Schrödinger operator with magnetic field in domain with corners

Virginie Bonnaillie Noël *

Abstract

We present here a simplified version of results obtained with F. Alouges, M. Dauge, B. Helffer and G. Vial (cf [4, 7, 9]). We analyze the Schrödinger operator with magnetic field in an infinite sector. This study allows to determine accurate approximation of the low-lying eigenpairs of the Schrödinger operator in domains with corners. We complete this analysis with numerical experiments.

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1 Introduction

Let $\Omega \subset \mathbb{R}^2$ be an open, simply connected domain with Lipschitz boundary and let ν be the unit outer normal on the boundary $\Gamma = \partial\Omega$. We assume that ν is well defined on Γ with the possible exception of a finite number of points (the corners of Ω). We consider a cylindrical superconducting sample of cross section Ω and we apply a constant magnetic field of intensity σ along the cylindrical axis. We denote by κ the characteristic of the sample, called the "Ginzburg-Landau parameter" and consider κ large (corresponding to a type II superconductor). Then, up

*IRMAR, Université Rennes 1, Campus de Beaulieu, 35042 Rennes Cedex, France

to normalization factors, the free energy writes

$$\mathcal{G}(\psi,\mathcal{A})=\frac{1}{2}\int_{\Omega}\left(|(\nabla-i\kappa\mathcal{A})\psi|^2+\frac{\kappa^2}{2}(|\psi|^2-1)^2+\kappa^2|\text{curl }\mathcal{A}-\sigma|^2\right)dx. \tag{1}$$

The superconducting properties are described by the minimizers $(\psi,\mathcal{A})$ of this Ginzburg-Landau functional $\mathcal{G}$. The complex-valued function ψ is the order parameter (cf [13]) ; the magnitude $|\psi|^2$ represents the density of superconducting electrons and the phase determines the current flow. The vector field $\mathcal{A}$ defined on $\mathbb{R}^2$ is the magnetic potential and $\mathcal{B}=\text{curl }\mathcal{A}$ is the induced magnetic field. To determine the onset of the superconductivity, we linearize the Euler equation associated with (1) near the normal state $(\psi,\mathcal{A})=(0,\sigma\mathcal{A}_{\mathbf{0}})$, where

$$\mathcal{A}_0 :\ =\frac{1}{2}(x_2,-x_1). \tag{2}$$

From now, we put $\mathcal{A}=\mathcal{A}_0$ and assume Ω bounded. Defining the change of parameter $h=\frac{1}{\kappa\sigma}$, we are interested in the asymptotic behavior, when $h\to 0$, of the Neumann realization P_h of the Schrödinger operator with a magnetic field and semi-classical parameter $h>0$. We define the associated quadratic form p_h on $H^1(\Omega)$ by :

$$p_h(u)=\int_{\Omega}|(h\nabla-i\mathcal{A})u(x)|^2\,dx.$$

This leads to define the operator $P_h=-(h\nabla-i\mathcal{A})^2$ on $\mathcal{D}(P_h)$ with :

$$\mathcal{D}(P_h)=\left\{u\in H^2(\Omega),\quad \nu\cdot(h\nabla-i\mathcal{A})u\big|_{\Gamma}=0\right\}.$$

It is well known that the spectrum of the operator $P_{h,\mathcal{A}}$ is invariant by gauge transformation. So, when Ω is simply connected, the spectrum of P_h depends only on the magnetic field and not on the choice of the corresponding magnetic potential. Then, we denote by $\mu_{h,n}$ the n-th eigenvalue of P_h for any $\mathcal{A}'$ such that $\text{curl }\mathcal{A}'=\text{curl }\mathcal{A}$.

Many papers have been devoted to this problem among which we quote the works by Bernoff-Sternberg [3], Lu-Pan [19, 20], Helffer-Mohamed [15, 16] and more recently Fournais-Helffer [12]. These papers deal with the case of regular domains and propose an asymptotics of the bottom of the spectrum. Although the interest for a non smooth domain is often mentioned in the physical literature, there are very few mathematical papers : We only know the contributions by Pan [22] and Jadallah [18] which deal with very particular domains like a square or a quarter plane. Our goal is to give asymptotics for the low-lying eigenvalues and localization of the corresponding eigenvectors in a domain with corners.

In the analysis of smooth domains, the model operator $-(\nabla - i\mathcal{A})^2$ on $\mathbb{R}^2$ and $\mathbb{R} \times \mathbb{R}^+$ was playing an important role. Our new model for domains with corners is the operator $-(\nabla - i\mathcal{A})^2$ in angular sectors. We analyze this model in Section 2. We recall results proved in [7]. We use these results, in Section 3, to construct quasi-modes for the operator P_h in polygonal domain. This gives the asymptotics of $\mu_{h,n}$ when the domain in a polygon in Section 4. We propose also some numerical experiments which show the decay of the eigenfunctions, the convergence of the eigenvalues and a numerical illustration of a tunnelling effect.

The bottom of the spectrum of the Schrödinger operator with magnetic field on an infinite sector is an eigenvalue when the opening is less than $\pi/2$ whereas it equals the bottom of the essential spectrum for the half-plane. This generates very different results for a polygonal domain and for a smooth domain.

2 The model case of an infinite sector

This section is devoted to the analysis of the Neumann realization of the Schrödinger operator with magnetic field $-(\nabla - i\mathcal{A})^2$ on an infinite sector. We recall results developed in [5, 7] and we just propose some sketches of proofs here.

