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Convergence of a finite volume scheme to the eigenvalues of a Schrödinger operator

Thomas Koprucki, Robert Eymard, and Jürgen Fuhrmann

Abstract. We consider the approximation of a Schrödinger eigenvalue problem arising from the modeling of semiconductor nanostructures by a finite volume method in a bounded domain $\Omega \subset \mathbb{R}^d$. In order to prove its convergence, a framework for finite dimensional approximations to inner products in the Sobolev space $H_0^1(\Omega)$ is introduced which allows to apply well known results from spectral approximation theory.

This approach is used to obtain convergence results for a classical finite volume scheme for isotropic problems based on two point fluxes, and for a finite volume scheme for anisotropic problems based on the consistent reconstruction of nodal fluxes. In both cases, for two- and three-dimensional domains we are able to prove first order convergence of the eigenvalues if the corresponding eigenfunctions belong to $H^2(\Omega)$.

The construction of admissible meshes for finite volume schemes using the Delaunay-Voronoï method is discussed.

As numerical examples, a number of one-, two- and three-dimensional problems relevant to the modeling of semiconductor nanostructures is presented. In order to obtain analytical eigenvalues for these problems, a matching approach is used. To these eigenvalues, and to recently published highly accurate eigenvalues for the Laplacian in the L-shape domain, the results of the implemented numerical method are compared. In general, for piecewise H^2 regular eigenfunctions, second order convergence is observed experimentally.

1. Introduction

A characteristic feature of semiconductor nanostructures is the abrupt change of the material properties such as chemical composition, band-edges or the effective mass parameters at the interface between two semiconductor materials on a distance smaller than a nanometer. This allows to utilize them for the confinement of the carriers in one-, two- or three-dimensional spatial domains corresponding to quantum well, quantum wire and quantum dot structures, respectively. Quantum effects due to the size-quantization given by the length scale of the nanostructure are arising and dominate the behavior for small structures. Therefore, it is appropriate to describe the carrier densities in a semiconductor nanostructure in terms of the quantum mechanical electronic states.

The basic model for the description of the electronic states in a semiconductor nanostructure is a stationary one-particle Schrödinger equation in $\mathbb{R}^d$ in the effective-mass approximation [**1**] (Ben-Daniel-Duke form) given by

$$-\nabla \cdot A(x)\nabla u_i + V(x)u_i = \lambda_i u_i. \tag{1.1}$$

Here, u_i is the wave function of the electronic state, λ_i the corresponding energy eigenvalue. Furthermore, $A(x) = \frac{\hbar^2}{2} m_{\text{eff}}^{-1}(x)$, where $m_{\text{eff}}(x)$ is the position dependent effective

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mass tensor of the carriers, $\hbar$ is Planck's constant. The potential V is a superposition of the variation of the band-edges and additional external potentials. Due to the rapid change of the material properties across interfaces, the variation of effective mass as well as the band-edges may experience a step-like change, leading to an eigenvalue problem with discontinuous coefficients. In graded heterostructures, the parameters between the two semiconductors change more smoothly corresponding to the chemical composition of the heterojunction.

In many applications one mainly is interested in the bounded states in the nanostructure, i.e. eigenfunctions which away from a certain central region - the region of confinement of the particles - decay exponentially. The standard approach for their computation is to consider the eigenvalue problem (1.1) in a finite spatial domain $\Omega \subset \mathbb{R}^d$ that is large enough to resolve the confinement region and to impose homogeneous Dirichlet boundary conditions on the wave function u at the boundary of the domain. Depending on the potential $V(x)$, there appears only a finite number of bounded states in the problem, and one is interested only in the lowest eigenmodes of the Schrödinger operator.

Following standard notations, by $L^2(\Omega)$ we denote the space of measurable functions whose moduli are square integrable. $L^\infty(\Omega)$ is the space of bounded measurable functions. By $H_0^1(\Omega)$ we denote the usual Sobolev space of functions $f : \Omega \to \mathbb{C}$, which belong to $L^2(\Omega)$, whose gradients belong to $L^2(\Omega)^d$ and whose trace on $\partial\Omega$ is equal to 0.

1.1. Assumption. *We consider in this paper the following basic assumptions on the data of the problem:*

(i) $\Omega \subset \mathbb{R}^d$ *– in general* $d = 1, 2, 3$ *– is an open bounded polygonal domain.*

(ii) The reciprocal effective mass tensor A *is a measurable mapping from* Ω *to the set of real symmetric positive definite* $d \times d$ *matrices such that there exists two reals* $\alpha > 0$ *and* $\beta > 0$ *with*

$$\alpha\xi \cdot \xi \leq A(x)\xi \cdot \xi \leq \beta\xi \cdot \xi \quad \text{for a.e. } x \in \Omega,\ \forall \xi \in \mathbb{R}^d. \tag{1.2}$$

(iii) For the potential V*, we assume* $V \in L^\infty(\Omega, \mathbb{R})$*,* $V \geq 0$*.*

Condition (ii) on A covers the case of abrupt heterojunctions as mentioned above as well as the case of graded heterostructures.

Optionally, we will regard isotropic effective mass tensors which are described as follows:

1.2. Assumption. *The effective mass is isotropic in the sense that there exists* $a \in L^\infty(\Omega, \mathbb{R}), a > 0$ *with*

$$A(x) = a(x)I_d \quad \text{for a.e. } x \in \Omega \tag{1.3}$$

where we denote by I_d *the* $d \times d$ *identity matrix.*

From the data of assumption 1.1, we define an inner product on $H_0^1(\Omega)$ by

$$\langle u, v\rangle = \int_\Omega [A(x)\nabla u(x) \cdot \nabla \bar{v}(x) + V(x)u(x)\bar{v}(x)]dx \quad \forall u, v \in H_0^1(\Omega). \tag{1.4}$$

This inner product is equivalent to the intrinsic inner product on $H_0^1(\Omega)$.

