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A posteriori error estimator for the eigenvalue problem associated to the Schrödinger operator with magnetic field

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Summary The ground state for the Neumann realization of the Schrödinger operator for constant and sufficiently large magnetic field presents a localization in the boundary of the domain and particularly in the corners where the angle is minimum. As the solution decreases exponentially fast away of the corner, it is rather difficult to catch it numerically. A natural idea is to try using a mesh refinement method coupled to a posteriori error estimates. The purpose of this paper is to provide such an estimator adapted to the problem.

Key words Eigenvalue problem, a posteriori error estimator, adaptative mesh refinement.

1 Introduction

A lot of papers have already been devoted to the Schrödinger operator with magnetic field among which we can quote those of Bernoff-Sternberg [7], Lu-Pan [21], Helffer-Morame [16] in the case of regular domains. Our goal is to establish similar results in a domain with edges. Physicists such as Brosens, Devreese, Fomin, Moshchalkov, Schweigert and Peeters and mathematicians like Jadallah and Pan contributed to the study of this problem in recent literature [13, 19, 24, 26]. A more general theoretical study can be found in [8, 9, 11] where we prove the exponential decay of the ground state outside corners with smallest angle for a constant and large magnetic field, we analyze the behavior according to the smallest angle and we give

an asymptotics of the eigenvalue for angle tending to 0.
In order to have a deeper understanding of the behavior of the first eigenpair according to the geometry of the domain, we employ numerical tools based on finite elements method. Since the first eigenvector decreases exponentially fast away of the smallest corner and is localized in a small neighborhood of the boundary, a numerical study is quite difficult and the problem badly conditioned. So it is necessary to find a criterion which determines, using only computed numerical solution and data of the problem, the spatial form of the error between numerical and exact solution. The fundamental tool is the a posteriori error estimator which allows to be more specific about local error and permit to adopt adaptive mesh-refinement techniques.

A posteriori error estimators have been studied in several domains. Maday, Patera and Peraire [23] propose a general formulation for a posteriori bounds for the eigenvalue problem but they consider uniform meshes. Their techniques are inefficient to use adaptative mesh refinement because they do not compute local error. For the Schrödinger operator with magnetic field, [11] proves that the first eigenvectors are localized in the boundary ; therefore adaptative mesh refinement techniques seem to be appropriate to gain computation time and for this, we need local error estimates. In this spirit, we can quote works of Babuška [2,4], Bernardi-Métivet [5], Bernardi-Métivet-Verfürth [6], Larson [20] who proposes a posteriori error estimates for the Laplacian operator with Dirichlet boundary conditions which can be extended to operators such $\sum_{i,j=1}^{d} \partial_{x_j} (a_{ij}(x)\partial_{x_i}) + b(x)$ with Robin boundary conditions, Maday-Turinici [22] who work more specifically about the nuclear hamiltonian. Some of these articles are based on the work of Verfürth [27] who tries to make a more systematic analysis of any problem. He begins with the Poisson equation with mixed boundary conditions and pursues with the nonlinear equation $F(u) = 0$. This permits to determine a posteriori error estimates for quasi-linear equations of second order or some eigenvalue problems for operators like $-\nabla \cdot (A\nabla) + d$ (cf Proposition 3.10 and Proposition 3.17 in [27]). We pursue in this way for another framework of operators and propose in this paper a posteriori error estimates in the case of the Neumann realization of the Schrödinger operator with constant magnetic field based also on the Verfürth techniques [27]. These estimates are able to give global and local information on the error of the numerical solution and so are efficient for using adaptative mesh refinement. We notice also that we obtain better estimates than Verfürth since the gap for the eigenvalue is of the order of the square of the estimate for the eigenvector, and so keep the same order of convergence as for a priori estimates (cf [3]). Heuveline-Rannacher [17] also deal with a posteriori error estimates for a convection-diffusion problem with a Galerkin finite element approximation of the problem. These estimates are based on the dual eigenvalue problem. We propose an easier formulation of a posteriori error estimates without using the dual problem.

This paper consists of two major parts. In Section 4, we adapt techniques of Verfürth. In order to do that, we use a functional F whose definition and study are developed in Section 3.2. To deal with this functional, we need an estimate of the gap between the numerical solution and the exact solution. This point is analyzed in Section 3 where Theorem 3.1 recalls classical a priori error estimates for the eigenvalue problem. Proofs of this result can be found in [3,11]. Let us begin with some notations in Section 2.

2 Notation and results

2.1 Physical problem

Let Ω be a bounded, open and polygonal set in $\mathbb{R}^2$. We denote by Γ the boundary of Ω and ν the unit outer normal where it is well defined. We consider the magnetic potential $\mathcal{A}$ with a constant magnetic field B defined by

$$\mathcal{A} = \frac{B}{2}(x_2, -x_1). \tag{2.1}$$

We are interested in the Neumann realization of $-(\nabla - i\mathcal{A})^2$ from $C_0^\infty(\overline{\Omega})$, which is the restriction to Ω of the functions in $C^\infty(\mathbb{R}^2)$ with a compact support. We define the sesquilinear form a in the form domain

$$Y := H^1_{\mathcal{A}}(\Omega) = \{u \in L^2(\Omega) | \nabla_{\mathcal{A}} u \in L^2(\Omega)\} \text{ with } \nabla_{\mathcal{A}} := \nabla - i\mathcal{A}, \tag{2.2}$$

by

$$a(u,v) = \int_\Omega \nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} v}\, dx,\ \forall u,\ v\ \in H^1_{\mathcal{A}}(\Omega). \tag{2.3}$$

The sesquilinear form a is semi bounded from below and so a admits a unique self-adjoint extension $-\Delta_{\mathcal{A}} := -\nabla^2_{\mathcal{A}}$ defined on the domain

$$\mathcal{D}^N(-\Delta_{\mathcal{A}}) := \left\{u \in H^1_{\mathcal{A}}(\Omega) |\ \nabla^2_{\mathcal{A}} u \in L^2(\Omega),\ \nu \cdot \nabla_{\mathcal{A}} u_{|\partial\Omega^*} = 0\right\},$$

where $\partial\Omega^*$ denotes points of the boundary of Ω where the unit outward normal is well defined. Furthermore, due to integration by parts, the following relation holds

$$\forall u \in \mathcal{D}^N(-\Delta_{\mathcal{A}}),\ \forall v \in Y,\ \langle -\Delta_{\mathcal{A}} u, v\rangle_{L^2(\Omega)} = a(u,v). \tag{2.4}$$

For every open set ω of Ω, we denote by γ the boundary of ω, $L^2(\omega)$, $H^1_{\mathcal{A}}(\omega)$ and $H^2_{\mathcal{A}}(\omega)$ the Sobolev spaces with the norms

$$||\phi||_{L^2(\omega)} = \left\{ \int_\omega |\phi|^2 \, dx \right\}^{1/2}, \tag{2.5}$$

$$||\phi||_{H^1_{\mathcal{A}}(\omega)} = \left\{ \int_\omega (|\phi|^2 + |\nabla_{\mathcal{A}}\phi|^2) \, dx \right\}^{1/2}, \tag{2.6}$$

$$||\phi||_{H^2_{\mathcal{A}}(\omega)} = \left\{ \int_\omega (|\phi|^2 + |\nabla_{\mathcal{A}}\phi|^2 + |\nabla^2_{\mathcal{A}}\phi|^2) \, dx \right\}^{1/2}. \tag{2.7}$$

Remark 2.1 As Ω is bounded, the norms $||\ ||_{H^1(\omega)}$ and $||\ ||_{H^1_{\mathcal{A}}(\omega)}$ are equivalent, like the norms $||\ ||_{H^2(\omega)}$ and $||\ ||_{H^2_{\mathcal{A}}(\omega)}$.

Our goal is to determine the ground state for the operator $-\Delta_{\mathcal{A}}$. Before being more specific about the first eigenvalue, we give the weak formulation to the eigenvalue problem, denoting by $X := \mathbb{R} \times Y$:

$$\text{Find } (\lambda, u) \in X \text{ s.t. } \forall (\mu, v) \in X,\ \begin{cases} \displaystyle\int_\Omega \nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} v} = \lambda \int_\Omega u\overline{v}, \\ \displaystyle\int_\Omega |u|^2 = 1. \end{cases} \tag{2.8}$$

We denote by $(\lambda_k, u_k)_k$ the solution of (2.8) with

$$0 < \lambda_1 \leq \lambda_2 \leq \ldots \lambda_k.$$

We omit the index 1 when there is no confusion. The min-max principle gives the expression of λ_1 by

$$\lambda_1 = \inf_{v \in H^1_{\mathcal{A}}(\Omega), v \neq 0} \frac{||\nabla_{\mathcal{A}} v||^2_{L^2(\Omega)}}{||v||^2_{L^2(\Omega)}}. \tag{2.9}$$

Due to spectral theory, we know that if (λ, u) is solution of (2.8), then $u \in \mathcal{D}^N(-\Delta_{\mathcal{A}})$ and $u \in H^2(\Omega)$ as soon as Ω is bounded.