2.1 Notations

Let G^α be the sector in $\mathbb{R}^2$ with opening α and $\mathsf{X} = (\mathsf{X}_1, \mathsf{X}_2)$ the coordinates on the sector. The Neumann realization Q^α of the Schrödinger operator with magnetic field $-(\nabla - i\mathcal{A})^2$ on G^α is associated with the quadratic form q^α defined on the variational space $\mathcal{V}(q^\alpha)$ as follows :

$$\mathcal{V}(q^\alpha) = \Big\{\Psi \in L^2(G^\alpha), \ \ (\nabla - i\mathcal{A})\Psi \in L^2(G^\alpha)\Big\}, \tag{3}$$

$$q^\alpha(\Psi) = \int_{G^\alpha} |(\nabla - i\mathcal{A})\Psi(\mathsf{X})|^2 \, d\mathsf{X}, \quad \forall \Psi \in \mathcal{V}(q^\alpha). \tag{4}$$

The norm attached with the space $\mathcal{V}(q^\alpha)$ is

$$||\Psi||^2_{\mathcal{V}(q^\alpha)} = ||\Psi||^2_{L^2(G^\alpha)} + ||(\nabla - i\mathcal{A})\Psi||^2_{L^2(G^\alpha)}.$$

Note that if $\Psi \in \mathcal{V}(G^\alpha)$, then for any ball B, $\Psi \in H^1(G^\alpha \cap B)$. We denote by Q^α the operator associated with the form q^α. Then,

$$Q^\alpha = -(\nabla - i\mathcal{A})^2,$$

is defined on $\mathcal{D}(Q^\alpha)$ with :

$$\mathcal{D}(Q^\alpha) = \Big\{\Psi \in \mathcal{V}(q^\alpha),\ \ (\nabla - i\mathcal{A})^2\Psi \in L^2(G^\alpha),\ \ \nu \cdot (\nabla - i\mathcal{A})\Psi\big|_{\partial G^\alpha} = 0\Big\}.$$

Definition 2.1. *Let $\mu_k(\alpha)$ be the $k-$th smallest element of the spectrum of Q^α, given by the max-min principle:*

$$\mu_k(\alpha) = \max_{\Psi_1,\cdots,\Psi_{k-1}} \min \left\{ \frac{q^\alpha(\Psi)}{\langle \Psi, \Psi\rangle},\ \ \Psi \in \mathcal{V}(q^\alpha),\ \ \Psi \in [\Psi_1, \cdots, \Psi_{k-1}]^\perp \right\}. \quad (5)$$

Here $\langle\cdot,\cdot\rangle$ denotes the hermitian scalar product of $L^2(G^\alpha)$.

2.2 Essential spectrum

Proposition 2.2. *The infimum of the essential spectrum of Q^α is equal to $\Theta_0 := \mu_1(\pi)$.*

Proof. This result is a consequence of the Persson Lemma (cf [23]) which can be generalized to unbounded domains of $\mathbb{R}^2$ and Neumann realizations :

Lemma 2.3. *Let Ω be an unbounded domain of $\mathbb{R}^2$ with Lipschitz boundary. We denote by* $\inf \sigma_{\text{ess}}(-(\nabla - i\mathcal{A})^2)$ *the bottom of the essential spectrum, then :*

$$\inf \sigma_{\text{ess}}(-(\nabla - i\mathcal{A})^2) = \lim_{r\to\infty} \Sigma_r(-(\nabla - i\mathcal{A})^2), \quad (6)$$

with, denoting $\Omega_r = \{\mathsf{X} \in \overline{\Omega} |\ |\mathsf{X}| > r\}$:

$$\Sigma_r(-(\nabla - i\mathcal{A})^2) :\ = \inf_{\phi \in C_0^\infty(\Omega_r), \phi\neq 0} \frac{\displaystyle\int_\Omega |(\nabla - i\mathcal{A})\phi(\mathsf{X})|^2\ d\mathsf{X}}{\displaystyle\int_\Omega |\phi(\mathsf{X})|^2\, d\mathsf{X}}. \quad (7)$$

Relying on this lemma, we use a partition of unity which splits the sector into three subdomains which can be compared to the models $\mathbb{R}^2$ or $\mathbb{R} \times \mathbb{R}^+$ respectively. $\square$

2.3 Decay of eigenfunctions

Proposition 2.4. *Let k be a positive integer and $\alpha > 0$ such that $\mu_k(\alpha) < \Theta_0$. We denote by Ψ_k^α a normalized eigenfunction associated with $\mu_k(\alpha)$. Then Ψ_k^α satisfies the following exponential decay estimate*

$$\forall \varepsilon > 0, \exists C_{\varepsilon,\alpha} : \quad \left|\left| \mathrm{e}^{\left(\sqrt{\Theta_0 - \mu_k(\alpha)} - \varepsilon\right)|\mathsf{X}|} \, \Psi_k^\alpha \right|\right|_{\mathcal{V}(q^\alpha)} \leq C_{\varepsilon,\alpha}. \tag{8}$$

Proof. Agmon's estimates (cf [1]) are useful to prove this result. We recall their principle. Let ϕ be a uniformly lipschitzian function on G^α, then, by assumption on Ψ_k^α :

$$\int_{G^\alpha} \left(\mu_k(\alpha) + |\nabla\phi|^2\right) \, \mathrm{e}^{2\phi} |\Psi_k^\alpha|^2 \, d\mathsf{X} = \int_{G^\alpha} |(\nabla - i\mathcal{A})(\mathrm{e}^{\phi}\Psi_k^\alpha)|^2 \, d\mathsf{X}. \tag{9}$$

