ON THE SEMI-CLASSICAL ANALYSIS OF THE GROUNDSTATE ENERGY OF THE DIRICHLET PAULI OPERATOR III: MAGNETIC FIELDS THAT CHANGE SIGN

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Abstract. We consider the semi-classical Dirichlet Pauli operator in bounded connected domains in the plane, and focus on the case when the magnetic field changes sign. We show, in particular, that the ground state energy of this Pauli operator will be exponentially small as the semi-classical parameter tends to zero and estimate this decay rate, extending previous results by Ekholm–Kovařík–Portmann and Helffer–Sundqvist.

1. Introduction

1.1. **The Pauli operator.** Let Ω be a bounded, open, and connected domain in $\mathbb{R}^2$, let $B : \Omega \to \mathbb{R}$ be a bounded magnetic field and $h > 0$ a semi-classical parameter. We are interested in the analysis of the ground state energy $\Lambda^D(h, B, \Omega)$ of the Dirichlet realization of the Pauli operator

$$P(B,h) = \begin{pmatrix} P_+(B,h) & 0 \\ 0 & P_-(B,h) \end{pmatrix}, \tag{1}$$

in $L^2(\Omega, \mathbb{C}^2)$. Here, the spin-up component $P_+(B, h)$ and spin-down component $P_-(B, h)$ are defined by

$$P_\pm(B,h) := (hD_{x_1} - A_1)^2 + (hD_{x_2} - A_2)^2 \pm hB(x), \tag{2}$$

$D_{x_j} = -i\partial_{x_j}$ for $j = 1, 2$, and the vector potential $\mathbf{A} = (A_1, A_2)$ satisfies

$$B(x) = \partial_{x_1} A_2 - \partial_{x_2} A_1, \qquad \forall\, x \in \Omega. \tag{3}$$

The reference to $\mathbf{A}$ is not necessary when Ω is simply connected, in which case it will be omitted, but it could play an important role if the domain is not simply connected. In the sequel we will write

$$\lambda^D_\pm(h, \mathbf{A}, B, \Omega) = \inf \sigma(P_\pm(B,h)) \tag{4}$$

and skip the reference to $\mathbf{A}$ when not needed. The smallest eigenvalue $\Lambda^D(B, h, \Omega)$ of $P(B, h)$ is given by

$$\Lambda^D(B,h,\Omega) = \min\{\lambda^D_-(h,B,\Omega),\, \lambda^D_+(h,B,\Omega)\}. \tag{5}$$

The Pauli operator is non-negative (this follows from an integration by parts, or from the view-point that the Pauli operator is the square of a Dirac operator) and, as a consequence, the bottom of the spectrum is non-negative,

$$\lambda^D_\pm(h, \mathbf{A}, B, \Omega) \geq 0.$$

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Moreover, if Γ is defined by $\Gamma u = \bar{u}$, then

$$P_+(B,h)\Gamma = \Gamma P_-(-B,h).$$

It immediately follows that

$$\lambda_+^D(h,B,\Omega) = \lambda_-^D(h,-B,\Omega). \tag{6}$$

Hence, to understand the properties of $\Lambda^D(B,h,\Omega)$ it suffices to study $\lambda_-^D(h,\mathbf{A},B,\Omega)$, and we will mostly do so.

Let us now specify the amount of regularity we assume about our domain Ω and magnetic field B. To do so, we introduce the notation $C^{p,+}$ to mean the Hölder class $C^{p,\alpha}$, for some unspecified $\alpha > 0$.

Assumption 1. The boundary of Ω is continuous and piecewise in the Hölder class $C^{2,+}$. We allow the boundary to have at most a finite number of corners, each with aperture less than π. The magnetic field B is assumed to be in class $C^0(\overline{\Omega})$.

For later reference, we introduce the notation $C^{p,+}_{\mathrm{pw}}$ for the piecewise $C^{p,+}$ condition from the assumption. From now we will always work under Assumption 1.

1.2. **The state of art.** Given a magnetic field B, we introduce the sets Ω_B^+ and Ω_B^- as the subsets of Ω where the magnetic field B is positive and negative, respectively,

$$\Omega_B^+ = \{x\in\Omega : B(x) > 0\} \quad\text{and}\quad \Omega_B^- = \{x\in\Omega : B(x) < 0\}. \tag{7}$$

Assuming that Ω_B^+ is non-empty, we know from [3, 8] that $\lambda_-^D(h,\mathbf{A},B,\Omega)$ is exponentially small as the semi-classical parameter $h > 0$ tends to zero. More precisely, we have

Theorem 1.1 ([3, 8])**.** *Let Ω be a connected domain in $\mathbb{R}^2$. If B does not vanish identically in Ω there exists $\epsilon > 0$ such that, for all $h > 0$ and for all $\mathbf{A}$ such that* $\operatorname{curl}\mathbf{A} = B$*,*

$$\lambda_-^D(h,\mathbf{A},B,\Omega) \geq \lambda^D(\Omega)\, h^2 \exp(-\epsilon/h)\,. \tag{8}$$

Here, $\lambda^D(\Omega)$ denotes the ground state energy of the Dirichlet Laplacian in Ω.