Remark 2.2 It is proved in [11] that the bottom of the spectrum of $-\Delta_{\mathcal{A}}$ is simple if Ω has only one corner with a smallest angle α with α small enough. We think that λ_1 stays simple as soon as α is acute but it is not proved for the time being. From now, we assume that the smallest eigenvalue λ_1 is simple.

We can not determine an exact solution of (2.8), so we look for a numerical solution and want to determine the gap between the exact solution and the approximate solution given by the finite elements method. We use the same notations as Verfürth [27], p. 7-8. Let $\mathcal{T}_h$, $h > 0$ be a family of triangulations of Ω satisfying the conditions :

1. Any two triangles in $\mathcal{T}_h$ share at most a common complete edge or a common vertex.
2. The minimal angle of all triangles in the whole family $\mathcal{T}_h$ is bounded from below by a strictly positive constant.

Let $Y_h := \mathbb{P}^k(\mathcal{T}_h)$ be the space of all continuous piecewise polynomial function of degree k. We denote by $X_h := \mathbb{R} \times Y_h$ and consider the following eigenvalue problem

$$\text{Find } (\lambda_h, u_h) \in X_h \text{ s.t.}$$
$$\forall(\mu_h, v_h) \in X_h, \quad \begin{cases} \displaystyle\int_\Omega \nabla_{\mathcal{A}} u_h \cdot \overline{\nabla_{\mathcal{A}} v_h} = \lambda_h \int_\Omega u_h \overline{v}_h, \\ \displaystyle\int_\Omega |u_h|^2 = 1, \end{cases} \tag{2.10}$$

We denote by $(\lambda_{k,h}, u_{k,h})_k$ the solution of (2.10) with

$$0 < \lambda_{1,h} \leq \lambda_{2,h} \leq \ldots \lambda_{k,h}.$$

We omit the index 1 when there is no confusion. The min-max principle allows to write the approximate bottom of the spectrum by

$$\lambda_{1,h} = \inf_{v_h \in \mathbb{P}^k(\mathcal{T}_h), v_h \neq 0} \frac{||\nabla_{\mathcal{A}} v_h||^2_{L^2(\Omega)}}{||v_h||^2_{L^2(\Omega)}}. \tag{2.11}$$

For (λ_k, u_k) and $(\lambda_{k,h}, u_{k,h})$ respectively solution of (2.8) and (2.10), we want to estimate the gap $|\lambda_k - \lambda_{k,h}|$ and $||u_k - u_{k,h}||_{L^2(\Omega)}$.

2.2 Notation

For any element T of the triangulation $\mathcal{T}_h$, we denote by $\mathcal{E}(T)$ and $\mathcal{N}(T)$ the set of its edges and vertices respectively and we define

$$\mathcal{E}_h := \bigcup_{T \in \mathcal{T}_h} \mathcal{E}(T) \text{ and } \mathcal{N}_h := \bigcup_{T \in \mathcal{T}_h} \mathcal{N}(T).$$

For $T \in \mathcal{T}_h$ and $E \in \mathcal{E}_h$, we define ρ_T, h_T and h_E their radius of inscribed circle, diameter and length, respectively. We assume h_T, $h_E < h$. We remark that if the triangulation satisfies the condition 2, then the ratio $\frac{h_T}{h_E}$ and $\frac{h_T}{h_{T'}}$ are bounded from below independently of h for every $T,\ T' \in \mathcal{T}_h$ such that $\mathcal{N}(T) \cap \mathcal{N}(T') \neq \emptyset$, and for every $E \in \mathcal{E}(T)$. We split $\mathcal{E}_h$ and $\mathcal{N}_h$ as follow :

$$\mathcal{E}_h = \mathcal{E}_{h,\Omega} \cup \mathcal{E}_{h,\Gamma} \text{ and } \mathcal{N}_h = \mathcal{N}_{h,\Omega} \cup \mathcal{N}_{h,\Gamma},$$

with :

$$\mathcal{E}_{h,\Omega} := \{E \in \mathcal{E}_h | E \subset \Omega\},\ \mathcal{E}_{h,\Gamma} := \{E \in \mathcal{E}_h | E \subset \Gamma\},$$
$$\mathcal{N}_{h,\Omega} := \{x \in \mathcal{N}_h | x \in \Omega\},\ \mathcal{N}_{h,\Gamma} := \{x \in \mathcal{N}_h | x \in \Gamma\}.$$

For any $E \in \mathcal{E}_h$, we denote by $\mathcal{N}(E)$ the set of its vertices. For $T \in \mathcal{T}_h$, $E \in \mathcal{E}_h$ and $x \in \mathcal{N}_h$, we define :

$$\omega_T := \bigcup_{\mathcal{E}(T)\cap\mathcal{E}(T')\neq\emptyset} T' : \quad \text{elements with common edges with } T,$$
$$\omega_E := \bigcup_{E\in\mathcal{E}(T')} T' : \quad \text{elements which admit } E \text{ as edge},$$
$$\tilde{\omega}_T := \bigcup_{\mathcal{N}(T)\cap\mathcal{N}(T')\neq\emptyset} T' : \quad \text{elements with a common vertex with } T,$$
$$\tilde{\omega}_E := \bigcup_{\mathcal{N}(E)\cap\mathcal{N}(T')\neq\emptyset} T' : \quad \text{elements with a common vertex with } E.$$

For any edge $E \in \mathcal{E}_h$, we associate a unit vector n_E (equal to ν if $E \subset \Gamma$). For any $E \in \mathcal{E}_{h,\Omega}$ and $\phi \in L^2(\omega_E)$ such that $\phi_{|_{T'}}$ is continuous on T' for any $T' \subset \omega_E$, we denote by $[\phi]_E$ the jump of ϕ across E in the direction n_E.

We now recall a property of the interpolation operator of Clément or Scott-Zhang, denoted by I_h and developed in [15,12,25]. This interpolation I_h sends $H^1(\Omega)$ onto $\mathbb{P}^k(\mathcal{T}_h)$.

Lemma 2.1 *There exists a constant c which depends on the regularity parameter of the triangulation, such that for any $u \in H^1(\Omega)$, $T \in \mathcal{T}_h$ and $E \in \mathcal{E}_h$:*

$$||u - I_h u||_{L^2(T)} \leq c h_T ||u||_{H^1(\tilde{\omega}_T)}, \tag{2.12}$$
$$||u - I_h u||_{L^2(E)} \leq c h_E^{1/2} ||u||_{H^1(\tilde{\omega}_E)}. \tag{2.13}$$

2.3 Main result

For any $(\lambda, u),\ (\mu, v) \in X$, we define

$$||(\lambda, u)||_X := \left\{ |\lambda|^2 + ||u||^2_{H^1_{\mathcal{A}}(\Omega)} \right\}^{1/2}, \tag{2.14}$$

$$\langle F(\lambda, u), (\mu, v)\rangle := \int_\Omega \left(\nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} v} - \lambda u \overline{v}\right) dx + \mu \left(\int_\Omega |u|^2 dx - 1\right). \tag{2.15}$$

Our goal is to find $(\lambda, u) \in X$ and $(\lambda_h, u_h) \in X_h$ with the smallest λ and λ_h such that :

$$\forall(\mu, v) \in X, \quad \langle F(\lambda, u), (\mu, v)\rangle \;=\; 0, \tag{2.16}$$
$$\forall(\mu_h, v_h) \in X_h, \langle F(\lambda_h, u_h), (\mu_h, v_h)\rangle = 0. \tag{2.17}$$

We introduce the a posteriori error indicator

$$\eta_T^2 := h_T^2 \int_T \left|-\nabla_{\mathcal{A}}^2 u_h - \lambda_h u_h\right|^2 + \sum_{E \in \mathcal{E}(T) \cap \mathcal{E}_{h,\Omega}} h_E \int_E |[n_E \cdot \nabla_{\mathcal{A}} u_h]_E|^2 . \tag{2.18}$$

As we see in the following theorem, the estimator η_T has a fundamental role to see if we are close to the exact solution or not and to increase accuracy of the numerical solution :

Theorem 2.1 *Let $(\lambda, u) \in X$ be a solution for the problem (2.16) and $(\lambda_h, u_h) \in X_h$ be a solution for the problem (2.17) such that λ and λ_h are the smallest eigenvalues of the continuous and discrete operators. Then, there exist $h_0 > 0$ and constants c_1, c_2 which depend only on the regularity parameter of the triangulation such that for all $h \leq h_0$:*

$$c_1 \sum_{T \in \mathcal{T}_h} \eta_T^2 \leq |\lambda - \lambda_h| \leq c_2 \sum_{T \in \mathcal{T}_h} \eta_T^2, \tag{2.19}$$

$$c_1 \sum_{T \in \mathcal{T}_h} \eta_T^2 \leq ||u - u_h||^2_{H^1_{\mathcal{A}}(\Omega)} \leq c_2 \sum_{T \in \mathcal{T}_h} \eta_T^2. \tag{2.20}$$

Remark 2.3 Theorem 2.1 holds also for any simple eigenvalue λ_k : there exists $R > 0$ such that if $(\lambda_{k,h}, u_{k,h})$ is a solution of (2.17) with $||(\lambda_k - \lambda_{k,h}, u_k - u_{k,h})||_X \leq R$, then (2.19) and (2.20) hold.
Estimates (2.19) and (2.20) are better than those of Verfürth where the gap for the eigenvalue and the eigenvector have the same order.