This allows to formulate the eigenvalue problem (1.1) in the weak form by investigating the following variational eigenvalue problem and its approximation by the finite volume method:

1.3. Problem. *Given assumption 1.1, find* $u \in H_0^1(\Omega), \lambda \in \mathbb{C}$ *such that*

$$\langle u, v\rangle = \lambda \int_\Omega u\bar{v}dx\ \forall v \in H_0^1(\Omega). \tag{1.5}$$

Generalizing the setting of piecewise constant approximations in L^2 defined on families of finite volume meshes with mesh size parameter h, we will present our results for families $\mathcal{F}$ of finite dimensional approximations $\mathcal{D} \in \mathcal{F}$ with an associated defining parameter $h_\mathcal{D}$ such that $\inf_{\mathcal{D}\in\mathcal{F}} h_\mathcal{D} = 0$. Let X be a Banach space. Assume that for any $\mathcal{D} \in \mathcal{F}$ we are given $u_\mathcal{D} \in X$. We will write $\lim_{h_\mathcal{D}\to 0} u_\mathcal{D} = u \in X$ if for all sequences $(\mathcal{D}_n)_{n\in\mathbb{N}} \subset \mathcal{F}$ such that $\lim_{n\to\infty} h_{\mathcal{D}_n} = 0$, we have that $\lim_{n\to\infty} \|u_{\mathcal{D}_n} - u\|_X = 0$.

The paper is organized as follows. In section 2, we define the inverse of the Schrödinger operator defined by problem 1.3, and show that it is a self-adjoint and compact operator on $L^2(\Omega)$. This allows to apply well known results for spectral approximation for compact, selfadjoint operators which we summarize in the rest of the section. In section 3, we introduce an abstract framework for finite dimensional approximations to the inner product defined by (1.4). Based on consistency and compactness properties of families of discretizations, we establish the convergence of the discrete inverse operator to its continuous counterpart. In section 4, these results are used to prove the convergence of eigenfunctions and eigenvalues for two finite volume schemes, one for the isotropic case based on the classical two point flux approach, and another one for the anisotropic case, based on a strongly convergent reconstruction of nodal fluxes. Additionally, we provide error estimates for the case of H^2 regular eigenfunctions. In section 5, we discuss the Voronoï-Delaunay construction of admissible meshes. Based on this approach we apply the isotropic finite volume method to a number of numerical examples for one-, two- and three-dimensional semiconductor nanostructures. These examples include cases with continuous as well as discontinuous position-dependent effective mass. A matching approach allows to derive analytical eigenvalues to which the numerical results are compared. Our conclusions are presented in section 6.

2. Spectral approximation theory for compact, selfadjoint operators

From the Lax-Milgram theorem, we establish that for all $f \in L^2(\Omega)$, there exists an unique $u \in H_0^1(\Omega)$ such that

$$\langle u, v\rangle = \int_\Omega u\bar{v}dx \;\forall v \in H_0^1(\Omega).$$

By denoting $u = Tf$, we thus define the inverse operator $T : L^2(\Omega) \to H_0^1(\Omega) \subset L^2(\Omega)$. By concluding

$$\int_\Omega Tf\bar{g}dx = \int_\Omega u\bar{g}dx = \langle u, Tg\rangle = \int_\Omega f\bar{Tg}dx \quad \forall f, g \in L^2(\Omega)$$

we establish that it is selfadjoint. Using (1.2) and the Poincaré inequality, we estimate

$$\alpha\|u\|^2_{H_0^1(\Omega)} \le \left|\int_\Omega f\bar{u}dx\right| \le \|f\|_{L^2(\Omega)}\|u\|_{L^2(\Omega)} \le C\|f\|_{L^2(\Omega)}\|u\|_{H_0^1(\Omega)}$$

and obtain

$$\|Tf\|_{H_0^1(\Omega)} \le \frac{C}{\alpha}\|f\|_{L^2(\Omega)}. \tag{2.1}$$

Let now $(f_n)_{n\in\mathbb{N}}$ be a bounded sequence in $L^2(\Omega)$. By estimate (2.1), the sequence $(Tf_n)_{n\in\mathbb{N}}$ is bounded as well. By Rellich's theorem [**2**], the embedding $H_0^1(\Omega) \hookrightarrow L^2(\Omega)$ is compact , and we establish the existence of a converging subsequence of $(Tf_n)_{n\in\mathbb{N}}$. This proves the compactness of T. The two tools used here – compactness and Poincaré

inequality – will accompany us throughout the paper. The pair (λ, u) is a solution of problem 1.3 if and only if for $\mu = \lambda^{-1}$, the pair (μ, u) is a solution of

$$Tu = \mu u.$$

This construction allows to apply the results of spectral approximation theory for compact, selfadjoint operators which are the base for error estimates for the finite element method. These are reviewed in the following. The main textbook source is [**3**]. See also the references cited therein.

Let H be a real or complex Hilbert space with norm $\|\cdot\|_H$, and let $T : H \to H$ be a compact selfadjoint operator. Its *spectrum* $\sigma(T)$ consists of a countable number of real values μ called *eigenvalues* such that $\dim\ker(\mu I - T) > 0$. The space $E_\mu(T) = \ker(\mu I - T)$ is called *eigenspace*, and its dimension m is called *multiplicity* of the eigenvalue μ. A pair (μ, u) such that $\mu \in \sigma(T)$ and $u \in E_\mu(T)$ is called *eigenpair*.

Let $\gamma \subset \mathbb{R}$ be an open interval which separates μ from the other eigenvalues of T, i.e. $\mu \in \gamma$ and $\gamma \cap (\sigma(T) \setminus \{\mu\}) = \emptyset$.

Let $\mathcal{F}$ be an index set. For all $\mathcal{D} \in \mathcal{F}$, let $T_\mathcal{D} : H \to H$ be a compact, self-adjoint operator, and let $h_\mathcal{D}$ be an associated real value such that $\inf_{\mathcal{D}\in\mathcal{F}} h_\mathcal{D} = 0$. We assume that $\lim_{h_\mathcal{D}\to 0} \|T - T_\mathcal{D}\|_{H\to H} = 0$, where the operator norm

$$\|T\|_{H\to H} = \sup_{0\neq x\in H} \frac{\|Tx\|_H}{\|x\|_H} \tag{2.2}$$

is defined in the usual way as being induced by the norm $\|\cdot\|_H$.