Let B_R be the ball in $\mathbb{R}^2$ centered on 0 with radius R and χ_1, χ_2 be real, positive, smooth functions, with support respectively in B_2 and $\mathbb{R}^2 \setminus B_1$, and such that $|\chi_1|^2 + |\chi_2|^2 \equiv 1$. We define $\chi_j^R : = \chi_j\left(\frac{\cdot}{R}\right)$, then :

$$q_\alpha(\mathrm{e}^{\phi}\Psi_k^\alpha) = \sum_{j=1}^{2} q_\alpha(\chi_j^R \mathrm{e}^{\phi}\Psi_k^\alpha) - \frac{1}{R^2}\sum_{j=1}^{2} ||\mathrm{e}^{\phi}\Psi_k^\alpha \, |\nabla\chi_j^R| \, ||^2_{L^2(G^\alpha)}.$$

The two last relations combined with the positivity of $q_\alpha(\chi_1^R \mathrm{e}^{\phi}\Psi_k^\alpha)$ lead to :

$$q_\alpha(\chi_2^R \mathrm{e}^{\phi}\Psi_k^\alpha) \quad \leq \quad \int_{G^\alpha} \left(\mu_k(\alpha) + |\nabla\phi|^2 + \frac{C}{R^2}\right) \mathrm{e}^{2\phi}|\Psi_k^\alpha|^2 d\mathsf{X}. \tag{10}$$

We can prove (cf Lemma 2.3 and [7] for details) that :

$$q_\alpha(\chi_2^R \mathrm{e}^{\phi}\Psi_k^\alpha) \geq \left(\Theta_0 - \frac{C}{R^2}\right) ||\chi_2^R \mathrm{e}^{\phi}\Psi_k^\alpha||^2_{L^2(G^\alpha)}. \tag{11}$$

To obtain a L^2-estimate, we put together (10) and (11). We bound $||\chi_2^R \mathrm{e}^{\phi}\Psi_k^\alpha||^2_{L^2(G^\alpha)}$ from below by $||\mathrm{e}^{\phi}\Psi_k^\alpha||^2_{L^2(G^\alpha \setminus \mathcal{B}_{2R})}$, choose $\phi(x) : = \sqrt{\Theta_0 - \mu_k(\alpha) - \varepsilon} \, |\mathsf{X}|$ and split the integral over G^α in two parts, respectively over $G^\alpha \setminus B_{2R}$ and $B_{2R} \cap G^\alpha$. To end the proof, it is enough to use (9) again. ∎

2.4 Estimates of $\mu_1(\alpha)$

Theorem 2.5.
(i) For all $\alpha \in (0, \frac{\pi}{2}]$, $\mu_1(\alpha) < \Theta_0$ and, therefore, $\mu_1(\alpha)$ is an eigenvalue.
(ii) There exists a real sequence $(m_j)_{j\in\mathbb{N}}$, with $m_0 = 1/\sqrt{3}$, such that :

$$\mu_1(\alpha) \sim \alpha \sum_{j=0}^{\infty} m_j \alpha^{2j} \text{ as } \alpha \to 0.$$

Furthermore, $\mu_1(\alpha) \leq \alpha/\sqrt{3}$ for any $\alpha \in (0, \pi]$.

Proof. After a change of variables, a scaling and a gauge transformation, we get a new operator which is now defined on a constant domain $\omega\colon = \mathbb{R}^+ \times \left]-\frac{1}{2}, \frac{1}{2}\right[$ with coordinates (t, η) (instead of the constant operator $-(\nabla - i\mathcal{A})^2$ on an α-dependent domain G^α). This new operator is associated with the sequilinear form :

$$a_\alpha(u, v)\colon = \int_\omega \left(2\alpha t(D_t - \eta)u\, \overline{(D_t - \eta)v} + \frac{1}{2\alpha t} D_\eta u\, \overline{D_\eta v} \right)\, dt\, d\eta,$$

defined on :

$$\mathcal{V}\colon = \left\{ u \in L^2(\omega) |\ \sqrt{t}(D_t - \eta)u \in L^2(\omega),\ \frac{1}{\sqrt{t}} D_\eta u \in L^2(\omega) \right\}\ ,$$

We look for two sequences : $(u_k)_{k\in\mathbb{N}}$ and $(m_k)_{k\in\mathbb{N}}$ with m_k real such that for all $n \in \mathbb{N}^*$, if we define $U^{(n)} = \sum_{k=0}^{n} \alpha^{2k} u_k$ and $\mu^{(n)}(\alpha) = \sum_{k=0}^{n} \alpha^{2k} m_k$, then, modulo $\mathcal{O}_n(\alpha^{2n+2})$, we have :

$$a_\alpha(U^{(n)}, v) \equiv \mu^{(n)}(\alpha) \langle U^{(n)}, v\rangle_{L^2(\omega)},\ \forall v \in \mathcal{V}.$$

We expand the equation in powers of α and express that the coefficients of α^{2k} ($k \geq -1$) should cancel. The construction shows that functions u_k belong to the space of polynomial functions in η whose coefficients are in $\mathcal{S}(\overline{\mathbb{R}^+})$. □

Remark 2.6. From the expression of the form a_α, we immediately see that the function $\alpha \mapsto \alpha\mu_1(\alpha)$ is increasing and $\alpha \mapsto \mu_1(\alpha)/\alpha$ is decreasing over $(0, 2\pi)$. According to results on $\mu_1(\alpha)$ (cf [7]) and numerical computations (cf [4]), we conjecture that μ_1 is strictly increasing from $(0, \pi]$ onto $(0, \Theta_0]$ and equal to Θ_0 on $[\pi, 2\pi)$. Figure 1 presents numerical estimates of $\mu_1(\alpha)$ that we have obtained (with G. Vial) using a finite element method. To realize these computations, we consider a truncated sector G_c^α. We keep Neumann magnetic boundary conditions on the common boundary between G_c^α and G^α and a Dirichlet conditions on the other part of the boundary of G_c^α. So we are ensured to obtain an upper-bound of $\mu_1(\alpha)$, $\alpha \in \{k\pi/100, k = 1, \ldots, 85\}$. For any opening, we consider a uniform mesh with 48 quadrangular elements and a tensor product polynomial of degree 10.