In [3], the statement in the theorem is proved under the assumption that Ω is simply connected. The generalization to non-simply connected domains, given in [8], was relatively straight forward using domain monotonicity of the ground state energy in the case of the Dirichlet problem,

$$\lambda_-^D(h,\mathbf{A},B,\Omega) \geq \lambda_-^D(h,\widetilde{B},\widetilde{\Omega})\,,$$

as soon as extensions of $\mathbf{A}$ and B to the simply connected envelope $\widetilde{\Omega}$ of Ω were constructed.

The proof in [3] gives a way of computing a lower bound for ϵ, by considering the oscillation of the scalar potential ψ, i.e. of any solution of $\Delta\psi = B$, and optimizing over ψ. For future reference, we introduce a specific choice of the scalar potential by letting the function ψ_0 be a solution of

$$\Delta\psi_0 = B(x) \text{ in } \Omega\,, \quad \psi_0 = 0 \text{ on } \partial\Omega. \tag{9}$$

The regularity conditions in Assumption 1 guarantee that ψ_0 belongs to $C^0(\overline{\Omega}) \cap C^2(\Omega)$ and that it has C^1 regularity up to the boundary, away from the corners. With this particular choice, proposed for simply connected domains in [7], we have

Theorem 1.2 ([3]). *Assume that Ω is a simply connected domain in $\mathbb{R}^2$ and that ψ_0 satisfies* (9). *Then*

$$\lambda_-^D(h, \mathbf{A}, B, \Omega) \geq \lambda^D(\Omega)\, h^2 \, \exp(-2 \operatorname*{Osc}_{\Omega} \psi_0/h)\,. \tag{10}$$

For positive magnetic fields the following theorem was proved in [7]:

Theorem 1.3 ([7]). *Let Ω be a simply connected domain in $\mathbb{R}^2$. If $B > 0$, and if ψ_0 satisfies* (9)*, then, for any $h > 0$,*

$$\lambda_-^D(h, B, \Omega) \geq \lambda^D(\Omega)\, h^2 \, \exp(2 \inf_{\Omega} \psi_0/h)\,.$$

In the semi-classical limit,

$$\lim_{h\to 0} h \log \lambda_-^D(h, B, \Omega) = 2 \inf_{\Omega} \psi_0\,.$$

In the non-simply connected case, effects from the the circulations of the magnetic potential along different components of the boundary could in principle introduce a different constant than $\inf_\Omega \psi_0$ inside the exponential function. Thus, a modified scalar potential, taking the circulation along the holes into account, was used in [8]. It turns out, however, that in the semi-classical limit, such effects disappear, and it is again ψ_0 that gives the correct asymptotics.

Theorem 1.4 ([8]). *Assume that Ω is a connected domain in $\mathbb{R}^2$, and that $B > 0$. If ψ_0 is the solution of* (9)*, then, for any $\mathbf{A}$ such that* $\operatorname{curl} \mathbf{A} = B$,

$$\lim_{h\to 0} h \log \lambda_-^D(h, \mathbf{A}, B, \Omega) = 2 \inf_{\Omega} \psi_0\,.$$

2. Main results

The aim of this paper is to extend the above mentioned results to Pauli operators with sign changing magnetic fields.

2.1. The ground state energy of $P_\pm(B, h)$.

It turns out that the scalar potential ψ_0, the solution of (9), still plays a main role for the asymptotic of the bottom of the spectrum of the Pauli operator. If $B > 0$ then, by the maximum principle $\psi_0 < 0$ in Ω, and similarly, if $B < 0$ then $\psi_0 > 0$ in Ω. For B with varying sign, it might still be the case that ψ_0 is of constant sign in Ω, but that will depend on B, and the situation is delicate (we study some examples in the sections 5 and 6).

With (6) in mind we focus again on the eigenvalue $\lambda_-^D(h, B, \Omega)$. Our first result concerns the case when ψ_0 attains negative values in Ω.