2.4 Scheme of the proof of Theorem 2.1

We want to use the same scheme as Verfürth [27], p. 81-84 for the eigenvalue problem for the operator $-\nabla \cdot (A\nabla) + d$ with a Dirichlet boundary condition. The fundamental point is to study the functional F and particularly, we have to find a neighborhood of $(\lambda, u) \in X$ on which the differential of F denoted DF is invertible. We will use DF to estimate the gap between $F(\lambda, u)$ and $F(\lambda_h, u_h)$ and for this, we first recall an a priori estimate in Section 3 of $||u - u_h||$. This is the great difference between our problem and examples presented by

Verfürth because our problem is not linear and we can't use classical argument like Cea's Lemma. Therefore, we propose a priori error estimate appropriate for $-\Delta_{\mathcal{A}}$. The study of the functional F is presented in Section 3.2 and will be used to follow the same techniques as Verfürth in Section 4 to give an a posteriori error estimate.

3 A priori estimates and applications to the study of F

3.1 A priori estimates

We just recall a priori error estimates proposed by [3]. We notice that in our case, we obtain easily these estimates (cf [11]) by the self-adjointness of the operator. Indeed, the Neumann realization of the Schrödinger operator $-\Delta_{\mathcal{A}}$ with constant magnetic field is self-adjoint with compact resolvent and so we can decompose each function of $\mathcal{D}^N(-\Delta_{\mathcal{A}})$ in an orthogonal basis of eigenvectors to obtain the following theorem.

Theorem 3.1 *There exists a constant $C > 0$ such that for solutions (λ_k, u_k) and $(\lambda_{k,h}, u_{k,h})$ of the continuous problem (2.16) and the discrete problem (2.17) respectively, with λ_k simple, the following upper bounds hold :*

$$\begin{aligned} ||u_k - u_{k,h}||_{H^1_{\mathcal{A}}(\Omega)} &\leq Ch, \\ |\lambda_k - \lambda_{k,h}| &\leq Ch^2. \end{aligned}$$

3.2 Study of the functional F

Let us give some properties of the functional F :

Lemma 3.1 *Let $(\lambda, u) \in X$ be the solution of problem (2.16), then the differential $DF(\lambda, u)$ is an isomorphism from X onto X^*.*

Proof We begin with the calculus of the differential DF at the point (λ, u). Let $(\mu, v) \in X$ and $(\nu, w) \in X$, then :

$$\langle DF(\lambda, u)(\mu, v), (\nu, w)\rangle = \int_{\Omega} \nabla_{\mathcal{A}} v \cdot \overline{\nabla_{\mathcal{A}} w} - (\lambda v + \mu u)\overline{w} + 2\nu u\overline{v}. \quad (3.1)$$

To justify the fact that $DF(\lambda, u)$ is an isomorphism from X onto X^*, we will use the following theorem given in [12] p. 131 :

Theorem 3.2 *Let U, V be two Hilbert spaces, then the application $L: U \to V'$ is an isomorphism if and only if the associated sesquilinear form $a: U \times V \to \mathbb{R}$ satisfies the three following conditions :*

1. Continuity : there exists a constant C such that :

$$\forall (u,v) \in U \times V,\ \ |a(u,v)| \le C||u||_U ||v||_V.$$

2. Inf-Sup condition : there exists a constant $\gamma > 0$ such that :

$$\inf_{u\in U} \sup_{v\in V} \frac{|a(u,v)|}{||u||_U ||v||_V} \ge \gamma.$$

3. For all $v \in V$, $v \neq 0$, there exists $u \in U$ such that $a(u,v) \neq 0$.

Let us apply this theorem by choosing $U = V = X$ and $a = DF(\lambda, u)$. We have to verify each condition of Theorem 3.2 :
1. Continuity : we consider $(\mu, v), (\nu, w) \in X$ and estimate :

$$\begin{aligned} |\langle DF(\lambda,u)(\mu,v),(\nu,w)\rangle| &\le ||\nabla_{\mathcal{A}} v||_{L^2(\Omega)} ||\nabla_{\mathcal{A}} w||_{L^2(\Omega)} + 2|\nu| ||v||_{L^2(\Omega)} \\ &\quad +(\lambda ||v||_{L^2(\Omega)} + |\mu|)||w||_{L^2(\Omega)} \\ &\le (4+\lambda)||(\mu,v)||_X ||(\nu,w)||_X. \end{aligned}$$

The condition *1.* holds.
2. Let us verify the Inf-Sup condition. We want to prove that there exists a strictly positive constant γ such that for all $(\mu, v) \in X$, there is $(\nu, w) \in X$ with $|\langle DF(\lambda,u)(\mu,v),(\nu,w)\rangle|$ bounded from below by $\gamma ||(\mu,v)||_X ||(\nu,w)||_X$. In order to show this, we establish the lower bound for some $(\nu, w) \in X$, dependent on (μ, v) and so deduce a lower bound by taking the upper limit. We decompose v and w like

$$v = \alpha u + \tilde{v} \text{ and } w = \beta u + \tilde{w} \text{ with } \int_\Omega u\overline{\tilde{v}} dx = 0,\ \int_\Omega u\overline{\tilde{w}} dx = 0.$$

Since (λ, u) is solution of the problem (2.16), we deduce that

$$\int_\Omega \nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} \tilde{v}}\ dx = 0 \text{ and } \int_\Omega \nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} \tilde{w}}\ dx = 0.$$

The norms in X of (μ, v) and (ν, w) write :

$$\begin{aligned} ||(\mu,v)||_X^2 &= ||\nabla_{\mathcal{A}} \tilde{v}||^2_{L^2(\Omega)} + ||\tilde{v}||^2_{L^2(\Omega)} + (\lambda+1)\alpha^2 + \mu^2, \\ ||(\nu,w)||_X^2 &= ||\nabla_{\mathcal{A}} \tilde{w}||^2_{L^2(\Omega)} + ||\tilde{w}||^2_{L^2(\Omega)} + (\lambda+1)\beta^2 + \nu^2. \end{aligned}$$

We compute the form $\langle DF(\lambda,u)(\mu,v),(\nu,w)\rangle$:

$$\begin{aligned} &\langle DF(\lambda,u)(\mu,v),(\nu,w)\rangle \\ &= \alpha \int_\Omega \nabla_{\mathcal{A}} u \cdot \overline{\nabla_{\mathcal{A}} w} - \lambda u \overline{w} + \int_\Omega \nabla_{\mathcal{A}} \tilde{v} \cdot \overline{\nabla_{\mathcal{A}} w} - (\lambda \tilde{v} + \mu u)\overline{w} + 2\nu\alpha \\ &= 2\nu\alpha - \mu\beta + \int_\Omega \beta(\nabla_{\mathcal{A}} \tilde{v} \cdot \overline{\nabla_{\mathcal{A}} u} - \lambda \tilde{v}\overline{u}) + \nabla_{\mathcal{A}} \tilde{v} \cdot \overline{\nabla_{\mathcal{A}} \tilde{w}} - (\lambda\tilde{v} + \mu u)\overline{\tilde{w}} \\ &= 2\nu\alpha - \mu\beta + \int_\Omega \nabla_{\mathcal{A}} \tilde{v} \cdot \overline{\nabla_{\mathcal{A}} \tilde{w}} - \lambda \tilde{v}\overline{\tilde{w}}. \end{aligned}$$