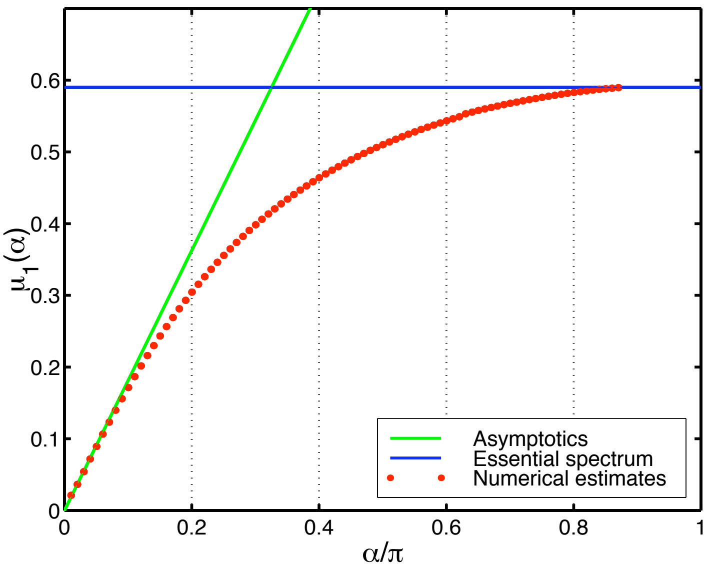

Figure 1: Estimates of $\mu_1(\alpha)$ by a finite element method.

3 Construction of quasi-modes for polygonal domains

Results presented in this section are proved in [9].

3.1 Notation and localized model operators

Let $\Omega \in \mathbb{R}^2$ be a convex bounded polygon with straight edges, Σ be the set of its vertices s, and α_{s} be its angle at $\mathsf{s} \in \Sigma$. The spectrum of P_h is in close relation with the spectra of the model operators $Q^{\alpha_{\mathsf{s}}}$, for s describing the set of corners Σ. As a first step in the explanation of this relation, we introduce, for each vertex s, the semi-model operator $\widetilde{Q}_{h,\mathsf{s}}$ defined by the same operator as P_h, but on the infinite plane sector $\widetilde{G}_{\mathsf{s}}$ which coincides with Ω near the vertex s: Let $d = \min_{\mathsf{s}\neq\mathsf{s}'\in\Sigma} d(\mathsf{s},\mathsf{s}')$ and $\mathcal{R}_{\mathsf{s}}$ be the rotation of angle β_{s} such that

$$\{\mathcal{R}_{\mathsf{s}}(x-\mathsf{s}),\ \ x\in\Omega\cap\mathcal{B}(\mathsf{s},d)\}\subset G^{\alpha_{\mathsf{s}}},$$

and let us denote

$$\widetilde{G}_{\mathsf{s}} = \{\mathcal{R}_{\mathsf{s}}^{-1}\mathsf{X}+\mathsf{s},\ \ \mathsf{X}\in G^{\alpha_{\mathsf{s}}}\}.$$

Finally $\widetilde{Q}_{h,\mathsf{s}}$ is the operator $-(h\nabla - i\mathcal{A})^2$ on $\widetilde{G}_{\mathsf{s}}$.

Lemma 3.1. *The following relation holds between the spectra of the operators $\widetilde{Q}_{h,\mathsf{s}}$ and $Q^{\alpha_{\mathsf{s}}}$ respectively denoted by $\sigma(\widetilde{Q}_{h,\mathsf{s}})$ and $\sigma(Q^{\alpha_{\mathsf{s}}})$:*

$$\sigma(\widetilde{Q}_{h,\mathsf{s}}) = h\,\sigma(Q^{\alpha_{\mathsf{s}}}).$$

The corresponding eigenvectors are deduced from each other by a change of variables and a gauge transformation

$$\begin{array}{rcl}\mathcal{V}(q^{\alpha_{\mathsf{s}}}) & \longrightarrow & \mathcal{V}(\widetilde{q}_{h,\mathsf{s}}) = \left\{\psi\in L^2(\widetilde{G}_{\mathsf{s}}),\quad (h\nabla - i\mathcal{A})\psi\in L^2(\widetilde{G}_{\mathsf{s}})\right\},\\ \Psi_k^{\alpha} & \longmapsto & \widetilde{\psi}_{h,\mathsf{s},k}\quad \text{s.t.}\quad \widetilde{\psi}_{h,\mathsf{s},k}(x) = \frac{1}{\sqrt{h}}\exp\left(\frac{i}{2h}x\wedge\mathsf{s}\right)\Psi_k^{\alpha}\left(\frac{\mathcal{R}_{\mathsf{s}}(x-\mathsf{s})}{\sqrt{h}}\right).\end{array} \tag{12}$$

We now use results on angular sectors and Lemma 12 to construct functions which are good approximations of the eigenfunctions of P_h.