2.1. Theorem. *Convergence of the eigenvalues.*
Let $\mathcal{D} \in \mathcal{F}$. We define the closed subspace

$$E_{\mu,\mathcal{D}}(T_\mathcal{D}) = \sum_{\mu_\mathcal{D}\in\gamma\cap\sigma(T_\mathcal{D})} \ker(\mu_\mathcal{D} - T_\mathcal{D}). \tag{2.3}$$

Then, if $h_\mathcal{D}$ is small enough, $\gamma \cap \sigma(T_\mathcal{D})$ consists of eigenvalues converging to μ as $h_\mathcal{D} \to 0$ and $\dim E_\mu = \dim E_{\mu,\mathcal{D}}$.

For the proof, see [**3, 4**].

Given two closed subspaces M and N of H, we denote by

$$\delta(M, N) = \sup_{\substack{u\in M\\ \|u\|_H=1}} \operatorname{dist}(u, N) = \sup_{\substack{u\in M\\ \|u\|_H=1}} \inf_{v\in N} \|u - v\|_H \tag{2.4}$$

the largest principal angle between M and N. We note, that $\delta(M, N) = \delta(N, M)$.

2.2. Theorem. *Let $\mu \neq 0$ be an eigenvalue of T with multiplicity m. Let $\mathcal{D} \in \mathcal{F}$. Let $\mu_{\mathcal{D},1} \dots \mu_{\mathcal{D},m}$ be the eigenvalues of $T_\mathcal{D}$ converging to μ. Let $\phi_1 \dots \phi_m \in H$ be a basis of E_μ. Then there are constants C_1, C_2 independent of $\mathcal{D}$ such that for small $h_\mathcal{D}$,*

$$\delta(E_\mu, E_{\mu,\mathcal{D}}) \le C_1 \|(T - T_\mathcal{D})|_{E_\mu}\|_{H\to H} \tag{2.5}$$

$$|\mu - \mu_{\mathcal{D},j}| \le C_2 \left(\sum_{i,j=1}^{m} |((T - T_\mathcal{D})\phi_i, \phi_j)| + \|(T - T_\mathcal{D})|_{E_\mu}\|^2_{E_\mu\to H} \right). \tag{2.6}$$

This result combines theorems 7.1 and 7.3 in [**3**] and the specialization for the selfadjoint case at the end of section 7.

2.3. Corollary. *Under the conditions of theorem 2.2, concerning the approximation of eigenvalues and eigenvectors, we have the following results:*

(i) Let μ be an eigenvalue of T with multiplicity m. Let $\mu_{\mathcal{D},j}$ $(j = 1 \dots m)$ denote the eigenvalues of $T_{\mathcal{D}}$ converging to μ. Then there exists a constant C such that

$$|\mu - \mu_{\mathcal{D},j}| \leq C\|(T - T_{\mathcal{D}})|_{E_\mu}\|_{E_\mu \to H} \quad (j = 1 \dots m) \tag{2.7}$$

(ii) Let $w_{\mathcal{D}}$ be an unit eigenvector of $T_{\mathcal{D}}$ corresponding to $\mu_{\mathcal{D}}$ and let $\mu_{\mathcal{D}}$ converge to μ, an eigenvalue of T. Then there is an unit eigenvector u of T corresponding to μ such that

$$\|u - w_{\mathcal{D}}\| \leq C\|(T - T_{\mathcal{D}})|_{E_\mu}\|_{E_\mu \to H} \tag{2.8}$$

(iii) Let w be an unit eigenvector of T corresponding to μ, then there is an eigenvalue $\mu_{\mathcal{D}}$ of $T_{\mathcal{D}}$ converging to μ, and an eigenvector $u_{\mathcal{D}}$ of $T_{\mathcal{D}}$ corresponding to $\mu_{\mathcal{D}}$ such that

$$\|w - u_{\mathcal{D}}\| \leq C\|(T - T_{\mathcal{D}})|_{E_\mu}\|_{E_\mu \to H} \tag{2.9}$$

We note that in [**3**], the results concerning higher order convergence of the eigenvalues are based on the Galerkin approach which allows an $O(h^2)$-estimate for $|((T - T_{\mathcal{D}})\phi_i, \phi_j)|$ which does not work for the finite volume framework we are using here.

3. A framework for finite dimensional approximations

In this section, we define an abstract framework for finite dimensional approximations to the inner product defined by 1.4. This framework is formulated in a general setting, without referring to the concept of neither finite volume nor finite element methods. It will allow us to establish the connection between the discrete operators obtained by the finite volume method and the theory of spectral approximations based on the concept of compact, selfadjoint discrete operators converging to their continuous counterparts.

3.1. Definition (Admissible family of finite dimensional approximations). *Given assumption 1.1, an admissible family of finite dimensional approximations is a set of finite dimensional spaces $H^{\mathcal{D}} \subset L^2(\Omega)$ indexed by $\mathcal{D} \in \mathcal{F}$ equipped with inner products $\langle \cdot, \cdot \rangle_{\mathcal{D}}$ such that for all $\mathcal{D} \in \mathcal{F}$, there exists a real value $h_{\mathcal{D}} > 0$ with $\inf_{\mathcal{D} \in \mathcal{F}} h_{\mathcal{D}} = 0$. Furthermore, for each $\mathcal{D} \in \mathcal{F}$, there exists an interpolation operator $P_{\mathcal{D}} : C_c^\infty(\Omega) \to H^{\mathcal{D}}$ such that, for all $\varphi \in C_c^\infty(\Omega)$, $\lim_{h_{\mathcal{D}} \to 0} P_{\mathcal{D}}\varphi = \varphi$ in $L^2(\Omega)$.*

For any sequence $(\mathcal{D}_n)_{n \in \mathbb{N}} \subset \mathcal{F}$ such that $\lim_{n \to \infty} h_{\mathcal{D}_n} = 0$ and for any sequence of functions $(v_n)_{n \in \mathbb{N}}$ with $v_n \in H^{\mathcal{D}_n}$ such that there exists $C > 0$ with $\langle v_n, v_n \rangle_{\mathcal{D}_n} \leq C$ for all $n \in \mathbb{N}$, we assume the following properties:

(i) (Compactness) There exists $\hat{v} \in H_0^1(\Omega)$ and a subsequence of $(\mathcal{D}_n)_{n \in \mathbb{N}}$, again denoted $(\mathcal{D}_n)_{n \in \mathbb{N}}$, such that $\lim_{n \to \infty} v_n = \hat{v}$ in $L^2(\Omega)$.