We choose $(\nu, w) \in X$ such that $\tilde{w} = \tilde{v}$, $\beta = -\mu$ and $\nu = \alpha$ then

$$\langle DF(\lambda, u)(\mu, v), (\nu, w)\rangle = ||\nabla_{\mathcal{A}}\tilde{v}||^2_{L^2(\Omega)} - \lambda||\tilde{v}||^2_{L^2(\Omega)} + \mu^2 + 2\alpha^2. \quad (3.2)$$

We bound from below $||\nabla_{\mathcal{A}}\tilde{v}||^2_{L^2(\Omega)} - \lambda||\tilde{v}||^2_{L^2(\Omega)}$ according to $||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)}$. We know that λ is the first eigenvalue of $-\Delta_{\mathcal{A}}$, then the second eigenvalue λ_2 is given by the min-max principle :

$$\lambda_2 = \inf_{\phi \in H^1_{\mathcal{A}}(\Omega) \cap <u>^{\perp}, \phi \neq 0} \frac{||\nabla_{\mathcal{A}}\phi||^2_{L^2(\Omega)}}{||\phi||^2_{L^2(\Omega)}}. \quad (3.3)$$

As we have decomposed w so that $\tilde{w} \perp u$,

$$||\nabla_{\mathcal{A}}\tilde{v}||^2_{L^2(\Omega)} \geq \lambda_2 ||\tilde{v}||^2_{L^2(\Omega)}. \quad (3.4)$$

Let $\delta \in]0, 1[$ be determined later. Relation (3.4) leads to the lower bound

$$||\nabla_{\mathcal{A}}\tilde{v}||^2_{L^2} - \lambda||\tilde{v}||^2_{L^2} \geq \delta||\nabla_{\mathcal{A}}\tilde{v}||^2_{L^2(\Omega)} + ((1-\delta)\lambda_2 - \lambda)||\tilde{v}||^2_{L^2(\Omega)}. \quad (3.5)$$

We choose δ such that $\delta = (1-\delta)\lambda_2 - \lambda$, then $\delta = \dfrac{\lambda_2 - \lambda}{\lambda_2 + 1} > 0$. We plug equality (3.2) into (3.5) :

$$\langle DF(\lambda, u)(\mu, v), (\nu, w)\rangle \geq \frac{\lambda_2 - \lambda}{\lambda_2 + 1}||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + \mu^2 + 2\alpha^2. \quad (3.6)$$

We have now to compare $\frac{\lambda_2 - \lambda}{\lambda_2 + 1}||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + \mu^2 + 2\alpha^2$ with the product of norms of (μ, v) and (ν, w). With the previous choice on (ν, w),

$$||(\nu, w)||^2_X = ||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + (\lambda + 1)\mu^2 + \alpha^2.$$

This implies $||(\nu, w)||_X ||(\mu, v)||_X \leq ||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + (\lambda + 1)(\mu^2 + \alpha^2)$. We take $\gamma = \inf\left(\dfrac{\lambda_2 - \lambda}{\lambda_2 + 1}, \dfrac{1}{\lambda + 1}\right)$, then :

$$\begin{aligned}\frac{\lambda_2 - \lambda}{\lambda_2 + 1}||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + \mu^2 + 2\alpha^2 &\geq \gamma\left(||\tilde{v}||^2_{H^1_{\mathcal{A}}(\Omega)} + (\mu^2 + \alpha^2)(\lambda + 1)\right) \\ &\geq \gamma||(\mu, v)||_X ||(\nu, w)||_X.\end{aligned}$$

We so have proved that for all $(\mu, v) \in X$:

$$\begin{aligned}\sup_{(\nu_1, w_1) \in X} \frac{|\langle DF(\lambda, u)(\mu, v), (\nu_1, w_1)\rangle|}{||(\nu_1, w_1)||_X} &\geq \frac{|\langle DF(\lambda, u)(\mu, v), (\nu, w)\rangle|}{||(\nu, w)||_X} \\ &\geq \gamma||(\mu, v)||_X,\end{aligned}$$

and the Inf-Sup condition holds.
3. Let us justify the last condition. Let $(\nu, w) \in X$, we decompose w in the form $w = \beta u + \tilde{w}$ such that $\tilde{w} \perp u$ and we consider :

$$(\mu, v) = (-\beta, \nu u + \tilde{w}) \in X.$$

As we have seen in the justification of the Inf-Sup condition, we have :

$$\frac{|\langle DF(\lambda, u)(\mu, v), (\nu, w)\rangle|}{||(\nu, w)||_X ||(\mu, v)||_X} \geq \gamma > 0,$$

so the third condition holds.
We get that $DF(\lambda, u)$ is an isomorphism from X onto X^* and the proof of Lemma 3.1 is achieved.

Remark 3.1 Let us notice that we can prove by this way that the differential $DF(\lambda_k, u_k)$ is an isomorphism from X onto X^* for any (λ_k, u_k) solution of (2.8) such that λ_k is a simple eigenvalue.
This result was proved by Verfürth for the operator $-\nabla \cdot (A\nabla) + d$ with a Dirichlet or Neumann condition. We extend this result for the Schrödinger operator with magnetic field.

Corollary 3.1 *Let* $(\lambda, u) \in X$ *be the solution of problem (2.16) with the smallest* λ*, so there exist* $R > 0$ *and constants* $c_1,\ c_2 > 0$ *such that for any* $(\mu, v) \in \mathcal{B}_X((\lambda, u), R)$*, the following bound holds :*

$$c_1 ||F(\mu, v)||_{X^*} \leq ||(\lambda, u) - (\mu, v)||_X \leq c_2 ||F(\mu, v)||_{X^*}.$$

Proof First, we show that DF is Lipschitz-continuous in (λ, u). Let $(\tilde{\lambda}, \tilde{u})$, (μ, v), $(\nu, w) \in X$. We denote

$$(\Delta\lambda, \Delta u) = (\tilde{\lambda} - \lambda, \tilde{u} - u),$$

then :

$$\begin{aligned} &\left|\left\langle DF(\lambda, u)(\mu, v) - DF(\tilde{\lambda}, \tilde{u})(\mu, v), (\nu, w)\right\rangle\right| \\ &= \left|\int_\Omega (\tilde{\lambda} - \lambda) v\overline{w} + \mu(\tilde{u} - u)\overline{w} + 2\nu(u - \tilde{u})\overline{v}\right| \\ &\leq 4||(\Delta\lambda, \Delta u)||_X ||(\mu, v)||_X ||(\nu, w)||_X. \end{aligned}$$

Therefore, for any $(\tilde{\lambda}, \tilde{u}) \in X$,

$$\frac{||DF(\lambda, u) - DF(\tilde{\lambda}, \tilde{u})||_{\mathcal{L}(X, X^*)}}{||(\lambda, u) - (\tilde{\lambda}, \tilde{u})||_X} \leq 4. \tag{3.7}$$

We have already seen that $DF(\lambda,u)$ is an isomorphism, so we can express $(\tilde\lambda,\tilde u)$ with (λ,u) by :

$$(\Delta\lambda,\Delta u) = (\tilde\lambda,\tilde u) - (\lambda,u) = (DF(\lambda,u))^{-1}\Big(F(\tilde\lambda,\tilde u) + \int_0^1 \left(DF(\lambda,u) - DF((\lambda,u)+t(\Delta\lambda,\Delta u))\right)(\Delta\lambda,\Delta u)\ dt\Big).$$

This expression gives an estimate of the gap between (λ,u) and $(\tilde\lambda,\tilde u)$ according to the triangular inequality and relation (3.7) :

$$\begin{aligned}||(\Delta\lambda,\Delta u)||_X &\le ||(DF(\lambda,u))^{-1}||_{\mathcal{L}(X^*,X)} \times \left(||F(\tilde\lambda,\tilde u)||_X + 4\int_0^1 t\ dt||(\Delta\lambda,\Delta u)||_X^2\right)\\ &\le ||(DF(\lambda,u))^{-1}||_{\mathcal{L}(X^*,X)} \times \left(||F(\tilde\lambda,\tilde u)||_X + 2||(\Delta\lambda,\Delta u)||_X^2\right).\end{aligned}$$

We take $0 < R < R_1 := \frac{1}{4||DF(\lambda,u)^{-1}||_{\mathcal{L}(X^*,X)}}$, then for all $(\tilde\lambda,\tilde u)$ such that $(\tilde\lambda,\tilde u) \in \mathcal{B}_X((\lambda,u),R)$:

$$\begin{aligned}||(\tilde\lambda,\tilde u) - (\lambda,u)||_X &\le \frac{||DF(\lambda,u)^{-1}||_{\mathcal{L}(X^*,X)}||F(\tilde\lambda,\tilde u)||_{X^*}}{1-2R||DF(\lambda,u)^{-1}||_{\mathcal{L}(X^*,X)}}\\ &\le 2||DF(\lambda,u)^{-1}||_{\mathcal{L}(X^*,X)}||F(\tilde\lambda,\tilde u)||_{X^*}. \qquad (3.8)\end{aligned}$$