3.2 Quasi-modes

Lemma 3.2. *Let $\mathsf{s}\in\Sigma$ and d_{s} be the distance to other vertices*

$$d_{\mathsf{s}} = \operatorname{dist}(\mathsf{s},\Sigma\setminus\{\mathsf{s}\}).$$

Let $d' < d_{\mathsf{s}}$ and χ_{s} be a smooth cut-off function with support in $\mathcal{B}(\mathsf{s},d_{\mathsf{s}})$, equal to 1 in $\mathcal{B}(\mathsf{s},d')$ and such that $0\le\chi_{\mathsf{s}}\le 1$.
We consider $\Psi^{\alpha_{\mathsf{s}}}$ a normalized eigenfunction of $Q^{\alpha_{\mathsf{s}}}$ on $G^{\alpha_{\mathsf{s}}}$ for the eigenvalue $\mu_k(\alpha_{\mathsf{s}})$. Using the transformation (12), we define :

$$\widetilde{\psi}_{h,\mathsf{s},k}(x) \;=\; \frac{\mathrm{e}^{\frac{i}{2h}x\wedge\mathsf{s}}}{\sqrt{h}}\,\Psi_k^{\alpha_{\mathsf{s}}}\left(\frac{\mathcal{R}_{\mathsf{s}}(x-\mathsf{s})}{\sqrt{h}}\right)\ \ \textit{on}\ \widetilde{G}_{\mathsf{s}}, \tag{13}$$

$$\psi_{h,\mathsf{s},k}(x) = \chi_{\mathsf{s}}(x)\,\widetilde{\psi}_{h,\mathsf{s},k}(x) \text{ on } \Omega. \tag{14}$$

Then, for any $\varepsilon > 0$, there exists C_ε such that

$$\begin{aligned}
\left|1 - ||\psi_{h,\mathsf{s},k}||_\Omega^2\right| &\leq C_\varepsilon \exp\left(-\frac{2}{\sqrt{h}}\left(d'\sqrt{\Theta_0 - \mu_k(\alpha_{\mathsf{s}})} - \varepsilon\right)\right),\\
\left|\frac{p_h(\psi_{h,\mathsf{s},k})}{||\psi_{h,\mathsf{s},k}||_\Omega^2} - h\mu_k(\alpha_{\mathsf{s}})\right| &\leq C_\varepsilon \exp\left(-\frac{2}{\sqrt{h}}\left(d'\sqrt{\Theta_0 - \mu_k(\alpha_{\mathsf{s}})} - \varepsilon\right)\right),\\
||P_h\psi_{h,\mathsf{s},k} - h\mu_k(\alpha_{\mathsf{s}})\psi_{h,\mathsf{s},k}||_\Omega &\leq C_\varepsilon \exp\left(-\frac{1}{\sqrt{h}}\left(d'\sqrt{\Theta_0 - \mu_k(\alpha_{\mathsf{s}})} - \varepsilon\right)\right),
\end{aligned}$$

where $||\cdot||_\Omega$ denotes the L^2-norm on Ω.

The proof relies on the decay of the eigenfunctions $\Psi_k^{\alpha_{\mathsf{s}}}$. The following lemma shows how we can split the corners of the polygon to obtain global informations.

3.3 Partition of unity

Lemma 3.3. *For any $\mathsf{s} \in \Sigma$, we consider a real-valued cut-off function χ_{s} with support in $\mathcal{B}(\mathsf{s}, d_{\mathsf{s}})$. We assume furthermore that for any $\mathsf{s} \neq \mathsf{s}'$, $\mathrm{supp}\chi_{\mathsf{s}} \cap \mathrm{supp}\chi_{\mathsf{s}}' = \emptyset$. We define χ_0 on Ω by $\chi_0^2 = 1 - \sum_{\mathsf{s}\in\Sigma}\chi_{\mathsf{s}}^2$. Then, for any $\widetilde{\psi} \in H^1(\Omega)$,*

$$p_h(\widetilde{\psi}) = \sum_{\mathsf{s}\in\Sigma\cup\{0\}} p_h(\chi_{\mathsf{s}}\widetilde{\psi}) - h^2 \sum_{\mathsf{s}\in\Sigma\cup\{0\}} ||\widetilde{\psi}\nabla\chi_{\mathsf{s}}||_{L^2(\Omega)}^2.$$

4 Approximation of $\sigma(P_h)$ with the model operators

4.1 Asymptotics

Notation 4.1. Let us denote by λ_n the $n-$th eigenvalue of $\oplus_{\mathsf{s}\in\Sigma}Q^{\alpha_{\mathsf{s}}}$ counted with multiplicity as defined by the min-max principle, and let N be the largest integer such that $\lambda_N < \Theta_0$. We assume that $N \geq 1$. For any $n \leq N$, we denote by Σ_n the subset of vertices

$$\Sigma_n = \left\{\mathsf{s} \in \Sigma, \ \ \lambda_n \text{ is an eigenvalue for } Q^{\alpha_{\mathsf{s}}}\right\},$$

and by r_n the distance

$$r_n = r(\lambda_n) = \min_{\mathsf{s}\in\Sigma_n} d(\mathsf{s}, \Sigma \setminus \{\mathsf{s}\}).$$

Let $n \leq N$. We denote by $\mu_{h,n}$ the $n-$th eigenvalue of P_h counted with multiplicity. For any $\mathsf{s} \in \Sigma_n$, we denote by Ψ^{α_s} a normalized eigenvector for Q^{α_s} associated with λ_n and by $\widetilde{\psi}_{h,\mathsf{s}}$ the function deduced from Ψ^{α_s} by (13), then $\widetilde{\psi}_{h,\mathsf{s}}$ is a normalized eigenfunction of $\widetilde{Q}_{h,\mathsf{s}}$ for $h\lambda_n$. Let $\varepsilon > 0$. We consider a smooth cut-off function $\chi_\mathsf{s} \in \mathcal{C}_0^\infty(\Omega, [0,1])$ as in Lemma 3.2 with $d' < r_n$ and we define $\psi_{h,\mathsf{s}} = \chi_\mathsf{s}\widetilde{\psi}_{h,\mathsf{s}}$ as in (14).