(ii) (Consistency) If there exists $\hat{v} \in H_0^1(\Omega)$ with $\lim_{n \to \infty} v_n = \hat{v}$ in $L^2(\Omega)$, it follows that $\lim_{n \to \infty} \langle v_n, P_{\mathcal{D}_n}\varphi \rangle_{\mathcal{D}} = \langle v, \varphi \rangle$ $\forall \varphi \in C_c^\infty(\Omega)$.

3.2. Lemma (Discrete Poincaré inequality). *Given an admissible family of finite dimensional approximations $\mathcal{F}$, there exists $\alpha > 0$ such that*

$$\forall \mathcal{D} \in \mathcal{F}\ \forall v \in H^{\mathcal{D}}, \|v\|_{L^2(\Omega)}^2 \leq \alpha \langle v, v \rangle_{\mathcal{D}}. \tag{3.1}$$

Proof. Assume that (3.1) is wrong. Then, for all $n \in \mathbb{N}$, there exists $\mathcal{D}_n \in \mathcal{F}$ and $u_n \in H^{\mathcal{D}_n}$ such that $\langle u_n, u_n \rangle_{\mathcal{D}_n} = 1$ and $\|u_n\|_{L^2(\Omega)} > n$. By compactness, there exists $\hat{u} \in H_0^1(\Omega)$ such that we can extract a strictly monotonically increasing subsequence, $\phi(n)$ such that $\lim_{n \to \infty} u_{\phi(n)} = \hat{u}$ in $L^2(\Omega)$. This is in contradiction with $\|u_{\phi(n)}\|_{L^2(\Omega)} > \phi(n)$. □

The following theorem provides the link between admissible families of finite dimensional approximations and the convergence of the inverse operators associated to the inner products $\langle \cdot, \cdot \rangle_{\mathcal{D}}$ to their continuous counterpart, as it is used in spectral approximation theory reviewed in section 2.

3.3. Theorem (Convergence of operator approximation). *Under assumption 1.1, let $T : L^2(\Omega) \to L^2(\Omega)$ be such that, for all $f \in L^2(\Omega)$, Tf is the solution $u \in H_0^1(\Omega)$ of*

$$\langle u, v \rangle = \int_\Omega f(x)\bar{v}(x)dx \quad \forall v \in H_0^1(\Omega). \tag{3.2}$$

Let $\mathcal{F}$ be an admissible family of finite dimensional approximations in the sense of definition 3.1, and, for all $\mathcal{D} \in \mathcal{F}$, let $T_{\mathcal{D}} : L^2(\Omega) \to L^2(\Omega)$ be such that $T_{\mathcal{D}} f = u_{\mathcal{D}} \in H^{\mathcal{D}}$ is the unique solution of

$$\langle u_{\mathcal{D}}, v \rangle_{\mathcal{D}} = \int_\Omega f(x)\bar{v}(x)dx \quad \forall v \in H^{\mathcal{D}}. \tag{3.3}$$

Then

$$\lim_{h_{\mathcal{D}} \to 0} \|T - T_{\mathcal{D}}\|_{L^2(\Omega) \to L^2(\Omega)} = 0. \tag{3.4}$$

Proof. Let us prove the above theorem by contradiction. Let us assume that there exists $\varepsilon > 0$, such that for all $\eta > 0$, there exists an approximation $\mathcal{D} \in \mathcal{F}$ such that $h_{\mathcal{D}} < \eta$ and there exists $f \in L^2(\Omega)$ such that $\|f\|_{L^2(\Omega)} = 1$ with $\|T_{\mathcal{D}} f - Tf\|_{L^2(\Omega)} > \varepsilon$. Taking $\eta = 1/(n+1)$, we get the existence of a sequence $(\mathcal{D}_n)_{n \in \mathbb{N}}$ with $h_{\mathcal{D}_n} < 1/(n+1)$ and a sequence $(f_n)_{n \in \mathbb{N}}$ with $\|f_n\|_{L^2(\Omega)} = 1$ such that $\|T_{\mathcal{D}_n} f_n - Tf_n\|_{L^2(\Omega)} > \varepsilon$. We remark that, for all $n \in \mathbb{N}$, the function $u_n = T_{\mathcal{D}_n} f_n$ defined by (3.3) fulfills

$$\langle u_n, u_n \rangle_{\mathcal{D}} = \int_\Omega f_n(x)\bar{u}_n(x)dx.$$

Hence, applying the Cauchy-Schwarz inequality, we get

$$\langle u_n, u_n \rangle_{\mathcal{D}} \leq \|f_n\|_{L^2(\Omega)} \|u_n\|_{L^2(\Omega)} = \|u_n\|_{L^2(\Omega)}.$$

Applying lemma 3.2, we get $\langle u_n, u_n \rangle_{\mathcal{D}} \leq (\alpha \langle u_n, u_n \rangle_{\mathcal{D}})^{1/2}$ which leads to $\langle u_n, u_n \rangle_{\mathcal{D}} \leq \alpha$. Hence, from compactness property (point (i) of definition 3.1), we get that we can define a strictly increasing mapping $\psi : \mathbb{N} \to \mathbb{N}$ such that there exists $\hat{u} \in H_0^1(\Omega)$ with $u_{\psi(n)}$ tending to $\hat{u}$ in $L^2(\Omega)$. Since the sequence of functions $(f_{\psi(n)})_{n \in \mathbb{N}}$ is bounded in $L^2(\Omega)$, we can define a strictly increasing mapping $\phi : \mathbb{N} \to \mathbb{N}$ such that there exists $\hat{f} \in L^2(\Omega)$ with $f_{\psi(\phi(n))}$ weakly tending to $\hat{f}$ in $L^2(\Omega)$.