Theorem 2.1. *Assume that Ω is a simply connected domain in $\mathbb{R}^2$, and that $\inf_\Omega \psi_0 < 0$, where ψ_0 is satisfying* (9)*. Then*

$$\limsup_{h\to 0} h \log \lambda_-^D(h, B, \Omega) \leq 2 \inf_{\Omega} \psi_0.$$

We recall from (7) the definitions of Ω_B^+ and Ω_B^-, and will now turn to the case when both of them are non-void.

We assume in addition that $\Gamma := B^{-1}(0) \subset \overline{\Omega}$ is of class $C^{2,+}$ and that $\Gamma \cap \partial\Omega$ is either empty or, if non empty, that the intersection is a finite set, avoiding the corner points, with transversal intersection.

Under this assumption $\Omega_B^\pm$ satisfies the same condition as Ω from Assumption 1, and we will denote by $\hat{\psi}_0$ the solution of

$$\Delta\hat{\psi}_0 = B(x) \text{ in } \Omega_B^+, \quad \hat{\psi}_0 = 0 \text{ on } \partial\Omega_B^+. \tag{11}$$

By domain monotonicity, with $\Omega_B^+ \subset \Omega$, we can apply Theorem 2.1 with Ω replaced by Ω_B^+ and get

Corollary 2.2. *Assume that Ω is a connected domain in $\mathbb{R}^2$. Assume further that $\hat{\psi}_0$ satisfies* (11). *Then*

$$\limsup_{h\to 0} h \log \lambda_-^D(h, B, \Omega) \leq 2 \inf_{\Omega_B^+} \hat{\psi}_0 \,. \tag{12}$$

Now, the main problem is to determine if one of the bounds above, i.e. (10) and (12), is optimal. We have two possibly enlightening statements on this question. The first one gives a simple criterion under which the upper bound given in Corollary 2.2 is not optimal.

Theorem 2.3. *Assume that Ω is a simply connected domain in $\mathbb{R}^2$, $\Omega_B^+ \neq \varnothing$, and that $\hat{\psi}_0$ satisfies* (11). *If $B^{-1}(0)$ either is a compact $C^{2,+}$ closed curve in Ω or a $C^{2,+}$ line crossing $\partial\Omega$ transversally away from the corners, then*

$$\limsup_{h\to 0} h \log \lambda_-^D(h, B, \Omega) < 2 \inf_{\Omega_B^+} \hat{\psi}_0 \,.$$

Two examples where this condition is satisfied is when Ω is a disk, and the magnetic field is either radial, vanishing on a circle, or affine, vanishing on a line. We will return to them later.

We mentioned earlier that even though B changes sign, it might happen that the scalar potential ψ_0 does not. Our second statement says that in this case we actually have the optimal result.

Theorem 2.4. *Suppose that Ω is a simply connected domain in $\mathbb{R}^2$. If $\psi_0 < 0$ in Ω, where ψ_0 is the solution of* (9), *then*

$$\lim_{h\to 0} h \log \lambda_-^D(h, B, \Omega) = 2 \inf_{\Omega} \psi_0 \,.$$

2.2. **The ground state energy of the Pauli operator.** We have already mentioned, that from (6) it follows that to understand the lowest eigenvalue of each of the components of $P(B,h)$, it suffices to study one of them, with the extra price that we must do it both for B and $-B$. To discuss the lowest eigenvalue $\Lambda^D(B,h,\Omega)$ of the Pauli operator $P(B,h)$, we will compare the eigenvalues for the spin-up and spin-down components.

If the scalar potential ψ_0 does not changes sign in Ω, we can transfer the earlier results to $\Lambda^D(B,h,\Omega)$.

Theorem 2.5. *Let Ω be a simply connected domain in $\mathbb{R}^2$, and let ψ_0 be given by* (9). *If ψ_0 does not change sign in Ω, then*

$$\lim_{h\to 0} h \log \Lambda^D(h, B, \Omega) = -2 \operatorname*{Osc}_{\Omega} \psi_0. \tag{13}$$

Our final result concerns a case when ψ_0 changes sign.

Theorem 2.6. *Let Ω be a simply connected domain in $\mathbb{R}^2$, and let ψ_0 be given by* (9)*. Assume that*

$$\psi_{\min} = \inf_{\Omega} \psi_0 < 0 < \sup_{\Omega} \psi_0 = \psi_{\max}.$$

Assume further that $\psi_0^{-1}(\psi_{\max})$ contains a $C^{2,+}$ closed curve enclosing a non-empty part of $\psi_0^{-1}(\psi_{\min})$ or that $\psi_0^{-1}(\psi_{\min})$ contains a $C^{2,+}$ closed curve enclosing a non-empty part of $\psi_0^{-1}(\psi_{\max})$. Then

$$\lim_{h\to 0} h \log \Lambda^D(h, B, \Omega) = -2 \operatorname{Osc} \psi_0. \tag{14}$$