As we will see in the following theorem, according to repetitions of the same values in $\{\lambda_1, \cdots, \lambda_N\}$, the eigenvalues $\mu_{h,n}$ are gathered into clusters.

Theorem 4.2. *With Notation 4.1, for any $\varepsilon > 0$, there exists C_ε such that for any $n \leq N$,*

$$\begin{aligned}
\mu_{h,1} &\leq h\lambda_1 + C_\varepsilon \exp\left(-\frac{2}{\sqrt{h}}\left(r_1\sqrt{\Theta_0 - \lambda_1} - \varepsilon\right)\right), \\
|\mu_{h,n} - h\lambda_n| &\leq C_\varepsilon \exp\left(-\frac{1}{\sqrt{h}}\left(r_n\sqrt{\Theta_0 - \lambda_n} - \varepsilon\right)\right).
\end{aligned}$$

Proof. Upper-bound of $\mu_{h,1}$ is a consequence of Lemma 3.2 applied with $\mu_k(\alpha_\mathsf{s}) = \lambda_1$ and $d' = r_1 - \varepsilon$ and the min-max principle.
Let $n \leq N$, $\mathsf{s} \in \Sigma_n$ and $d' = r_n - \varepsilon$. We deduce from Lemma 3.2 and the spectral theorem that :

$$d(\sigma(P_h), h\lambda_n) \leq C_\varepsilon \exp\left(-\frac{1}{\sqrt{h}}\left(r_n\sqrt{\Theta_0 - \lambda_n} - \varepsilon\right)\right). \tag{15}$$

To prove a lower bound of $\mu_{h,n}$, we use [10, 24]. □

To approximate eigenvectors of P_h, we have to take account of clusters as explained in the following result.

Notation 4.3. Using Notations 4.1, we denote by $\{\Lambda_1 < \cdots < \Lambda_M\}$ the set of distinct values in $\{\lambda_1, \cdots, \lambda_N\}$. Let $m \leq M$, we define the distances

$$\rho_m = r(\Lambda_m).$$

For $n \leq N$, we denote by $(\mu_{h,n}, u_{h,n})$ the n-th eigenpair of P_h. We introduce the cluster of eigenspaces of P_h by

$$F_{h,m} = \text{span}\{u_{h,n} \text{ for any } n \text{ such that } \lambda_n = \Lambda_m\},$$

and the cluster of quasi-modes

$$E_{h,m} = \text{span}\{\psi_{h,\mathsf{s},k} = \chi_{\mathsf{s}}\widetilde{\psi}_{h,\mathsf{s},k} \text{ for any } \mathsf{s} \in \Sigma, k \geq 1 \text{ such that } \mu_k(\alpha_{\mathsf{s}}) = \Lambda_m\}.$$

Here, χ_{s} is a real-valued smooth cut-off function equal to 1 in $\mathcal{B}(\mathsf{s}, \rho_m - \delta)$.

Theorem 4.4. *Under Notation 4.1 and 4.3, for any $\varepsilon > 0$, there exists C_ε such that for any $m \leq M$,*

$$d(E_{h,m}; F_{h,m}) \leq C_\varepsilon \exp\left(-\frac{1}{\sqrt{h}}\left((\rho_m - \delta)\sqrt{\Theta_0 - \Lambda_m} - \varepsilon\right)\right),$$

where, if we denote $\Pi_{E_{h,m}}$, $\Pi_{F_{h,m}}$ the orthogonal projections on $E_{h,m}$ and $F_{h,m}$ respectively, d is the distance defined by :

$$d(E_{h,m}; F_{h,m}) = ||\Pi_{E_{h,m}} - \Pi_{F_{h,m}}\Pi_{E_{h,m}}||_{L^2(\Omega)}.$$

Proof. The proof of this theorem relies on Proposition 4.1.1, p. 30 of [14] (cf also [17]) which we recall now :

Theorem 4.5. *Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$. Let $I \subset \mathbb{R}$ be a compact interval, $\psi_1, \ldots, \psi_N \in \mathcal{H}$ linearly independents in $\mathcal{D}(A)$ and $\mu_1, \ldots, \mu_N$ such that :*

$$A\psi_j = \mu_j\psi_j + r_j \text{ with } ||r_j||_{\mathcal{H}} \leq \eta. \tag{16}$$

Let $a > 0$ and assume that $\sigma(A) \cap (I + \mathcal{B}(0, 2a) \setminus I) = \emptyset$. Then, if E is the space spanned by $\psi_1, \ldots, \psi_N$ and if F is the space associated with $\sigma(A) \cap I$, we have :

$$d(E, F) \leq \frac{\eta\sqrt{N}}{a\sqrt{\lambda_S^{\min}}}, \tag{17}$$

where $\lambda_S^{\min}$ is the smallest eigenvalue of $S = (\langle\psi_j, \psi_k\rangle_{\mathcal{H}})$ and d is the non-symmetric distance as :

$$d(E, F) = ||\Pi_E - \Pi_F\Pi_E||_{\mathcal{H}},$$

denoting by Π_E, Π_F the orthogonal projections on E and F respectively.