We now have to prove the second inequality. Let $(\mu,v) \in X$ with $||(\mu,v)||_X = 1$, then :

$$\left\langle F(\tilde\lambda,\tilde u),(\mu,v)\right\rangle = \langle DF(\lambda,u)(\Delta\lambda,\Delta u),(\mu,v)\rangle + \left\langle \int_0^1 \left(DF((\lambda,u)+t(\Delta\lambda,\Delta u)) - DF(\lambda,u)\right)(\Delta\lambda,\Delta u)dt,(\mu,v)\right\rangle.$$

We deduce an upper bound of $||F(\tilde\lambda,\tilde u)||_{X^*}$:

$$\begin{aligned}||F(\tilde\lambda,\tilde u)||_{X^*} &\le ||DF(\lambda,u)||_{\mathcal{L}(X,X^*)}||(\Delta\lambda,\Delta u)||_X + 4\int_0^1 t\ dt||(\Delta\lambda,\Delta u)||_X^2\\ &\le ||DF(\lambda,u)||_{\mathcal{L}(X,X^*)}||(\Delta\lambda,\Delta u)||_X + 2||(\Delta\lambda,\Delta u)||_X^2.\end{aligned}$$

Taking $0 < R < R_2 := \frac{||DF(\lambda,u)||_{\mathcal{L}(X,X^*)}}{2}$, we see that for all $(\tilde\lambda,\tilde u)$ in $\mathcal{B}_X((\lambda,u),R)$:

$$||F(\tilde\lambda,\tilde u)||_{X^*} \le 2||DF(\lambda,u)||_{\mathcal{L}(X,X^*)}||(\Delta\lambda,\Delta u)||_X. \qquad (3.9)$$

Choosing $R := \min(R_1, R_2)$, relations (3.8) and (3.9) justify Corollary 3.1 with $c_1 = \frac{||DF(\lambda,u)||^{-1}_{\mathcal{L}(X,X^*)}}{2}$ and $c_2 = 2||(DF(\lambda,u))^{-1}||_{\mathcal{L}(X^*,X)}$.

4 Adaptation of Verfürth's techniques

4.1 Preliminary lemmas

We have defined the projector I_h from $H^1_{\mathcal{A}}(\Omega)$ onto $\mathbb{P}^k(\mathcal{T}_h)$ and we consider $R_h := (0, I_h)$.

Lemma 4.1 *Let $(\lambda_h, u_h) \in X_h$ be solution of (2.17) and $(\mu, v) \in X$, then :*

$$\langle F(\lambda_h, u_h), (\mu, v)\rangle = \sum_{T\in\mathcal{T}_h} \left(\int_T (-\nabla^2_{\mathcal{A}} - \lambda_h) u_h \overline{v} + \sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} \int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \, \overline{v} \right). \quad (4.1)$$

Proof Since $(\lambda_h, u_h) \in X_h$ is solution of (2.17), u_h is normalized, so

$$\langle F(\lambda_h, u_h), (\mu, v)\rangle = \int_\Omega \nabla_{\mathcal{A}} u_h \cdot \overline{\nabla_{\mathcal{A}} v} - \lambda_h u_h \overline{v},$$

An integration by parts on each $T \subset \Omega$ gives :

$$\int_T \nabla_{\mathcal{A}} u_h \cdot \overline{\nabla_{\mathcal{A}} v} = -\int_T \nabla^2_{\mathcal{A}} u_h \overline{v} + \sum_{E\in\mathcal{E}(T)} \int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \, \overline{v}.$$

Furthermore, if $E \in \mathcal{E}_{h,\Gamma}$, then $[n_E \cdot \nabla_{\mathcal{A}} u_h]_E$ vanishes since we deal with the Neumann realization and $n_E \cdot \nabla_{\mathcal{A}} u_{h|_E} = 0$. We deduce (4.1).

Lemma 4.2 *Let $(\lambda_h, u_h) \in X_h$ be solution of (2.17), then there exists a constant C which depends only on the regularity parameter such that :*

$$||(Id - R_h)^* F(\lambda_h, u_h)||_{X^*} \le C \left\{ \sum_{T\in\mathcal{T}_h} \eta_T^2 \right\}^{1/2}. \quad (4.2)$$

Proof We begin with writing the definition of the norm $||.||_{X^*}$:

$$||(Id - R_h)^* F(\lambda_h, u_h)||_{X^*} = \sup_{||(\mu,v)||_X = 1} \langle F(\lambda_h, u_h), (\mu, v - I_h v)\rangle . \quad (4.3)$$

We compute the right hand side of (4.3) with Lemma 4.1

$$\langle F(\lambda_h, u_h), (\mu, v - I_h v)\rangle = \sum_{T\in\mathcal{T}_h} \Big[\int_T (-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h \overline{(v - I_h v)} \qquad (4.4)$$
$$+ \sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} \int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{(v - I_h v)} \Big].$$

We estimate each term with a Cauchy-Schwarz inequality coupled with Lemma 2.1 to obtain

$$\left| \int_T (-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h \overline{(v - I_h v)} \right| \le c_1 h_T ||v||_{H^1(\tilde\omega_T)} ||(-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h||_{L^2(T)}, \qquad (4.5)$$

$$\left| \int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{(v - I_h v)} \right| \le c_2 h_E^{1/2} ||v||_{H^1(\tilde\omega_E)} ||[n_E \cdot \nabla_{\mathcal{A}} u_h]_E||_{L^2(E)}. \qquad (4.6)$$

We report (4.6) in (4.4) and use the Hölder inequality :

$$\sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} \int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{(v - I_h v)}$$
$$\le C_2 \sqrt{\sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} h_E \int_E |[n_E \cdot \nabla_{\mathcal{A}} u_h]_E|^2} \sqrt{\sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} ||v||^2_{H^1(\tilde\omega_E)}}.$$

Since $||v||^2_{H^1(\tilde\omega_E)} \le ||v||^2_{H^1(\Omega)}$, there exists a constant c only depending on the regularity parameter of the triangulation such that

$$\sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} ||v||^2_{H^1(\tilde\omega_E)} \le c||v||^2_{H^1(\Omega)}. \qquad (4.7)$$

According to the inequality $\sqrt{A} + \sqrt{B} \le \sqrt{2}\sqrt{A+B}$ used in (4.4) coupled with (4.5), (4.6) and (4.7), there exists $C > 0$ depending only on the regularity parameter of the triangulation such that :

$$\langle F(\lambda_h, u_h), (\mu, v - I_h v)\rangle \le C||v||_{H^1(\Omega)} \Big(\sum_{T\in\mathcal{T}_h} h_T^2 \int_T |(-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h|^2$$
$$+ \sum_{E\in\mathcal{E}_{h,\Omega}\cap\mathcal{E}(T)} h_E \int_E |[n_E \cdot \nabla_{\mathcal{A}} u_h]_E|^2 \Big)^{\frac{1}{2}}.$$

Since the norms $H^1(\Omega)$ and $H^1_{\mathcal{A}}(\Omega)$ are equivalent, we deduce

$$\langle F(\lambda_h, u_h), (\mu, v - I_h v)\rangle \le \tilde C \left(\sum_{T\in\mathcal{T}_h} \eta_T^2 \right)^{1/2} ||v||_{H^1_{\mathcal{A}}(\Omega)}. \qquad (4.8)$$

To come back to the calculation of $||(Id - R_h)^* F(\lambda_h, u_h)||_{X^*}$, we use (4.3) and (4.8) and the fact that $||v||_{H^1_{\mathcal{A}}(\Omega)} \leq ||(\mu, v)||_X = 1$. Therefore, we achieve the proof of Lemma 4.2.

Before the following lemma, we recall some notations and properties developed in [27]. For every $T \in \mathcal{T}_h$ and $E \in \mathcal{E}_{h,\Omega}$, we define the triangle-bubble function b_T and the edge-bubble function b_E by

$$b_T = \begin{cases} 27\lambda_{T,1}\lambda_{T,2}\lambda_{T,3} & \text{on } T \\ 0 & \text{on } \Omega \setminus T, \end{cases} \tag{4.9}$$

where $\lambda_{T,1}$, $\lambda_{T,2}$ and $\lambda_{T,3}$ are the barycentric coordinates of T. Given an $E \in \mathcal{E}_{h,\Omega}$ such that $\omega_E = T_1 \cup T_2$. We enumerate the vertices of T_1 and T_2 in the such way the vertices of E are numbered first. We define the edge-bubble function b_E by

$$b_E = \begin{cases} 4\lambda_{T_i,1}\lambda_{T_i,2} & \text{on } T_i, \; i = 1, 2 \\ 0 & \text{on } \Omega \setminus \omega_E. \end{cases} \tag{4.10}$$

We consider the lifting prolongation operator $P\colon L^\infty(E) \to L^\infty(T)$ by

$$Pu(x) \colon= u(x'), \; \forall x \in T, x' \in E \; s.\,t. \; \lambda_j(x') = \lambda_j(x).$$

We denote by $\tilde{X}_h \colon= \mathbb{R} \times \tilde{Y}_h$ with

$$\tilde{Y}_h \colon= span\{b_T v, b_E P\sigma | \; v \in \Pi_{k+2|_T}, \sigma \in \Pi_{k+1|_E}, T \in \mathcal{T}_h, E \in \mathcal{E}_{h,\Omega}\}.$$

We use a particular case of Lemma 3.3 of [27] p. 59 and recall it now.