Remark 2.7. *Since ψ_0 can attain its minimum only in $\overline{\Omega_B^+}$ and its maximum only in $\overline{\Omega_B^-}$, see equation* (7)*, a necessary condition for the hypothesis of Theorem 2.6 is that $B^{-1}(0)$ contain a closed curve. A radial magnetic field which changes sign on a disc is a typical example in which this condition is satisfied, see Section 5.*

3. Proof of Theorems 2.1, 2.4, 2.5, and 2.6

We assume in this section that Ω is simply connected. As it is standard, we can assume up to a gauge transform that

$$\operatorname{div} \mathbf{A} = 0 \text{ in } \Omega\,,\ \mathbf{A}\cdot\nu \text{ on } \partial\Omega\,.$$

In this case, the solution ψ_0 of (9) satisfies: $\mathbf{A} = \nabla^\perp \psi_0 = (-\partial_{x_2}\psi_0\,,\,\partial_{x_1}\psi_0)$. We let $\psi_{\min} = \inf_\Omega \psi_0$ and $\psi_{\max} = \sup_\Omega \psi_0$, and assume that

$$\psi_{\min} < \psi_{\max} = 0\,. \tag{15}$$

We note that this is the case when $B > 0$ in Ω and that this condition implies that $\int_\Omega B(x)\,dx > 0$. An example of such a magnetic field will be given in Section 6.

Proof of Theorem 2.4. Under Assumption (15), the proofs of Section 4 in [8] go through. One can first consider trial states in the form $v_\eta \exp(-\psi_0/h)$ with v_η compactly supported in Ω and v_η being equal to 1 outside a sufficiently small neighborhood of the boundary, or in the form (this equality defines v)

$$\exp(-\psi_0/h) - \exp(\psi_0/h) := \exp(-\psi_0/h)v.$$

The only change consists in replacing [8, equation (4.4)] by

$$h^2 \int_\Omega \exp\Big(-\frac{2\psi}{h}\Big)\big|(\partial_{x_1} + i\partial_{x_2})v\big|^2\,dx \le 4h \int_\Omega |B(x)|\,dx. \tag{16}$$

Hence all the statements are unchanged under the condition of replacing $\Phi = \int B(x)dx$ by $2\int |B(x)|dx$. In particular, the statement in Theorem 2.4 follows. □

Proof of Theorem 2.1. If we only assume $\psi_{\min} < 0$, we get by the same calculation as above that

$$\begin{aligned} 2(\psi_{\min} - \psi_{\max}) &\le \liminf_{h\to 0} h \log \lambda_-^D(h, \mathbf{A}, B, \Omega) \\ &\le \limsup_{h\to 0} h \log \lambda_-^D(h, \mathbf{A}, B, \Omega) \le 2\psi_{\min}\,. \end{aligned} \tag{17}$$

This proves Theorem 2.1. □

Proof of Theorem 2.5. We first note that, since $\operatorname{Osc}_\Omega \psi_0 = \operatorname{Osc}_\Omega(-\psi_0)$, Theorem 1.2 in combination with (6) gives

$$\liminf_{h\to 0} h \log \lambda_\pm^D(h,B,\Omega) \ \geq\ -2 \operatorname*{Osc}_\Omega \psi_0 \,. \tag{18}$$

If $\psi_0 < 0$ in Ω, the claim follows from Theorem 2.4 and (18). If $\psi_0 > 0$ in Ω, then Theorem 2.4 together with equation (6) implies that

$$\lim_{h\to 0} h \log \lambda_+^D(h,B,\Omega) = 2 \inf_\Omega(-\psi_0) = -2 \operatorname*{Osc}_\Omega \psi_0. \tag{19}$$

The lower bound (18) then again completes the proof. □

Proof of Theorem 2.6. Suppose first that $\psi_0^{-1}(\psi_{\max})$ contains a $C^{2,+}$ closed curve γ_1 enclosing a non-empty part of $\psi_0^{-1}(\psi_{\min})$. Let $\Omega_1 \subset \Omega$ be the region enclosed by γ_1 and define on Ω_1 the function $\psi_1 = \psi_0 - \psi_{\max}$. Then $\Delta\psi_1 = B$, $\psi_1 < 0$ and $\psi_1 = 0$ on $\partial\Omega_1 = \gamma_1$. The domain monotonicity and Theorem 2.1 thus imply that

$$\begin{aligned} \limsup_{h\to 0}\ h \log \lambda_-^D(h,B,\Omega) &\leq \limsup_{h\to 0}\ h \log \lambda_-^D(h,B,\Omega_1) \\ &\leq\ -2 \inf_{\Omega_1} \psi_1 = -2 \operatorname*{Osc}_\Omega \psi_0. \end{aligned}$$