□

4.2 Numerical experiments

This section is devoted to numerical computations on a square. In this case, we have

$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 \approx 0.509905.$$

We present computations of the eigenpairs realized by M. Dauge with the Finite Element Method code MELINA (cf [21]). For any h, we use a uniform mesh with 64 elements and tensor product polynomial of degree 10. When h is very small, very fast oscillations (cf Figure 4) appear on the eigenfunctions as expected in (12) and it is better to increase the degree of the polynomial than reduce the size of the mesh. We can note this by looking at [8, 2, 6] where we use an adapted mesh refinement based on a posteriori error estimates and a low order degree; we need many elements.
Figure 2 presents the behavior of the twelve first eigenvalues $\mu_{h,n}/h$ for $n = 1, \dots, 12$, as function of $1/h$. We draw the exponential tube

$$\lambda_1 \pm \exp\left(-\frac{r_1\sqrt{\Theta_0 - \lambda_1}}{\sqrt{h}}\right).$$

According to Theorem 4.2, we expect that the four first eigenvalues are concentrated in this tube.

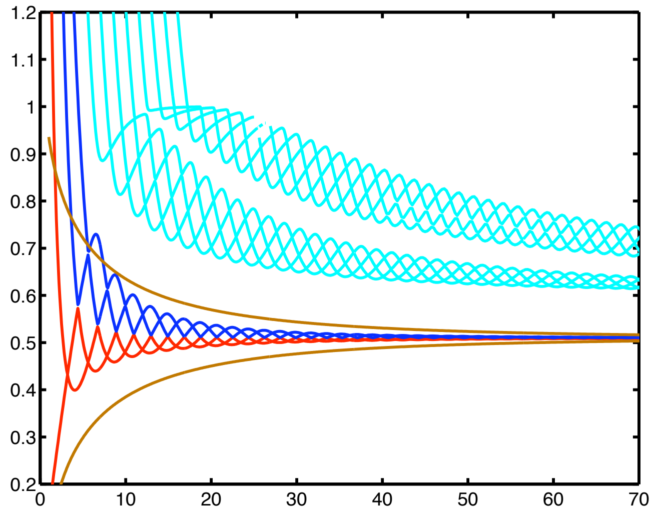

Figure 2: $h^{-1}\mu_{h,n}$ versus h^{-1}

Let us now present the modulus and the real part of the first eigenfunction according h in Figures 3 and 4 respectively. We can observe the exponential concentration near the corners in $\sqrt{h}$. Figure 4 displays concentration in $\mathrm{e}^{-c/\sqrt{h}}$ together with oscillations in $1/h$ which appear in the construction of the quasi-modes in (13). Looking at the symmetry of these figures, we see the linear combination of the four modes constructed from the quarter plane. Figure 2 is a numerical illustration of a tunnelling effect. We hope to propose a theoretical interpretation by analyzing an interaction matrix.

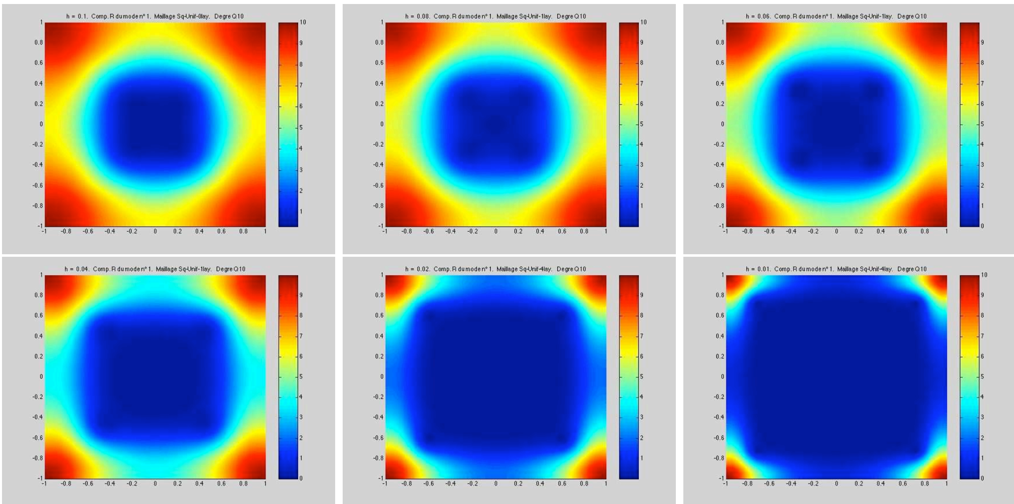

Figure 3: $h = 0.1,\ 0.08,\ 0.06,\ 0.04,\ 0.02,\ 0.01$

5 Conclusion

Even if we have given some informations about the bottom of the spectrum of Q^α as a function of α, an open problem is to prove the monotonicity of $\mu_1(\alpha)$.
Furthermore, this paper completes the results of Helffer-Morame [16], Jadallah [18], Pan [22] by dealing with the low-lying eigenstates of the Schrödinger operator with constant magnetic field in a polygon and proving the localization of the eigenfunctions. We can generalize these results (with some assumptions, cf [9]) to the Schrödinger operator with non constant magnetic field in a bounded open domain with a curvilinear boundary.