Denoting again $u_n = u_{\psi(\phi(n))}$ and $f_n = f_{\psi(\phi(n))}$, we get

$$\langle u_n, P_{\mathcal{D}_n} \varphi \rangle_{\mathcal{D}} = \int_\Omega f_n(x) P_{\mathcal{D}_n} \bar{\varphi}(x)dx \quad \forall \varphi \in C_c^\infty(\Omega).$$

Applying the consistency property (point (ii) of definition (3.1)), we pass to the limit $n \to \infty$ in the above equation. Since in the right hand side, the two sequences converge weakly and strongly, respectively, we get

$$\langle \hat{u}, \varphi \rangle = \int_\Omega \hat{f}(x)\bar{\varphi}(x)dx \quad \forall \varphi \in C_c^\infty(\Omega).$$

This proves that $\hat{u} = T\hat{f}$, which means that $\|T_{\mathcal{D}_n} f_n - T\hat{f}\|_{L^2(\Omega)} \to 0$ for $n \to \infty$. From the continuity of the inner product defined by (1.4), we get that Tf_n converges in $L^2(\Omega)$ to $T\hat{f}$. Hence, passing to the limit $n \to \infty$, we get a contradiction with $\|T_{\mathcal{D}_n} f_n - Tf_n\|_{L^2(\Omega)} \geq \varepsilon$. Therefore, for all $\varepsilon > 0$, there exists $\eta > 0$, such that for all approximations $\mathcal{D} \in \mathcal{F}$ such

that $h_{\mathcal{D}} < \eta$ and for all $f \in L^2(\Omega)$ such that $\|f\|_{L^2(\Omega)} = 1$, then $\|T_{\mathcal{D}_n} f - Tf\|_{L^2(\Omega)} \leq \varepsilon$. This proves the convergence of the operator $T_{\mathcal{D}}$ to T as $h_{\mathcal{D}} \to 0$. □

Concluding this section, we remark that with this result, the convergence in norm of the inverse $T_{\mathcal{D}}$ of the finite dimensional approximation in $L^2(\Omega)$ to the inverse T of the original operator has been established. From the basic results of spectral approximation theory reviewed in section 2, the convergence of eigenvalues and eigenfunctions follows.

To show the convergence of a particular discretization method, it suffices to prove that the compactness and consistency properties of definition 3.1 hold.

In the case that $H^{\mathcal{D}} \subset H = H_0^1(\Omega)$ and $\langle \cdot, \cdot \rangle_{\mathcal{D}}$ is defined by the Rayleigh-Ritz-Galerkin method, it is easy to establish these properties with standard finite element arguments. So, let $H^{\mathcal{D}} \subset H$ be spanned by the finite element basis functions ψ_i. Let $P_{\mathcal{D}} : C_0^\infty \to H^{\mathcal{D}}$ be the usual finite element interpolation operator. Let $\langle \cdot, \cdot \rangle_{\mathcal{D}}^g$ be the restriction of $\langle \cdot, \cdot \rangle$ to $H_{\mathcal{D}}$. Then the compactness property (i) of definition 3.1 is a direct consequence of Rellich's theorem [**2**]. Another consequence of Rellich's theorem is the weak convergence $\nabla v_n \to \nabla v$. Furthermore, from the well known H^1 estimates of the finite element interpolation operator, we obtain strong convergence $\nabla P_{\mathcal{D}_n} \phi \to \nabla \phi$. Therefore, using the weak-strong convergence property [**2**], we obtain $\lim_{n\to\infty} \langle v_n, P_{\mathcal{D}_n} \varphi \rangle_{\mathcal{D}}^g = \langle v, \varphi \rangle$.

4. Convergence of finite volume methods

In this section, the concept of admissible finite dimensional approximations is applied to finite volume discretization of isotropic and anisotropic Hamiltonians.

4.1. Admissible finite volume discretization. We define an admissible finite volume discretization and the discrete function space using the concepts of [**5**] which allow that nodes can be located at the boundaries of control volumes.

4.1. Definition (Admissible discretization). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$, with $d \in \mathbb{N}, d > 0$. An admissible finite volume discretization of Ω, denoted by $\mathcal{D}$, is given by $\mathcal{D} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$, where:*

- *$\mathcal{T}$ is a finite family of non empty open polygonal convex disjoint subsets of Ω (the "control volumes") such that $\overline{\Omega} = \cup_{K \in \mathcal{T}} \overline{K}$. We then denote, for all $K \in \mathcal{T}$, by $m_K > 0$ the d-dimensional Lebesgue measure of K.*
- *$\mathcal{E}$ is a finite family of disjoint subsets of $\overline{\Omega}$ (the "edges" of the mesh), such that, for all $\sigma \in \mathcal{E}$, there exists a hyperplane E of $\mathbb{R}^d$ and $K \in \mathcal{T}$ with $\overline{\sigma} = \partial K \cap E$ and σ is a non empty open subset of E. We then denote by $m_\sigma > 0$ the $(d-1)$-dimensional measure of σ and we denote by x_σ the center of gravity of σ. We assume that, for all $K \in \mathcal{T}$, there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K = \cup_{\sigma \in \mathcal{E}_K} \overline{\sigma}$. It then results from the previous hypotheses that, for all $\sigma \in \mathcal{E}$, either $\sigma \subset \partial\Omega$ or there exists a pair $(K, L) \in \mathcal{T}^2$ of neighbouring control volumes with $K \neq L$ such that $\overline{K} \cap \overline{L} = \overline{\sigma}$; we denote in the latter case $\sigma = K|L$. We denote by N_K the set of neigbouring control volumes $L \neq K$ such that there exists $\sigma \in \mathcal{E}_K$ with $\sigma = K|L$. The subset of interior edges of $\mathcal{E}$ - of the edges σ such that there exist two control volumes K and L with $\sigma = K|L$ is denoted by $\mathcal{E}_{\text{int}}$.*
- *$\mathcal{P}$ is a family of points of Ω indexed by $\mathcal{T}$, denoted by $\mathcal{P} = (x_K)_{K \in \mathcal{T}}$. This family is such that, for all $K \in \mathcal{T}$, $x_K \in \bar{K}$. For all $\sigma \in \mathcal{E}$ such that there exists $(K, L) \in \mathcal{T}^2$ with $\sigma = K|L$, it is assumed that $x_K \neq x_L$ and that the straight line (x_K, x_L) going through x_K and x_L is orthogonal to $K|L$. For all $K \in \mathcal{T}$ such that $\text{meas}(\partial K \cap \partial\Omega) \neq 0$ we assume that $x_K \in \partial\Omega$ (the set of such control volumes is denoted $\mathcal{T}_{\text{ext}}$, the set of control volumes such that $\text{meas}(\partial K \cap \partial\Omega) = 0$ is denoted $\mathcal{T}_{\text{int}}$).*