On the other hand, if $\psi_0^{-1}(\psi_{\min})$ contains a $C^{2,+}$ closed curve γ_2 enclosing a non-empty part of $\psi_0^{-1}(\psi_{\max})$, then we denote by $\Omega_2 \subset \Omega$ the region enclosed by γ_2 and define $\psi_2 = -\psi_0 + \psi_{\min}$. Hence $\Delta\psi_2 = -B$, $\psi_2 < 0$ and $\psi_2 = 0$ on $\partial\Omega_2 = \gamma_2$. In view of equation (6), Theorem 2.1 and the domain monotonicity we then get

$$\begin{aligned} \limsup_{h\to 0}\ h \log \lambda_+^D(h,B,\Omega) &\leq \limsup_{h\to 0}\ h \log \lambda_+^D(h,B,\Omega_2) \\ &= \limsup_{h\to 0}\ h \log \lambda_-^D(h,-B,\Omega_2) \\ &\leq\ -2 \inf_{\Omega_2} \psi_2 = -2 \operatorname*{Osc}_\Omega \psi_0. \end{aligned}$$

In either case, an application of inequality (18) completes the proof. □

4. Proof of Theorem 2.3

4.1. **A deformation argument.** We have seen that we can have $\psi < 0$ in Ω without to assume $B > 0$ and that once this property is satisfied we can obtain an upper bound by restricting to the subset of Ω where ψ is negative instead. Hence a natural idea is to consider the family of subdomains of Ω defined by

$$\mathcal{F} = \{\omega \subset \Omega,\, \partial\omega \in C^{2,+}_{\rm pw} :\ \Delta\psi = B \text{ in } \omega \ \text{ and } \ \psi|_{\partial\omega} = 0 \ \Rightarrow\ \psi < 0 \text{ in } \ \omega\}\,.$$

We know that $\Omega_B^+ \in \mathcal{F}$. The idea behind the proof of Theorem 2.3 is to show that there exists $\omega \in \mathcal{F}$ such that $\Omega_B^+ \subset \omega$ with strict inclusion. More precisely, we have

Proposition 4.1. *Let $\omega \in \mathcal{F}$ and let ψ_ω be the solution of $\Delta\psi = B$ in ω such that $\psi_\omega = 0$ on $\partial\omega$. If $\partial_\nu\psi_\omega > 0$ at some point M_ω of $\partial\omega \cap \Omega$, there exists $\psi_{\tilde\omega}$ attached to $\tilde\omega$, with $\omega \subset \tilde\omega$ such that*

$$\inf_{\tilde\omega} \psi_{\tilde\omega} < \inf_\omega \psi_\omega\,. \tag{20}$$

Proof. First we deform ω into $\tilde{\omega}$ (smooth and small perturbation). We refer to [10, Chapter 5] for different ways to do this. We can for example extend the outward normal vector field to a vector field defined in a tubular neighborhood of $\partial\omega$ near M_ω. We call this vector field X_0, and take a function θ in $C_0^\infty(\mathbb{R}^2)$ with compact support near M_ω and equal to 1 near M_ω. We then consider the vector field $X := \theta X_0$, which is naturally defined in $\mathbb{R}^2$. If we consider the associated flow Φ_t of the vector field X, $t \mapsto \Phi_t(\omega)$ defines he desired deformation for t small t. We then define $\tilde{\omega} = \Phi_{t_0}(\omega)$ for some $t_0 > 0$, and construct the corresponding scalar potential $\psi_{\tilde{\omega}}$. We claim that comparing ψ_ω and $\psi_{\tilde{\omega}}$, which can be done by comparing ψ_ω and $\psi_{\tilde{\omega}} \circ \Phi_{t_0}^{-1}$ which are defined on ω and arbitrarily close (for t_0 small enough) in $H^2(\omega)$, hence in $C^0(\bar{\omega})$, we get, noting that $\psi_{\tilde{\omega}} - \psi_\omega$ is harmonic in ω, non positive on $\partial\omega$, strictly negative near M_ω and using the maximum principle, that $\psi_{\tilde{\omega}} < \psi_\omega$ in ω. In particular, we get (20). □

4.2. **Proof of Theorem 2.3.** With the deformation argument at hand, we are now ready to give a

Proof of Theorem 2.3. This is now an immediate application of Proposition 4.1 if we can show that at some point of $B^{-1}(0)$, $\partial_\nu \hat{\psi}_0 \neq 0$. However, from the Hopf boundary lemma it follows that at every regular point of $\partial(\Omega_B^+ \cap \Omega)$ we have $\partial_\nu \hat{\psi}_0 > 0$. Hence the claim. □

5. Radial magnetic fields

A typical application of the general theorems concerns radial magnetic fields in $\Omega = D(0, R)$, the disk of radius R centered at 0. The following result is a combination of the theorems appearing in Section 2.