Lemma 4.3 (Verfürth [27], Lemma 3.3 p. 59) *There exist constants $c_1, \ldots, c_7$ such that for any $T \in \mathcal{T}_h$, $E \in \mathcal{E}(T)$, $u \in \Pi_{k+2|_T}$ and $\sigma \in \Pi_{k+1|_E}$, the following inequalities hold :*

$$c_1 ||u||_{L^2(T)} \leq \sup_{v \in \Pi_{k+2|_T}} \frac{\int_T u \overline{b_T v}}{||v||_{L^2(T)}} \leq ||u||_{L^2(T)}, \tag{4.11}$$

$$c_2 ||\sigma||_{L^2(E)} \leq \sup_{\tau \in \Pi_{k+1|_E}} \frac{\int_E \sigma \overline{b_E \tau}}{||\tau||_{L^2(E)}} \leq ||\sigma||_{L^2(E)}, \tag{4.12}$$

$$c_3 h_T^{-1} ||b_T u||_{L^2(T)} \leq ||\nabla(b_T u)||_{L^2(T)} \leq c_4 h_T^{-1} ||b_T u||_{L^2(T)}, \tag{4.13}$$

$$c_5 h_T^{-1} ||b_E P\sigma||_{L^2(T)} \leq ||\nabla(b_E P\sigma)||_{L^2(T)} \leq c_6 h_T^{-1} ||b_E P\sigma||_{L^2(T)}, \tag{4.14}$$

$$||b_E P\sigma||_{L^2(T)} \leq c_7 h_T^{1/2} ||\sigma||_{L^2(E)}. \tag{4.15}$$

Lemma 4.4 *Let* $(\lambda_h, u_h) \in X_h$ *be a solution of (2.17), then there exists a constant* $\tilde{C}$ *which depends on the regularity parameter such that :*

$$\eta_T \leq \tilde{C} \sup_{(0,v)\in\tilde{X}_h, \operatorname{supp} v\subset\omega_T} \frac{\langle F(\lambda_h, u_h), (0, v)\rangle}{||(0, v)||_X}. \tag{4.16}$$

Proof Let us give $T \in \mathcal{T}_h$ and $E \in \mathcal{E}_{h,\Omega} \cap \mathcal{E}(T)$. We recall that

$$\eta_T^2 = h_T^2 \int_T \left|-\nabla_{\mathcal{A}}^2 u_h - \lambda_h u_h\right|^2 + \sum_{E\in\mathcal{E}(T)\cap\mathcal{E}_{h,\Omega}} h_E \int_E |[n_E \cdot \nabla_{\mathcal{A}} u_h]_E|^2 . \tag{4.17}$$

We consider $\omega \in \{T, \omega_E, \omega_T\}$ and denote :

$$\tilde{Y}_{h|_\omega} := \{\phi \in \tilde{Y}_h | \ \operatorname{supp}(\phi) \subset \omega\}.$$

We first study $|| - \nabla_{\mathcal{A}}^2 u_h - \lambda_h u_h||_{L^2(T)}$ by using Lemma 4.3 whose relation (4.13) gives the following bound for all $v \in \Pi_{k+2|_T}$

$$c_4^{-1} h_T \leq \frac{||b_T v||_{L^2(T)}}{||\nabla(b_T v)||_{L^2(T)}}. \tag{4.18}$$

Now we use inequality (4.11) with $u = -\nabla_{\mathcal{A}}^2 u_h - \lambda_h u_h$

$$c_1||(-\nabla_{\mathcal{A}}^2 - \lambda_h)u_h||_{L^2(T)} \leq \sup_{v\in\Pi_{k+2|_T}} \int_T \frac{(-\nabla_{\mathcal{A}}^2 u_h - \lambda_h u_h)\overline{b_T v}}{||v||_{L^2(\Omega)}}. \tag{4.19}$$

But, we know that $0 \leq b_T \leq 1$, so $||b_T v||_{L^2(\Omega)} \leq ||v||_{L^2(\Omega)}$. Then taking account of (4.18) and (4.19), we deduce

$$\begin{aligned}\tfrac{c_1 h_T}{c_4}||(-\nabla_{\mathcal{A}}^2 - \lambda_h)u_h||_{L^2(T)} &\leq \sup_{v\in\Pi_{k+2|_T}} \frac{||b_T v||_{L^2(\Omega)}\int_T (-\nabla_{\mathcal{A}}^2 - \lambda_h)u_h\overline{b_T v}}{||\nabla(b_T v)||_{L^2(T)}||v||_{L^2(\Omega)}} \\ &\leq \sup_{v\in\Pi_{k+2|_T}} \frac{\langle F(\lambda_h, u_h), (0, b_T v)\rangle}{||\nabla(b_T v)||_{L^2(T)}}.\end{aligned}$$

By construction of b_T, $b_T v \in H_0^1(T)$ and we apply the Poincaré inequality. So there exists a constant C_Ω such that for any $T \in \mathcal{T}_h$ and any function $v \in \Pi_{k+2|_T}$, the following inequality holds by using also the equivalence between norms $H^1(\Omega)$ and $H_{\mathcal{A}}^1(\Omega)$:

$$||\nabla(b_T v)||_{L^2(\Omega)} \geq C_\Omega||b_T v||_{H_{\mathcal{A}}^1(\Omega)}.$$

Furthermore, if $v \in \Pi_{k+2_{|T}}$, then $b_T v \in \tilde{Y}_{h|_T}$ and it follows that

$$\frac{c_1}{c_4} h_T ||(-\nabla^2_{\mathcal{A}} - \lambda_h) u_h||_{L^2(T)} \leq C \sup_{\phi \in \tilde{Y}_{h|_T}, ||\phi||_Y = 1} \langle F(\lambda_h, u_h), (0, \phi) \rangle . \tag{4.20}$$

We now estimate the term $||[n_E \cdot \nabla_{\mathcal{A}} u_h]_E||_{L^2(E)}$. We look at inequality (4.12) with $\sigma = [n_E \cdot \nabla_{\mathcal{A}} u_h]_E$. By the construction of the prolongation operator P, for any $\sigma \in \Pi_{k+1_{|T}}$, the equality $P\sigma_{|_E} = \sigma$ holds. Then :

$$\sup_{\sigma \in \Pi_{k+1_{|T}}} \frac{\int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{b_E \sigma}}{||\sigma||_{L^2(E)}} = \sup_{\sigma \in \Pi_{k+1_{|T}}} \frac{\int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{b_E P\sigma}}{||P\sigma||_{L^2(E)}}$$
$$\geq c_2 ||[n_E \cdot \nabla_{\mathcal{A}} u_h]_E||_{L^2(E)}. \tag{4.21}$$

But, according to Lemma 4.1 with $\mu = 0,\ v = b_E P\sigma$, we obtain

$$\int_E [n_E \cdot \nabla_{\mathcal{A}} u_h]_E \overline{b_E P\sigma} = \langle F(\lambda_h, u_h), (0, b_E P\sigma) \rangle + \int_{\omega_E} (\nabla^2_{\mathcal{A}} + \lambda_h) u_h \overline{b_E P\sigma}.$$

Then

$$c_2 ||[n_E \cdot \nabla_{\mathcal{A}} u_h]_E||_{L^2(E)} \leq \tag{4.22}$$
$$\sup_{\sigma \in \Pi_{k+1_{|E}} \setminus \{0\}} \frac{\left| \langle F(\lambda_h, u_h), (0, b_E P\sigma) \rangle - \int_{\omega_E} (-\nabla^2_{\mathcal{A}} - \lambda_h) u_h \overline{b_E P\sigma} \right|}{||P\sigma||_{L^2(E)}}.$$

Relation (4.14) leads to

$$c_6^{-1} \leq h_T^{-1} ||b_E P\sigma||_{L^2(T)} ||\nabla(b_E P\sigma)||^{-1}_{L^2(T)}. \tag{4.23}$$

