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Computations of the first eigenpairs for the Schrödinger operator with magnetic field

V. Bonnaillie-Noël [a], M. Dauge [b,*], D. Martin [b], G. Vial [a]

[a] IRMAR, ENS Cachan Bretagne, CNRS, UEB F-35170 Bruz, France
[b] IRMAR (UMR CNRS 6625), Université de Rennes 1, F-35042 Rennes Cedex, France

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Abstract

This paper is devoted to computations of eigenvalues and eigenvectors for the Schrödinger operator with constant magnetic field in a domain with corners, as the semi-classical parameter h tends to 0. The eigenvectors corresponding to the smallest eigenvalues concentrate in the corners: They have a two-scale structure, consisting of a corner layer at scale $\sqrt{h}$ and an oscillatory term at scale h. The high frequency oscillations make the numerical computations particularly delicate. We propose a high order finite element method to overcome this difficulty. Relying on such a discretization, we illustrate theoretical results on plane sectors, squares, and other straight or curved polygons. We conclude by discussing convergence issues.

Keywords: Schrödinger operator: eigenvalues; Eigenvectors

1. Introduction

Superconductivity theory, modelled by Ginzburg and Landau, motivates investigations of the Schrödinger operator with magnetic field and Neumann boundary conditions in two-dimensional domains. The Schrödinger operator $-(h\nabla - i\mathscr{A})^2$ derives from a linearization of the Ginzburg–Landau functional and the behavior of its eigenvalues and eigenvectors as $h \to 0$ gives information about the onset of superconductivity in the material, see [6,7,13,14,20,29] for the general framework and [2,15–19,24,26,28] for more closely related questions concerning the Schrödinger operator.

We give the mathematical framework we will work within: let Ω denote a bounded polygonal domain in $\mathbb{R}^2$ and $\mathscr{A}$ the magnetic potential $\frac{1}{2}(-x_2, x_1)$ defined on $\mathbb{R}^2$. We investigate the behavior of the eigenpairs of the Neumann realization P_h on Ω for the Schrödinger operator $-(h\nabla - i\mathscr{A})^2$ as $h \to 0$. The variational space associated with P_h is $H^1(\Omega)$ and its domain is the subspace of functions u such that $P_h u \in L^2(\Omega)$ and $\nu \cdot (h\nabla - i\mathscr{A})u = 0$ on $\partial\Omega$, with ν denoting the unit normal to $\partial\Omega$.

Let us first mention that the Schrödinger operator P_h is gauge invariant in the sense of the following proposition:

Proposition 1.1. *Let $\phi \in H^2(\Omega)$, then u is an eigenvector associated with the eigenvalue μ for the operator $-(h\nabla - i\mathscr{A})^2$ if and only if $u_\phi := e^{i\phi/h}u$ is an eigenvector associated with the eigenvalue μ for the operator $-(\nabla - i(\mathscr{A} + \nabla\phi))^2$.*

In particular, the eigenvalues of the Schrödinger operator are the same for any potential $\tilde{\mathscr{A}}$ such that $\text{curl}\tilde{\mathscr{A}} = \text{curl}\mathscr{A}$. This allows the use of adapted gauges according to the domain.

In [10], a complete asymptotic expansion of low-lying eigenstates is exhibited for curvilinear polygonal domains and refined results are proved in the case when the domain has straight sides and the magnetic field is constant. The eigenmodes have a two-scale structure, in the form of the product of a corner layer at scale $\sqrt{h}$ with an oscillatory term at scale h. The latter makes the numerical

* Corresponding author. Tel.: +33 29 928 6049; fax: +33 29 928 6790.
E-mail address: monique.dauge@univ-rennes1.fr (M. Dauge).

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approximation delicate. *A posteriori* error estimates are used in [3,9] to determine localized mesh refinement in a low degree finite element method. We investigate here a finite element method using high degree polynomials, as described in Section 2.

It is proved in [10] that the study of the Schrödinger operator P_h in a domain with corners of openings $\alpha_1, \ldots, \alpha_J$, relies on those of the Schrödinger operator $Q^\alpha := -(\nabla - i\mathscr{A})^2$ on an infinite sector of opening α, for $\alpha = \alpha_1, \ldots, \alpha_J$. Section 3 is devoted to this operator. We show computations which make theoretical results more complete.

The next sections deal with the asymptotic behavior of the eigenstates of P_h as h goes to 0. We give numerical solutions which illustrate the clustering of eigenvalues, depending on the symmetries of the domain. Several particular polygonal domains are investigated, highlighting different points of the theory: Tunneling effect for the square, concentration in the lowest corners for the trapezoid, the rhombus or the L-shaped domain. We end with a curvilinear polygon for which the asymptotics is appreciably different.