Theorem 5.1. *Assume that $\Omega = D(0, R)$, and that the magnetic field B is radial and continuous. Then,*

$$\lim_{h \to 0} h \log \Lambda^D(h, B, \Omega) = -2 \operatorname{Osc} \psi_0.$$

Proof. We observe that the solution ψ_0 of (9) is radial, and write $r = (x_1^2 + x_2^2)^{1/2}$ and $\phi_0(r) = \psi_0(x_1, x_2)$. In view of Theorem 2.5 we may assume without loss of generality that ϕ_0 changes sign in $(0, R)$. The claim then follows from Theorem 2.6. □

Example. As an example of a radial field we consider the function

$$B_\beta(x_1, x_2) = \beta^2 - r^2$$

on the unit disc $D(0, 1)$. An explicit solution of

$$\Delta\psi_0 = B_\beta \text{ in } D(0,1), \quad \psi_0 = 0 \text{ on } \partial D(0,1),$$

is radial, and given by

$$\psi_0(x_1, x_2) = \frac{1}{16}\,(r^2 + 1 - 4\beta^2)(1 - r^2).$$

Hence for $\beta \in (0, \frac{1}{2}) \cup (\frac{1}{\sqrt{2}}, 1)$ we can apply Theorem 2.5, while the case $\beta \in [\frac{1}{2}, \frac{1}{\sqrt{2}}]$ is covered by Theorem 5.1. A simple calculation then shows that

$$\lim_{h\to 0} h \log \Lambda^D(h, B_\beta, D(0,1)) = -2 \operatorname{Osc} \psi_0 = -\begin{cases} \frac{1}{8}(2\beta^2-1)^2 & \beta \in (0, \frac{1}{2}) \\ \frac{1}{2}\beta^4 & \beta \in [\frac{1}{2}, \frac{1}{\sqrt{2}}] \\ \frac{1}{8}(4\beta^2-1) & \beta \in (\frac{1}{\sqrt{2}}, 1). \end{cases}$$

Remark 5.2. *Since $\Lambda^D(h, B_\beta, D(0,1)) = \Lambda^D(h, -B_\beta, D(0,1))$ the example above also covers the magnetic field $-B_\beta$, i.e. the case when the magnetic field is negative inside the domain delimited by the circle $B_\beta^{-1}(0)$.*

6. A magnetic field vanishing on a line joining two points of the boundary

6.1. **Preliminaries.** We present a numerical study for the case when the zero-set of the magnetic field, $B^{-1}(0)$, is a line joining two points of the boundary. We consider again $\Omega = D(0,1)$, the disk of radius 1, and assume that

$$B_\beta(x_1, x_2) = \beta - x_1, \quad -1 < \beta < 1.$$

This means that $B_\beta^{-1}(0)$ is given by the line $x_1 = \beta$. The solution of

$$\Delta\psi_\beta = (\beta - x_1) \text{ in } D(0,1)\,,\ \psi_\beta = 0 \text{ on } \partial D(0,1)\,,$$

is given by

$$\psi_\beta(x_1, x_2) = \frac{1}{8}(x_1 - 2\beta)(1 - x_1^2 - x_2^2). \tag{21}$$

A straightforward calculation shows that

$$\max \psi_\beta = \begin{cases} \psi_\beta\Big(\frac{2\beta+\sqrt{3+4\beta^2}}{3}, 0\Big) & \text{for } -1 < \beta < 1/2\,, \\ 0 & \text{for } 1/2 \le \beta < 1\,, \end{cases} \tag{22}$$

and

$$\min \psi_\beta = \begin{cases} 0 & \text{for } -1 < \beta \le -1/2\,, \\ \psi_\beta\Big(\frac{2\beta-\sqrt{3+4\beta^2}}{3}, 0\Big) & \text{for } -1/2 < \beta < 1\,. \end{cases} \tag{23}$$