Using now (4.15), we deduce

$$c_7^{-1} ||\sigma||^{-1}_{L^2(E)} = c_7^{-1} ||P\sigma||^{-1}_{L^2(E)} \leq h_T^{1/2} ||b_E P\sigma||^{-1}_{L^2(T)}. \tag{4.24}$$

We group together relations (4.23) and (4.24) to obtain :

$$\frac{h_E^{1/2}}{c_6 c_7} ||\sigma||^{-1}_{L^2(E)} \leq \sqrt{\frac{h_E}{h_T}} ||\nabla(b_E P\sigma)||^{-1}_{L^2(T)} \leq c_8 ||\nabla(b_E P\sigma)||^{-1}_{L^2(T)}, \tag{4.25}$$

where c_8 depends only on the regularity parameter. We use this upper bound to study (4.22) multiplied by $c_6^{-1} c_7^{-1} h_E^{1/2}$ and consider each term separately. We begin with the term :

$$\sup_{\sigma \in \Pi_{k+1_{|E}} \setminus \{0\}} \frac{h_E^{1/2}}{c_6 c_7} \frac{\langle F(\lambda_h, u_h), (0, b_E P\sigma) \rangle}{||\sigma||_{L^2(E)}} \leq$$
$$\sqrt{\frac{h_E}{h_T}} \sup_{\sigma \in \Pi_{k+1_{|E}} \setminus \{0\}} \frac{\langle F(\lambda_h, u_h), (0, b_E P\sigma) \rangle}{||\nabla(b_E P\sigma)||_{L^2(T)}}.$$

We use the Poincaré inequality on ω_E since $b_E P\sigma \in H_0^1(\omega_E)$, so there exists a constant c independent of E such that

$$\sup_{\sigma \in \Pi_{k+1|_E}\setminus\{0\}} \frac{\langle F(\lambda_h, u_h), (0, b_E P\sigma)\rangle}{||\nabla(b_E P\sigma)||_{L^2(T)}} \leq c \sup_{(0,v)\in \tilde{X}_{h|\omega_E}} \frac{\langle F(\lambda_h, u_h), (0, v)\rangle}{||(0,v)||_X}. \tag{4.26}$$

Let us look at the term $\frac{h_E^{1/2}}{c_7 c_6} \sup_{\sigma \in \Pi_{k+1|_E}\setminus\{0\}} \frac{\int_{\omega_E} (-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h \overline{b_E P\sigma}}{||\sigma||_{L^2(E)}}$.

We know that $0 \leq b_E \leq 1$ so $||b_E P\sigma||_{L^2(E)} \leq ||\sigma||_{L^2(E)}$. We use also relation (4.15) to deduce that :

$$||b_E P\sigma||_{L^2(\omega_E)} \leq 2c_7 \sqrt{h_{T_E}} ||\sigma||_{L^2(E)},$$

by defining $h_{T_E} := \sup_{T\in\omega_E} h_T$. Then :

$$\begin{aligned}
\frac{\sqrt{h_E}}{c_6 c_7} \sup_{\sigma \in \Pi_{k+1|_E}\setminus\{0\}} \frac{\int_{\omega_E} (-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h \overline{b_E P\sigma}}{||\sigma||_{L^2(E)}} &\leq 2\frac{\sqrt{h_E h_{T_E}}}{c_6} \\
&\times \sup_{\sigma \in \Pi_{k+1|_E}\setminus\{0\}} \frac{\int_{\omega_E} (-\nabla_{\mathcal{A}}^2 - \lambda_h) u_h \overline{b_E P\sigma}}{||b_E P\sigma||_{L^2(\omega_E)}} \\
&\leq C \sup_{\phi \in \tilde{Y}_{h|\omega_E}, ||\phi||_Y = 1} \langle F(\lambda_h, u_h), (0, \phi)\rangle .
\end{aligned} \tag{4.27}$$

Putting together relations (4.26), (4.27) and (4.22), we conclude :

$$\begin{aligned}
\sup_{\sigma \in \Pi_{k+1|_E}\setminus\{0\}} \frac{c_2 h_E^{1/2}}{c_6 c_7} ||[n_E \cdot \nabla_{\mathcal{A}} u_h]_E||_{L^2(E)} \leq \\
c \sup_{\phi \in \tilde{Y}_{h|\omega_E}, ||\phi||_Y = 1} \langle F(\lambda_h, u_h), (0, \phi)\rangle .
\end{aligned} \tag{4.28}$$

We just put upper bounds (4.28), (4.20) in the expression (4.17) of η_T, so there exists a constant $\tilde{C}$ which depends on the regularity parameter such that

$$\eta_T \leq \tilde{C} \sup_{(0,v)\in \tilde{X}_h, \operatorname{supp} v \subset \omega_T} \frac{\langle F(\lambda_h, u_h), (0, v)\rangle}{||(0,v)||_X}. \tag{4.29}$$

This concludes the proof of Lemma 4.4.

Lemma 4.5 *Let $(\lambda_h, u_h) \in X_h$ be a solution of (2.17), then there exists a constant C which depends on the regularity parameter such that :*

$$\left(\sum_{T\in\mathcal{T}_h} \eta_T^2\right)^{1/2} \leq C||F(\lambda_h, u_h)||_{\tilde{X}_h^*}. \tag{4.30}$$

Proof From the definition of the norm and the assumptions on (λ_h, u_h), we notice that :

$$||F(\lambda_h, u_h)||_{\tilde{X}_h^*} = \sup_{(0,v)\in\tilde{X}_h} \frac{\langle F(\lambda_h, u_h), (0, v)\rangle}{||(0, v)||_X}.$$

So, for all $\epsilon > 0$ and all $T \in \mathcal{T}_h$, there exists a function $v_T \in \tilde{Y}_h$ with support included in ω_T such that :

$$\begin{cases} \langle F(\lambda_h, u_h), (0, v_T)\rangle \geq 0, \\ \sup_{f\in\tilde{Y}_h, \operatorname{supp} f\subset\omega_T} \left|\frac{\langle F(\lambda_h, u_h), (0, f)\rangle}{||(0, f)||_X}\right|^2 \leq \left|\frac{\langle F(\lambda_h, u_h), (0, v_T)\rangle}{||(0, v_T)||_X}\right|^2 + \epsilon. \end{cases}$$

We define the function :

$$v := \sum_{T\in\mathcal{T}_h} \frac{v_T}{||(0, v_T)||_X},$$

then $v \in \tilde{Y}_h$ as a linear combination of elements of $\tilde{Y}_h$ and due to the triangular inequality, $||v||_Y \leq 1$. We take again the result of Lemma 4.4 and sum η_T^2 on elements of $\mathcal{T}_h$, then :

$$\sum_{T\in\mathcal{T}_h} \eta_T^2 \leq \tilde{C}^2 \sum_{T\in\mathcal{T}_h} \sup_{(0,w)\in\tilde{X}_h, \operatorname{supp} w\subset\omega_T} \left|\frac{\langle F(\lambda_h, u_h), (0, w)\rangle}{||(0, w)||_X}\right|^2. \quad (4.31)$$

Using the functions v_T :

$$\begin{aligned} \sum_{T\in\mathcal{T}_h} \eta_T^2 &\leq \tilde{C}^2 \sum_{T\in\mathcal{T}_h} \left(\left|\frac{\langle F(\lambda_h, u_h), (0, v_T)\rangle}{||(0, v_T)||_X}\right|^2 + \epsilon\right) \\ &\leq \tilde{C}^2 \left(\sum_{T\in\mathcal{T}_h} \frac{\langle F(\lambda_h, u_h), (0, v_T)\rangle}{||(0, v_T)||_X}\right)^2 + \tilde{C}^2 N\epsilon \\ &\leq \tilde{C}^2 |\langle F(\lambda_h, u_h), (0, v)\rangle|^2 + \tilde{C}^2 N\epsilon, \end{aligned} \quad (4.32)$$

with N an upper bound of the number of the triangulation's elements. Next, we take the upper limit on $(0, w)$ in $\tilde{X}_h$:

$$\sum_{T\in\mathcal{T}_h} \eta_T^2 \leq \tilde{C}^2 ||F(\lambda_h, u_h)||^2_{\tilde{X}_h^*} + \tilde{C}^2 N\epsilon. \quad (4.33)$$

So, making ϵ going to 0 leads to :

$$\left\{\sum_{T\in\mathcal{T}_h} \eta_T^2\right\}^{1/2} \leq \tilde{C}||F(\lambda_h, u_h)||_{\tilde{X}_h^*}, \quad (4.34)$$

with $\tilde{C}$ depending on the regularity parameter.