We conclude the paper in Section 7 by numerical error curves for the specific case of a standard square of length 2, and $h = 0.02$. We compare the performances of "p-extensions" (increasing the polynomial degree on a fixed mesh), and of "h-extensions" (refining the mesh with a fixed degree). According to the magnitude of h, a locking phenomenon is present, stronger and stronger as $h \to 0$. A disturbing feature of this locking is the preasymptotic convergence to interior modes, corresponding to the lowest Landau level, significantly larger than the correct eigenvalues. Our conclusion is the necessity for using "p-extensions" if we wish to capture fine effects like the tunneling effect in symmetric domains.

2. General results on eigenvalue approximation

In the sequel, we will show numerical results of spectral approximations for the Schrödinger operator in various domains. We wish first to recall some facts on the numerical computation of eigenvalues and eigenvectors by a finite element Galerkin method, which serve as a basis to justify the relevance of our results.

Let us fix some notation:

- $\mu_{h,n}$ is the nth eigenvalue of the operator P_h,
- $u_{h,n}$ is a normalized associated eigenfunction in $\mathscr{V} = H^1(\Omega)$,
- $(\mathscr{T}^\ell)_{\ell>0}$ is a family of quadrilateral meshes, where ℓ is the maximum size of the elements (we changed the traditional h into ℓ since the letter h already stands for the small semi-classical parameter),
- $\mathbb{Q}_p$ is the standard space of polynomials of partial degree p in the reference square element,
- $\mathscr{V}^{\ell,p}$ is the conforming discrete variational space associated with the $\mathbb{Q}_p$-reference square element on the mesh $\mathscr{T}^\ell$,
- $(\mu_{h,n}^{\ell,p}, u_{h,n}^{\ell,p})$ is the nth discrete eigenpair of P_h in $\mathscr{V}^{\ell,p}$:
$$\int_\Omega (h\nabla - i\mathscr{A})u_{h,n}^{\ell,p} \cdot \overline{(h\nabla - i\mathscr{A})v}\,\mathrm{d}x = \mu_{h,n}^{\ell,p} \int_\Omega u_{h,n}^{\ell,p}\bar{v}\,\mathrm{d}x, \quad \forall v \in \mathscr{V}^{\ell,p}.$$

For the first eigenpair ($n = 1$) or, more generally, if $\mu_{h,n} \neq \mu_{h,n-1}$, it is known from [4,5,11] that the following Céa-like estimate holds

$$|\mu_{h,n} - \mu_{h,n}^{\ell,p}| \leqslant L_{h,n}^{\ell,p} \sup_{u\in M_{h,n}} \inf_{\chi\in\mathscr{V}^{\ell,q}} \|u - \chi\|_{\mathscr{V}}^2, \tag{1}$$

where $M_{h,n}$ is the set of normalized eigenvectors[1] associated with $\mu_{h,n}$ and $L_{h,n}^{\ell,p}$ a positive constant which, for each fixed $h > 0$ and $n \in \mathbb{N}$, is bounded as $\ell \to 0$ or $p \to \infty$. Moreover the corresponding estimate for eigenvectors reads: There exists an eigenvector $\tilde{u}_{h,n}$ associated with $\mu_{h,n}$ satisfying

$$\|\tilde{u}_{h,n} - u_{h,n}^{\ell,p}\|_{\mathscr{V}} \leqslant L_{h,n}^{\ell,p} \sup_{u\in M_{h,n}} \inf_{\chi\in\mathscr{V}^{\ell,q}} \|u - \chi\|_{\mathscr{V}}. \tag{2}$$

Thus, discretization errors on the eigenpairs are essentially bounded by the best approximation errors on the eigenvectors of P_h. We have to keep in mind that the latter closely depends on the semi-classical parameter h.

In the following, we will interpret the Galerkin approximations obtained for the eigenpairs, with respect to the asymptotic results of [10]. We emphasize the fact that, since by construction $\mathscr{V}^{\ell,p} \subset \mathscr{V}$, the computed eigenvalues will always be *greater* than the exact eigenvalue of same rank.

All the results displayed in this paper have been obtained with the Finite Elements Library Mélina, see [27]. Computations are mostly done with pretty coarse meshes (consisting of less than 100 quadrilaterals), but with high polynomial degree (10 in general, referred to as $\mathbb{Q}_{10}$-approximation). We justify our choice of a "p-extension" (where the degree p of polynomials is increased), rather than a "h-extension" (where the size ℓ of the elements is decreased), by the fact that– for the same number of degrees of freedom– a p-extension captures oscillations more accurately than a h-extension, see [1,22,23] for related questions concerning the Helmholtz equation and dispersion relations at high wave number. This point is discussed in more detail in Section 7.

3. Model operators in infinite sectors

This section is devoted to the study of the Schrödinger operator $-(\nabla - i\mathscr{A})^2$ in an infinite sector: The analysis of the operator P_h in a bounded domain with corners relies on this model situation. We first recall some theoretical results from [8] concerning the spectrum of the operator and, next, we show some numerical experiments which illustrate some of these results or give hints on how to extend them.

[1] If $\mu_{h,n} = \mu_{h,n-1}$, the set $M_{h,n}$ has to be modified accordingly.