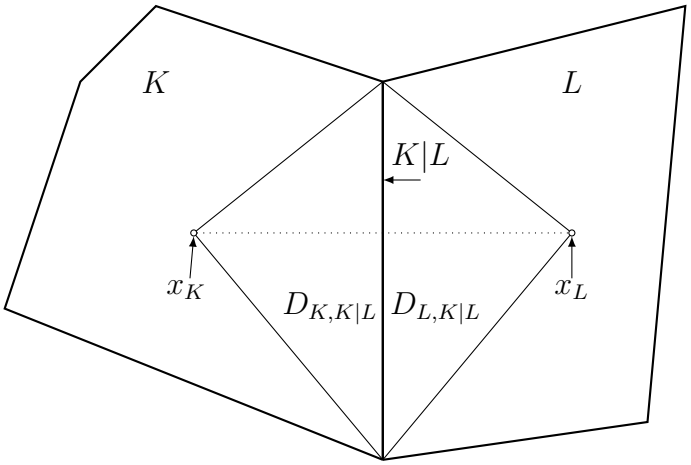

FIGURE 4.1. A pair of neigboring control volumes K, L with shared edge $K|L$, associated points x_K and x_L, and half-diamond domains $D_{L,K|L}$, and $D_{K,K|L}$

We define, for all $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_K$, the open half-diamond

$$D_{K,\sigma} = \{tx_K + (1-t)y \mid t \in (0,1),\ y \in \sigma\} \tag{4.1}$$

and we assume that for all $K \in \mathcal{T}$, $\bar{K} = \bigcup_{L \in N_K} \bar{D}_{K,K|L}$.

Define the mesh size of the discretization by

$$h_{\mathcal{D}} = \sup\{\mathrm{diam}(K), K \in \mathcal{T}\}. \tag{4.2}$$

For all $K \in \mathcal{T}$ and $L \in N_K$, we denote by $\mathbf{n}_{K,L}$ the unit vector normal to $K|L$ outward to K. For all $K \in \mathcal{T}$ and $L \in N_K$, we define the geometric factors

$$h_{KL} = |x_K - x_L|, \quad \tau_{KL} = \frac{m_{K|L}}{h_{KL}}. \tag{4.3}$$

4.2. Discrete function spaces and discrete functional analysis tools. Let $\mathcal{D} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible finite volume discretization of Ω. The *discrete function space* $H^{\mathcal{D}} \subset L^2(\Omega)$ is the space of step functions which admit a constant complex value u_K in each $K \in \mathcal{T}$. We denote by $H_0^{\mathcal{D}} \subset H^{\mathcal{D}}$ the subspace of functions which vanish in all $K \in \mathcal{T}_{\mathrm{ext}}$.

For $u, v \in H^{\mathcal{D}}$ and for any coefficient function $a \in L^\infty(\Omega, \mathbb{R})$, we introduce a weighted discrete *inner product* corresponding to the main part of (1.4):

$$\begin{aligned}[u,v]_{\mathcal{D},a} &= -\sum_{K \in \mathcal{T}} \bar{v}_K \sum_{L \in N_K} \tau_{KL} a_{KL}(u_L - u_K) \\ &= \sum_{K|L \in \mathcal{E}_{\mathrm{int}}} \tau_{KL} a_{KL}(u_L - u_K)(\bar{v}_L - \bar{v}_K),\end{aligned}$$

where the weights a_{KL} are obtained by arithmetic averaging of a over the union of the diamond domains adjacent to the edge σ_{KL}

$$a_{KL} = \frac{d}{m_{K|L} h_{KL}} \int_{D_{K,K|L} \cup D_{L,K|L}} a(x)dx. \tag{4.4}$$

The quantities $\tau_{KL} a_{KL}(u_L - u_K)$ are two point finite difference approximations to the normal flux $(a\nabla u) \cdot \mathbf{n}_{K,L}$ averaged over the edge $K|L$.

This allows to define the semi-norm

$$|u|_{\mathcal{D}} = ([u,u]_{\mathcal{D},1})^{1/2} \tag{4.5}$$

in $H^{\mathcal{D}}$.

We define the *interpolation* $P_{\mathcal{D}} : C^0(\Omega) \to H^{\mathcal{D}}$ by

$$(P_{\mathcal{D}}\varphi)_K = \varphi(x_K) \quad \forall K \in \mathcal{T}. \tag{4.6}$$

4.2. Lemma (Discrete Poincaré inequality). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$. Let $\mathcal{D}$ be an admissible finite volume discretization of Ω. Then for all $u \in H_0^{\mathcal{D}}$ one has*

$$\|u\|_{L^2(\Omega)} \leq \operatorname{diam}(\Omega)\ |u|_{\mathcal{D}}. \tag{4.7}$$

The proof is given in [**5**] and is not modified by the complex framework.

As shown in lemma 3.2, for an admissible family of finite dimensional approximations, a discrete Poincaré inequality can be obtained as a consequence of compactness and consistency, however with an unknown constant. Lemma 4.2 uses a direct proof and yields $\operatorname{diam}(\Omega)$ as the constant.

4.3. Corollary. *Due to the discrete Poincaré inequality* (4.7)*, the semi-norm defined by* (4.5) *is a norm.*

4.4. Lemma (Relative compactness in $L^2(\Omega)$). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$. Let $(\mathcal{D}_n, u_n)_{n\in\mathbb{N}}$ be a sequence such that for $n \in \mathbb{N}$, D_n is an admissible finite volume discretization of Ω and $u_n \in H_0^{\mathcal{D}_n}$. Assume that $\lim_{n\longrightarrow\infty} h_{\mathcal{D}_n} = 0$, and that there exists $C > 0$ such that, for all $n \in \mathbb{N}$, $|u_n|_{\mathcal{D}_n} \leq C$.*

Then there exist a subsequence of $(\mathcal{D}_n, u_n)_{n\in\mathbb{N}}$, again denoted $(\mathcal{D}_n, u_n)_{n\in\mathbb{N}}$, and $\hat{u} \in H_0^1(\Omega)$ such that $\lim_{n\longrightarrow\infty} u_n = \hat{u}$ in $L^2(\Omega)$.

Moreover, for all coefficient functions $a \in L^\infty(\Omega, \mathbb{R}_+)$ it holds that,

$$\int_\Omega a(x)|\nabla\hat{u}(x)|^2 dx \leq \liminf_{n\longrightarrow\infty} [u_n, u_n]_{\mathcal{D}_n,a}.$$

The proof of the convergence statement is based on the estimate of the space translates in terms of $|u_n|_{\mathcal{D}_n}$ and the application of the Kolmogorov compactness theorem. It has been given in [**5**]. The "lim inf" statement has been proven in [**6**], lemma 5.2.