4.2 Proof of Theorem 2.1

• We begin with justifying the first inequality :

$$|\lambda - \lambda| + ||u - u_h||_{H^1_{\mathcal{A}}(\Omega)} \leq c\sqrt{\sum_{T \in \mathcal{T}_h} \eta_T^2}. \qquad (4.35)$$

Let $(\mu, v) \in X$ such that $||(\mu, v)||_X = 1$, then

$$\begin{aligned} &\langle F(\lambda_h, u_h), (\mu, v)\rangle \\ &= \langle F(\lambda_h, u_h), (\mu, v) - R_h(\mu, v)\rangle + \langle F(\lambda_h, u_h), R_h(\mu, v)\rangle . \end{aligned} \qquad (4.36)$$

We estimate the second member (4.36) according to preliminary lemmas. Lemma 4.2 leads to an upper bound of the first term of (4.36)

$$\langle F(\lambda_h, u_h), (\mu, v) - R_h(\mu, v)\rangle \leq C_1 \left\{ \sum_{T \in \mathcal{T}_h} \eta_T^2 \right\}^{1/2} . \qquad (4.37)$$

Furthermore, as (λ_h, u_h) is a solution of problem (2.17), then for $(\mu_h, v_h) \in X_h$,

$$\langle F(\lambda_h, u_h), (\mu_h, v_h)\rangle = 0.$$

But, for all $(\mu, v) \in X$, the operator R_h is defined so as to $R_h(\mu, v)$ is in X_h, so particularly

$$\forall (\mu, v) \in X,\ \langle F(\lambda_h, u_h), R_h(\mu, v)\rangle = 0. \qquad (4.38)$$

We report relations (4.38) and (4.37) in (4.36) and obtain an estimate for all $(\mu, v) \in X$, this leads to the upper bound

$$||F(\lambda_h, u_h)||_{X^*} \leq C_1 \left\{ \sum_{T \in \mathcal{T}_h} \eta_T^2 \right\}^{1/2} . \qquad (4.39)$$

Let R given by Corollary 3.1. If λ and λ_h are the smallest eigenvalues of the continuous and discrete operators such that (λ, u) and (λ_h, u_h) are respectively solution of (2.16) and (2.17), then applying Lemma 3.1, there exists a constant C such that

$$|\lambda - \lambda_h| \leq Ch^2 \text{ and } ||u - u_h||_{H^1_{\mathcal{A}}(\Omega)} \leq Ch. \qquad (4.40)$$

So, if h is small enough, $||(\lambda, u) - (\lambda_h, u_h)||_X < R$, then relation (4.39), Corollary 3.1 and inequality $|\lambda - \lambda_h| + ||u - u_h||_{H^1_{\mathcal{A}}(\Omega)} \leq \sqrt{2}||(\lambda, u) - (\lambda_h, u_h)||_X$ lead to

$$|\lambda - \lambda_h| + ||u - u_h||_{H^1_{\mathcal{A}}(\Omega)} \leq \sqrt{2}||(\lambda, u) - (\lambda_h, u_h)||_X \leq \sqrt{2}c \left\{ \sum_{T \in \mathcal{T}_h} \eta_T^2 \right\}^{1/2} .$$

• We have now to justify the estimate

$$c\left\{\sum_{T\in\mathcal{T}_h}\eta_T^2\right\}^{1/2} \leq |\lambda-\lambda_h| + ||u-u_h||_{H^1_{\mathcal{A}}(\Omega)}. \qquad (4.41)$$

Lemma 4.5 shows that

$$\left\{\sum_{T\in\mathcal{T}_h}\eta_T^2\right\}^{1/2} \leq c||F(\lambda_h,u_h)||_{\tilde{X}_h^*}.$$

Since $\tilde{X}_h \subset X$ then $||F(\lambda_h,u_h)||_{\tilde{X}_h^*} \leq ||F(\lambda_h,u_h)||_{X^*}$ and so

$$\left\{\sum_{T\in\mathcal{T}_h}\eta_T^2\right\}^{1/2} \leq c||F(\lambda_h,u_h)||_{X^*}. \qquad (4.42)$$

Corollary 3.1 proves that for any $(\mu,v)\in\mathcal{B}_X((\lambda,u),R)$, we have

$$c_1||F(\mu,v)||_{X^*} \leq ||(\lambda,u)-(\mu,v)||_X \leq c_2||F(\mu,v)||_{X^*}.$$

Then, according to Lemma 3.1, $||(\lambda,u)-(\lambda_h,u_h)||_X < R$ if the triangulation is thin enough and this leads to (4.41).
• We now improve in (4.35) and (4.41) the estimate of $|\lambda-\lambda_h|$. We notice, using also (2.9) and (2.11), that :

$$\int_\Omega |\nabla_{\mathcal{A}}u_h-\nabla_{\mathcal{A}}u|^2 = \lambda-2\lambda\ \mathrm{Re}\ \langle u,u_h\rangle_{L^2(\Omega)}+\lambda_h \geq \lambda-\lambda_h \geq 0. \quad (4.43)$$

We deduce from (4.35) that

$$||u-u_h||^2_{H^1_{\mathcal{A}}(\Omega)} \leq \tilde{c}\sum_{T\in\mathcal{T}_h}\eta_T^2. \qquad (4.44)$$

Using (4.43), we conclude that

$$|\lambda-\lambda_h| \leq ||u-u_h||^2_{H^1_{\mathcal{A}}(\Omega)} \leq \tilde{c}\sum_{T\in\mathcal{T}_h}\eta_T^2. \qquad (4.45)$$

Relation (4.41) leads to

$$c\sum_{T\in\mathcal{T}_h}\eta_T^2 \leq |\lambda-\lambda_h|^2+||u-u_h||^2_{H^1_{\mathcal{A}}(\Omega)} \leq ||u-u_h||^4_{H^1_{\mathcal{A}}(\Omega)}+||u-u_h||^2_{H^1_{\mathcal{A}}(\Omega)}, \qquad (4.46)$$

using (4.45). We deduce that there exists a constant C depending only on the parameter of the triangulation such that

$$\sum_{T\in\mathcal{T}_h} \eta_T^2 \leq C||u-u_h||^2_{H^1_{\mathcal{A}}(\Omega)}. \tag{4.47}$$

Coming back to (4.46) with relation (4.44), we conclude that

$$\tilde{C}\sum_{T\in\mathcal{T}_h} \eta_T^2 \leq |\lambda-\lambda_h|, \tag{4.48}$$

as soon as $\sum_{T\in\mathcal{T}_h} \eta_T^2$ is small enough to have a positive constant $\tilde{C}$.

5 Conclusion

We construct an a posteriori error estimate as in Theorem 2.1. This theorem is appropriate to improve numerical computations by using adaptative mesh-refinement techniques. To illustrate this, we consider for Ω an angular sector cutting smoothly by a piece of circle. We want to determine the first eigenpair (λ, u) of $-(\nabla - i\mathcal{A})^2$ on Ω with the magnetic field $B = \operatorname{curl}\mathcal{A}$ constant equal to 30 Teslas. We compute a first numerical eigenpair $(\lambda_h, u_h = \rho_h e^{i\theta_h})$ for this operator by a finite elements method and the local error η_T on each element T of the triangulation $\mathcal{T}_h$ of Ω. As soon as η_T is too large for some $T \in \mathcal{T}_h$, we refine this element T and compute a new solution on the new adaptative refined mesh till the indicator of the error $\sum_{T\in\mathcal{T}_h} \eta_T^2$ is small enough. Figures 5.1 give the mesh obtained by using the a posteriori error estimator developed here, jointly with a mesh refinement technique. The right figure is a zoom of the left

Fig. 5.1. Mesh obtained by this adaptative refinement method

Fig. 5.2. Modulus ρ_h of the first eigenfunction for $-\Delta_{\mathcal{A}}$

figure near the corner. Figure 5.2 gives the numerical modulus ρ_h of the first eigenvector computed on the refined mesh. These figures are taken from [1, 10] where a more systematic study of the dependence of λ_1 to the angle of the corner is provided numerically. These numerical results developed in [8, 10, 11] are useful to determine where the superconductivity appears. The a posteriori error estimate we obtain is a prolongation of results by Larson [20], Bernardi-Métivet [5], Bernardi-Métivet-Verfürth [6], Maday-Turinici [22] or Verfürth [27] for another framework of operator with the Schrödinger operator with magnetic field and a Neumann magnetic boundary condition. We propose for this operator a better estimate than Verfürth [27] for $-\nabla\cdot(A\nabla)+d$ and the a posteriori error estimate in Theorem 2.1 has the same order of convergence than for the a priori error estimate proposed by Babuška-Osborn [3] and recalled in Theorem 3.1.

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