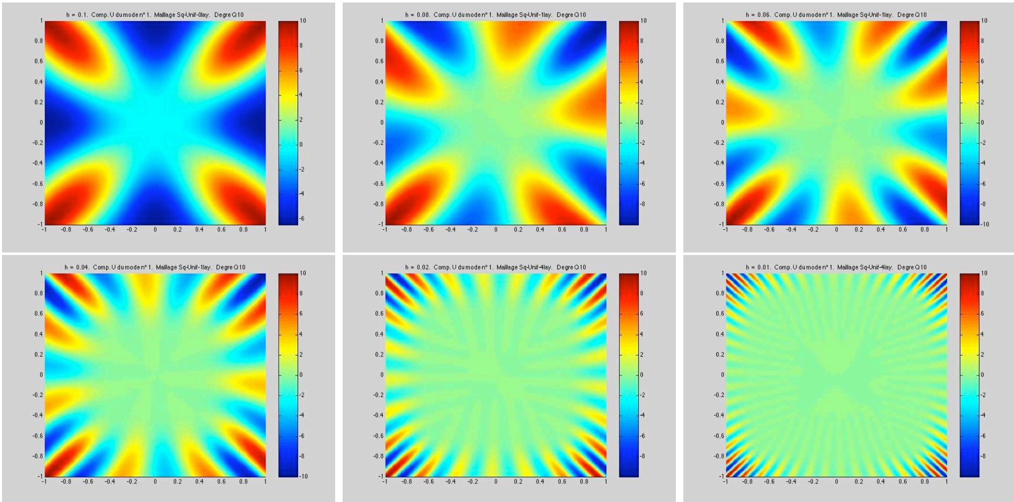

Figure 4: $h = 0.1,\ 0.08,\ 0.06,\ 0.04,\ 0.02,\ 0.01$

References

[1] AGMON, S. *Lectures on exponential decay of solutions of second-order elliptic equations: bounds on eigenfunctions of N-body Schrödinger operators*, vol. 29 of *Mathematical Notes*. Princeton University Press, Princeton, NJ, 1982.

[2] ALOUGES, F., AND BONNAILLIE, V. Analyse numérique de la supraconductivité. *C. R. Math. Acad. Sci. Paris 337*, 8 (2003), 543–548.

[3] BERNOFF, A., AND STERNBERG, P. Onset of superconductivity in decreasing fields for general domains. *J. Math. Phys. 39*, 3 (1998), 1272–1284.

[4] BONNAILLIE, V. *Analyse mathématique de la supraconductivité dans un domaine à coins; méthodes semi-classiques et numériques*. Thèse de doctorat, Université Paris XI - Orsay, 2003.

[5] BONNAILLIE, V. On the fundamental state for a Schrödinger operator with magnetic field in a domain with corners. *C. R. Math. Acad. Sci. Paris 336*, 2 (2003), 135–140.

[6] BONNAILLIE, V. Superconductivity in general domains. Prépublications d'Orsay 2004-09, 2004.

[7] BONNAILLIE, V. On the fundamental state energy for a Schrödinger operator with magnetic field in domains with corners. *Asymptot. Anal. 41*, 3-4 (2005), 215–258.

[8] BONNAILLIE NOËL, V. A posteriori error estimator for the eigenvalue problem associated to the Schrödinger operator with magnetic field. *Numer. Math. 99*, 2 (2004), 325–348.

[9] BONNAILLIE NOËL, V., AND DAUGE, M. Asymptotics for the low-lying eigenstates of the Schrödinger operator with magnetic field near corner. In preparation, 2005.

[10] CYCON, H. L., FROESE, R. G., KIRSCH, W., AND SIMON, B. *Schrödinger operators with application to quantum mechanics and global geometry*, study ed. Texts and Monographs in Physics. Springer-Verlag, Berlin, 1987.

[11] DAUGE, M., AND HELFFER, B. Eigenvalues variation. I. Neumann problem for Sturm-Liouville operators. *J. Differential Equations 104*, 2 (1993), 243–262.

[12] FOURNAIS, S., AND HELFFER, B. Accurate eigenvalue estimates for the magnetic neumann laplacian. *To appear in Annales Inst. Fourier* (2005).

[13] GINZBURG, V., AND LANDAU, L. On the theory of the superconductivity. *Soviet. Phys. JETP 20* (1950), 1064–1082.

[14] HELFFER, B. *Semi-classical analysis for the Schrödinger operator and applications*, vol. 1336 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1988.

[15] HELFFER, B., AND MOHAMED, A. Semiclassical analysis for the ground state energy of a Schrödinger operator with magnetic wells. *J. Funct. Anal. 138*, 1 (1996), 40–81.

[16] HELFFER, B., AND MORAME, A. Magnetic bottles in connection with superconductivity. *J. Funct. Anal. 185*, 2 (2001), 604–680.

[17] HELFFER, B., AND SJÖSTRAND, J. Multiple wells in the semiclassical limit. I. *Comm. Partial Differential Equations 9*, 4 (1984), 337–408.

[18] JADALLAH, H. T. The onset of superconductivity in a domain with a corner. *J. Math. Phys. 42*, 9 (2001), 4101–4121.

[19] LU, K., AND PAN, X.-B. Estimates of the upper critical field for the Ginzburg-Landau equations of superconductivity. *Phys. D 127*, 1-2 (1999), 73–104.

[20] LU, K., AND PAN, X.-B. Gauge invariant eigenvalue problems in $\mathbf{R}^2$ and in $\mathbf{R}^2_+$. *Trans. Amer. Math. Soc. 352*, 3 (2000), 1247–1276.

[21] MARTIN, D. http://perso.univ-rennes1.fr/daniel.martin/melina.

[22] PAN, X.-B. Upper critical field for superconductors with edges and corners. *Calc. Var. Partial Differential Equations 14*, 4 (2002), 447–482.

[23] PERSSON, A. Bounds for the discrete part of the spectrum of a semi-bounded Schrödinger operator. *Math. Scand. 8* (1960), 143–153.

[24] SIMON, B. Semiclassical analysis of low lying eigenvalues. I. Nondegenerate minima: asymptotic expansions. *Ann. Inst. H. Poincaré Sect. A (N.S.) 38*, 3 (1983), 295–308.