4.5. Lemma (Consistency). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$. Let $(\mathcal{D}_n, u_n)_{n\in\mathbb{N}}$ be a sequence such that for $n \in \mathbb{N}$, $\mathcal{D}_n$ is an admissible finite volume discretization of Ω and $u_n \in H_0^{\mathcal{D}_n}$. Assume that $\lim_{n\longrightarrow\infty} h_{\mathcal{D}_n} = 0$, and that there exists $\hat{u} \in H_0^1(\Omega)$ such that $\lim_{n\longrightarrow\infty} u_n = \hat{u}$. Then,*

$$\lim_{n\longrightarrow\infty} [u_n, P_{\mathcal{D}_n}\varphi]_{\mathcal{D},a} = \int_\Omega a(x)\nabla\hat{u}(x)\cdot\nabla\bar{\varphi}(x)dx \quad \forall\varphi \in C_c^\infty(\Omega). \tag{4.8}$$

The proof of the above lemma is given in [**7**], lemma 2.1 (the complex framework does not modify this proof).

4.3. Finite volume discretization of the Hamiltonian in the isotropic case. We consider in this section the heterogeneous isotropic case defined in (1.3), i.e. there is a scalar function $a(x)$ such that $a(x) = \frac{\hbar^2}{2} m_{\text{eff}}^{-1}(x)$. Let $\mathcal{D}$ be an admissible discretization

of Ω. We define the following inner product in $H_0^{\mathcal{D}}$:

$$\begin{aligned} &\forall u, v \in H_0^{\mathcal{D}}, \\ &\quad \langle u, v\rangle_{\mathcal{D}}^i = [u, v]_{\mathcal{D},a} + \int_\Omega V(x)u(x)\bar{v}(x)dx \\ &\quad\quad = \sum_{K|L\in\mathcal{E}_{\rm int}} \tau_{KL}a_{KL}(u_L - u_K)(\bar{v}_L - \bar{v}_K) + \sum_{K\in\mathcal{T}} m_K V_K u_K \bar{v}_K \end{aligned} \tag{4.9}$$

where

$$V_K = \frac{1}{m_K}\int_K V(x)dx,\ \forall K \in \mathcal{T} \tag{4.10}$$

are the averages of the potential over the control volumes.

4.6. Lemma (Finite volume schemes are admissible schemes). *Under the assumptions 1.1 and 1.2, consider a family $\mathcal{F}$ of admissible finite volume discretizations of Ω in the sense of definition 4.1 such that $\inf_{\mathcal{D}\in\mathcal{F}} h_{\mathcal{D}} = 0$. Then the family of spaces $H_0^{\mathcal{D}}$ with the inner product $\langle\cdot,\cdot\rangle_{\mathcal{D}}^i$ defined in* (4.9) *is an admissible family of finite dimensional approximations to the inner product $\langle\cdot,\cdot\rangle$ defined in* (1.4).

Proof. The compactness (i) of definition 3.1 results from lemma 4.4 and the fact that for all $u \in H_0^{\mathcal{D}}$, $[u, u]_{\mathcal{D},a} \le \langle u, u\rangle_{\mathcal{D}}^i$. The consistency (ii) is due to (4.8), the weak convergence of u_n and the strong convergence of $P_{\mathcal{D}_n}\varphi(x)$ which can be proven using the uniform continuity of φ. These allow to obtain the weak/strong convergence statement

$$\lim_{n\to\infty}\int_\Omega V(x)u_n P_{\mathcal{D}_n}\bar{\varphi}(x)\ dx = \int_\Omega V(x)u(x)\bar{\varphi}(x)\ dx.$$

□

Now, we regard the following discrete eigenvalue problem:

4.7. Problem. *Given assumptions 1.1,1.2, let $\mathcal{D}$ be an admissible finite volume discretization. Then, find $u \in H_0^{\mathcal{D}}, \lambda \in \mathbb{C}$ such that*

$$\langle u, v\rangle_{\mathcal{D}}^i = \lambda\int_\Omega u\bar{v}dx\ \forall v \in H_0^{\mathcal{D}}. \tag{4.11}$$

Combining the results of this section with the information from section 2, we arrive at

4.8. Theorem. *Under the assumptions 1.1 and 1.2, consider a family $\mathcal{F}$ of admissible finite volume discretizations of Ω in the sense of definition 4.1 such that $\inf_{\mathcal{D}\in\mathcal{F}} h_{\mathcal{D}} = 0$. Then, the eigenvalues of problem 4.7 converge to those of 1.3 in the following sense: for each eigenvalue λ of problem 1.3 with multiplicity m, for any sequence $(\mathcal{D}_n) \subset \mathcal{F}$ such that $\lim_{n\to\infty} h_{\mathcal{D}_n} = 0$, for n large enough, there are m eigenvalues $\lambda_{\mathcal{D}_n,1}\dots\lambda_{\mathcal{D}_n,m}$ of problem 4.7 converging to λ as $n \to \infty$.*

Proof. For the compact, self-adjoint inverse operators $T, T_{\mathcal{D}}$ corresponding to $\langle\cdot,\cdot\rangle$ and $\langle\cdot,\cdot\rangle_{\mathcal{D}}^i$, respectively, by lemma 4.6 and theorem 3.3 we have

$$\lim_{h_{\mathcal{D}}\to 0}\|T_{\mathcal{D}} - T\|_{L^2(\Omega)\to L^2(\Omega)} = 0.$$

The convergence statement then can be obtained by the spectral approximation result summarized in theorem 2.2. □

In order to obtain error estimates, we provide the following result.

