$$

Thanks to (2.6), we have $z_{n,\tau} \in \text{Dom}(\mathfrak{h}_{\tau}^{N})$ and we deduce (3.1).

This formula is not sufficient to give direct informations on the monotonicity of the functions $\tau \mapsto \zeta_n(\tau)$. However it provides the following comparison between the bottom of the spectrum of the 2D-hamiltonian $H_{\mathbf{A}^{\epsilon}}$ and the one of the 3D-hamiltonian $H_{\mathcal{A}}$:

Theorem 3.2. We have

$$\Theta_0 < \Xi_0$$
.

Proof. Let τ^* be a point such that $\zeta_1(\tau^*) = \Xi_0$ (see Proposition 2.5) and z_{τ^*} an associated eigenfunction such that $||z_{\tau^*}||_{L^2_r(\mathbb{R}_+)} = 1$. We get $\zeta'_1(\tau^*) = 0$ and thanks to Proposition 3.1:

$$\zeta_1(\tau^*) = \frac{\langle \mathbf{h}_{\tau^*}^{N} z_{\tau^*}, z_{\tau^*} \rangle_{L^2(\mathbb{R}_+)}}{\|z_{\tau^*}\|_{L^2}^2(\mathbb{R}_+)} \,.$$

We deduce from the min-max principle that $\zeta_1(\tau^*) \ge \mu_1^N(\tau^*)$. Let us suppose that we have the equality $\zeta_1(\tau^*) = \mu_1^N(\tau^*)$, then z_{τ^*} is a minimizer of the quadratic form associated to $\mathbf{h}_{\tau^*}^N$

and since z_{τ^*} satisfies the Neumann boundary condition (2.6), it is an eigenfunction of $\mathfrak{h}_{\tau^*}^N$ associated to $\mu_1^N(\tau^*)$ and it satisfies $\mathfrak{h}_{\tau^*}^N z_{\tau^*} = \mu_1^N(\tau^*) z_{\tau^*}$, that is

$$\forall r > 0, \quad -z_{\tau^*}''(r) + (r - \tau^*)^2 z_{\tau^*}(r) = \mu_1^{\mathrm{N}}(\tau^*) z_{\tau^*}(r) .$$

Combining this with (2.5a) we get $z'_{\tau^*} = 0$ on \mathbb{R}_+ , which is absurd. Therefore we have $\Xi_0 = \zeta_1(\tau^*) > \mu_1^N(\tau^*) \ge \Theta_0$.

We give here a criterion in order to characterize the critical points of ζ_1 .

Proposition 3.3. Let $\tau_{\rm C}$ be a critical point of ζ_1 . Then we have

$$\zeta_1''(\tau_{\rm C}) \ge \frac{\zeta_2(\tau_{\rm C}) - 3\zeta_1(\tau_{\rm C})}{\zeta_2(\tau_{\rm C}) - \zeta_1(\tau_{\rm C})} \,.$$

Proof. We follow the proof of [16, Lemma 7] (see also [17, Section 2]). The main ingredients are the Feynman-Hellmann formula and the Viriel Theorem. \Box

We know that $\zeta_2(0) - 3\zeta_1(0) = 0$ and that $\zeta_2 - 3\zeta_1$ goes to 0 for τ large. Moreover several numerical computations show that $\zeta_2 - 3\zeta_1$ seems to be positive on $(0, +\infty)$, see figure 2. We already know that ζ_1 is non-increasing on $(-\infty, 0)$, therefore using Proposition 3.3 we believe that all the critical points of ζ_1 are minima. Therefore we are led to make the following:

Conjecture 3.4. The band function $\tau \mapsto \zeta_1(\tau)$ has a unique and non-degenerate minimum.

Let us notice that similar conjectures can be found in the litterature: in [27], the characterization of the minimum of the band function of a related model problem would bring localization property for the semi-classical Laplacian of a domain with a curved edge. In [31] the author makes a conjecture on the monoticity of the derivative of a band function associated to a magnetic hamiltonian in \mathbb{R}^3 .

Using the technics from [31, Section 3] and [32, Section 5], the conjecture 3.4 can bring scattering properties for the hamiltonian $P_{\mathcal{A}, \mathbb{R}^3_+}$. Moreover if the conjecture 3.4 is true, we will be able to describe the number of eigenstates created under the action of a suitable electric perturbation V (see [7]). We hope to continue these investigations in the future.

APPENDIX A. NUMERICAL APPROXIMATIONS

The numerical approximations described here use the finite element library Mélina ([22]). We refer to [26, Subsection 6.2.4] for more simulations and computations details. We denote by $\check{\zeta}_n(\tau)$ a numerical approximation of $\zeta_n(\tau)$. The figure 1 presents the numerical approximation $\check{\zeta}_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \le k \le 500$. The numerical approximations have a unique minimum $\check{\Xi}_0 = 0.8630$ and the corresponding minimizing Fourier parameter is $\check{\tau}^* = 1.53$. We have also plotted the constant $\Theta_0 \approx 0.5901$ according to the computation of [6] and the upper bound $\sqrt{4 - \pi} \approx 0.9265$ given by Proposition 2.5.

The figure 2 presents the numerical approximation $\zeta_2(\tau) - 3\zeta_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \le k \le 500$. These quantities are positive for $\tau > 0$, therefore we think that $\zeta_2(\tau) - 3\zeta_1(\tau)$ is positive for all $\tau > 0$. Using Proposition 3.3, we believe that Conjecture 3.4 is true.



FIGURE 1. The numerical approximations $\xi_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \le k \le 500$ compared to the constant Θ_0 and the upper bound $\sqrt{4 - \pi}$.



FIGURE 2. The numerical approximations $\zeta_2(\tau) - 3\zeta_1(\tau)$ for $\tau = \frac{k}{100}$ with $0 \le k \le 500$.

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