It follows that

$$\operatorname{Osc} \psi_\beta = \begin{cases} \psi_\beta\Big(\frac{2\beta+\sqrt{3+4\beta^2}}{3}, 0\Big) & -1 < \beta \le -1/2\,, \\ \psi_\beta\Big(\frac{2\beta+\sqrt{3+4\beta^2}}{3}, 0\Big) - \psi_\beta\Big(\frac{2\beta-\sqrt{3+4\beta^2}}{3}, 0\Big) & -1/2 < \beta < 1/2\,, \\ -\psi_\beta\Big(\frac{2\beta-\sqrt{3+4\beta^2}}{3}, 0\Big) & 1/2 \le \beta < 1\,. \end{cases} \tag{24}$$

Next, we introduce B_β^+ as the subset of $D(0,1)$ where B_β is positive, i.e. $B_\beta^+ = \{(x_1, x_2) \in D(0,1) \mid x_1 < \beta\}$. The solution $\hat{\psi}_\beta$ of

$$\Delta\hat{\psi}_\beta = (\beta - x_1) \text{ in } \Omega_\beta^+, \quad \hat{\psi}_\beta = 0 \text{ on } \partial\Omega_\beta^+\,, \tag{25}$$

is not explicit, except in the case $\beta = 0$, where we have $\hat{\psi}_0 = \psi_0$ in Ω_0^+. The oscillation of $\hat{\psi}_\beta$ can be calculated numerically. When $\beta \in (\frac{1}{2}, 1)$, the oscillation of $\hat{\psi}_\beta$ is strictly smaller than the oscillation of ψ_β. Indeed, the function $\Psi_\beta = \psi_\beta - \hat{\psi}_\beta$ will in this case satisfy $\Delta\Psi_\beta = 0$ in Ω_β and $\Psi_\beta = 0$

on the circular part of the boundary of Ω_β and $\Psi_\beta = \psi_\beta \le 0$ on the line $x = \beta$. The Maximum principle gives $\Psi_\beta < 0$ in Ω_β, and so $\psi_\beta < \hat{\psi}_\beta$ in Ω_β. See also Figure 1.

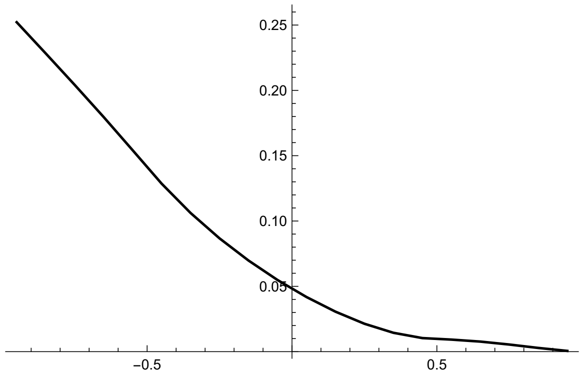

FIGURE 1. Here we have plotted $\operatorname{Osc}\psi_\beta - \operatorname{Osc}\hat{\psi}_\beta$ as a function of $\beta \in (-1, 1)$.

6.2. **Application.** We assume that

$$-\frac{1}{2} < \beta < \frac{1}{2}\,.$$

Using the restriction to $\Omega^+_{2\beta}$, we get by (17) an upper-bound (using (23)) involving $-\psi_\beta\big((2\beta - \sqrt{3+4\beta^2})/3\big)$. On the other hand we have a lower bound by the general theorem involving the oscillation of ψ_β (see (24) for the computation). Here we will discuss the application of Proposition 4.1 when applied with $\omega = \Omega_{2\beta}$. What we need is to compute

$$\partial_{x_1}\psi_\beta(2\beta, x_2) = \frac{1}{8}(1 - 4\beta^2 - x_2^2)\,,$$

with ψ_β defined in (21), and to observe that it does not vanish. As a consequence the upper bound of $\limsup_{h\to 0} h \log \lambda_1$ given by Corollary 2.2 with $\omega = \Omega_{2\beta+}$ is not optimal. Pushing the boundary will indeed improve the upper bound. The question of the optimality of the lower bound remains open.

6.3. **Researching a better upper bound.** Given β it is interesting to find the largest possible domain $\Omega_{\max} \subset D(0,1)$ such that the solution to

$$\Delta\psi = \beta - x_1,\ \text{in } \Omega_{\max}, \quad \psi = 0,\ \text{on } \partial\Omega_{\max} \tag{26}$$

is strictly negative in $\Omega_{\max}$. The oscillation of that solution could contribute to a candidate for the optimal constant in the asymptotics of the Pauli eigenvalue. We are only able to consider this problem numerically.

To find $\Omega_{\max}$ numerically, we follow (a slightly modified version of) an iterative procedure that was kindly suggested by Stephen Luttrell [11], described below. We start by numerically solving the problem on a regular polygon with (many) corners, positioned on the unit disk. Then we look at the sign of the solution close to each corner of the polygon, and move the corresponding points to make the new domain smaller if the calculated value is positive, and larger if it is negative. We also make sure that no point moves out from the disk. This gives us a new set of points. We build a new polygon, and repeat the procedure until the Euclidean distance between the corners of two iterations becomes as small as we wish (see Figure 2 for an example).

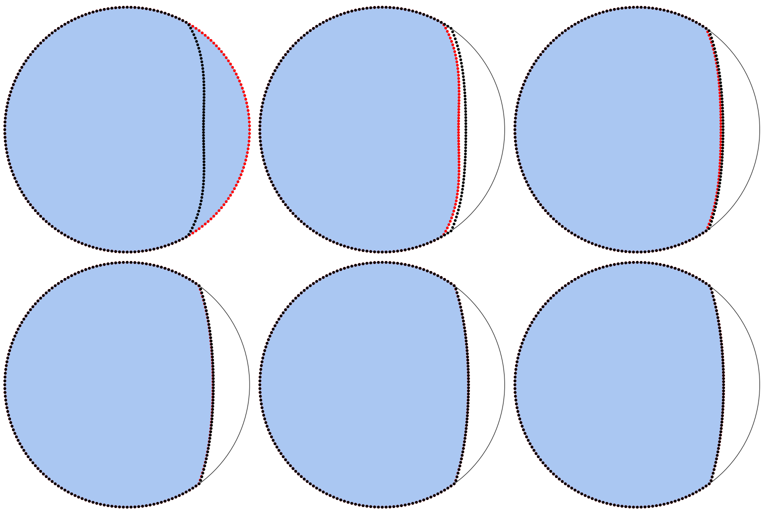

FIGURE 2. The set of domains converge quickly. In this example we start with 200 vertices, $\beta = 0.2$, and we exit the loop when the square norm of the difference between two consecutive iterations become less than 0.005 (after five steps). The red dots show the vertices used in the domain of the current step, and the black dots the ones that are calculated for the next step.

We denote by $\psi_{\beta,\mathrm{opt}}$ the function we end up with after the iterative procedure (ideally a solution of (26)). In Figure 3 we have made a comparison of the oscillation of $\psi_{\beta,\mathrm{opt}}$ and $\hat{\psi}_\beta$, and we find that the oscillation of $\psi_{\beta,\mathrm{opt}}$ is slightly larger than that of $\hat{\psi}_\beta$.

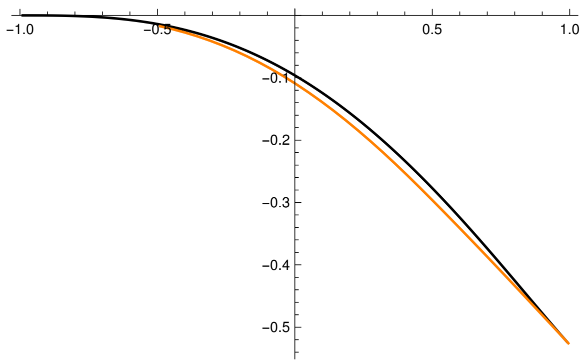

FIGURE 3. The oscillation of $\psi_{\beta,\mathrm{opt}}$ is slightly larger than that of $\hat{\psi}_\beta$. Here we show $-2\,\mathrm{Osc}\,\psi_{\beta,\mathrm{opt}}$ for $-0.5 \leq \beta \leq 1$ (orange) and $-2\,\mathrm{Osc}\,\hat{\psi}_\beta$ for $-1 \leq \beta \leq 1$ (black).

7. Conclusion

We have initially obtained from the previous papers [3, 7, 8] two natural upper bounds and a natural lower bound. We have shown that in general these two initial upper bounds cannot be true. We have also presented particular cases where the results are optimal. In all these cases, the oscillation of ψ_0 is shown to be optimal. If $\psi_0^{-1}(0,+\infty)\cap\Omega\neq\emptyset$, we have obtained the optimality by constructing an open set ω in Ω for which the solution ψ_ω of $\Delta\psi = B$ in ω and $\psi = 0$ on $\partial\omega$ satisfies in addition $\partial_\nu\psi = 0$ on $\partial\omega\cap\Omega$.

Numerically it could be interesting to see how to "push the boundary" in Proposition 4.1 in order to get a maximal domain.

Finally, as already observed in [7], one can also expect to get upperbounds by using previous results devoted to the asymptotics of the ground state energy of the Witten Laplacian (see [1, 2, 4, 5, 6, 13] and the quite recent note of B. Nectoux [12]). This unfortunately does not lead to any improvment in the cases we have considered.

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