4.9. Lemma (Error estimate). *Under the assumptions 1.1 and 1.2, let $\mathcal{D}$ be an admissible finite volume discretization of Ω in the sense of definition 4.1. Assume that $\mathcal{D}$ is regular in the sense that $\exists \zeta_{\mathcal{D}} > 0$ such that $\operatorname{dist}(x_K, \sigma) \geq \zeta_{\mathcal{D}} \operatorname{diam}(K)$ for all $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_{int}$. Furthermore, let $d = 2, 3$ and $a(x) = 1$.*

Let μ be an eigenvalue of the inverse operator T such that $E_\mu \subset H^2(\Omega)$. Then there exists a constant C, depending on $\Omega, \zeta_{\mathcal{D}}, d, w, E_\mu$, such that

$$\|(T_{\mathcal{D}} - T)|_{E_\mu}\|_{E_\mu \to L^2(\Omega)} \leq C h_{\mathcal{D}}. \tag{4.12}$$

Proof. Let $u \in E_\mu$ with $\|u\|_{L^2(\Omega)} = 1$. Let $\phi_1 \dots \phi_m$ be an orthonormal basis of E_μ. Then there exist complex numbers $u_1 \dots u_a$ such that $u = \sum_{j=1}^m u_j \phi_j$ and $\sum_{j=1}^m u_j \bar{u}_j = 1$, and we obtain

$$\|u\|_{H^2(\Omega)} \leq \sum_{j=1}^m |u_j| \|\phi_j\|_{H^2(\Omega)} \leq \left(\sum_{j=1}^m \|\phi_j\|^2_{H^2(\Omega)} \right)^{\frac{1}{2}}.$$

Consequently,

$$\|u\|_{H^2(\Omega)} \leq C_{E_\mu} := \inf_{\substack{\{\phi_1 \dots \phi_m\} \\ \text{o.n. basis of } E_\mu}} \left(\sum_{j=1}^m \|\phi_j\|^2_{H^2(\Omega)} \right)^{\frac{1}{2}}.$$

From the proof of [**8**], theorem 2 (H^2 regularity with homogeneous Dirichlet boundary conditions), we have

$$\|T_{\mathcal{D}} u - T u\|_{L^2(\Omega)} \leq C_{GHV} h_{\mathcal{D}} \|u\|_{H^2(\Omega)}$$

where C_{GHV} depends on $\Omega, \zeta_{\mathcal{D}}, d, w$, but not on $u, h_{\mathcal{D}}$. With $C = C_{E_\mu} C_{GHV}$, the statement 4.12 follows. □

4.10. Remark. *The statement of lemma 4.9 as well holds in the more general case when $a(x)|_K \in C^1(K)$ for all $K \in \mathcal{T}$ see* [**8**]*, assumption 2 and remark 1 (vi).*

4.11. Corollary. *Assume the conditions of theorem 4.8 and lemma 4.9. If $\zeta_D \geq \zeta > 0$ for all $\mathcal{D} \in \mathcal{F}$ we have the following statements*

(i) There exists a constant C such that

$$\left| \frac{1}{\lambda} - \frac{1}{\lambda_{\mathcal{D},j}} \right| \leq C h_{\mathcal{D}}$$

(ii) Let $w_{\mathcal{D}}$ be an unit eigenvector of problem 4.7 corresponding to $\lambda_{\mathcal{D}}$ and let $\lambda_{\mathcal{D}}$ converge to λ, an eigenvalue of problem 1.3. Then there is an unit eigenvector u of problem 1.3 corresponding to λ such that

$$\|u - w_{\mathcal{D}}\|_{L^2(\Omega)} \leq C h_{\mathcal{D}} \tag{4.13}$$

(iii) Let w be an unit eigenvector of problem 1.3 corresponding to λ, then there is an eigenvalue $\lambda_{\mathcal{D}}$ of problem 4.7 converging to λ, and an eigenvector $u_{\mathcal{D}}$ of problem 4.7 corresponding to $\lambda_{\mathcal{D}}$ such that

$$\|w - u_{\mathcal{D}}\|_{L^2(\Omega)} \leq C h_{\mathcal{D}} \tag{4.14}$$

Proof. The proof uses corollary 2.3 and lemma 4.9. □

4.12. Corollary. *Under the conditions of theorem 4.8, there exist constants C,$h_0 > 0$ such that for all $\mathcal{D} \in \mathcal{F}$ such that $h_{\mathcal{D}} \leq h_0$, we have*

$$|\lambda - \lambda_{\mathcal{D},j}| \leq C h_{\mathcal{D}}$$

PROOF. For $\mu = \lambda^{-1}, \mu_{\mathcal{D},j} = \lambda_{\mathcal{D},j}^{-1}$, statement (i) of corollary 2.3 implies that $|\mu - \mu_{\mathcal{D},j}| \leq Ch_{\mathcal{D}}$. Therefore

$$|\lambda - \lambda_{\mathcal{D},j}| = \left|\frac{1}{\mu} - \frac{1}{\mu_{\mathcal{D},j}}\right| \leq Ch_{\mathcal{D}} \frac{1}{|\mu||\mu_{\mathcal{D},j}|}$$

We have

$$|\mu_{\mathcal{D},j}| = |\mu - (\mu - \mu_{\mathcal{D},j})| \geq |\mu| - |\mu - \mu_{\mathcal{D},j}| \geq |\mu| - Ch_0$$

where h_0 is a fixed value such that $|\mu| - Ch_0 > 0$. Then, for $C^* = \frac{C}{|\mu|(|\mu| - Ch_0)}$, we obtain for $h_{\mathcal{D}} < h_0$, that

$$|\lambda - \lambda_{\mathcal{D},j}| \leq C^* h_{\mathcal{D}}.$$

□

4.13. REMARK. *The statement of corollary 4.12 is similar to that of theorem 8.3 in* [**3**]. *However, as we see in the proof, the constant C in the statement contains λ, and statement (i) of corollary 4.11 gives the more precise result. Interestingly, this is in accord with* [**4**] *which lays the ground for chapter 8 in* [**3**].

The very nature of this finite volume approximation allows to apply the M-matrix theory in order to obtain a statement which is equivalent to the fact that the eigenmode corresponding to the lowest eigenvalue has constant sign [**9**].

4.14. THEOREM. *Let $\mathcal{D} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible discretization of Ω in the sense of definition 4.1. Assume, that $\int_\Omega V(x)dx > 0$ and the the domain Ω is connected. Then, the lowest eigenvalue of the discrete eigenvalue problem 4.7 is positive with single multiplicity, and the corresponding eigenfunction has constant sign.*

PROOF. According to equation (4.9), the discretized system can be written in matrix form as

$$A_{\mathcal{D}} u + M_{\mathcal{D}} V_{\mathcal{D}} u = \lambda M_{\mathcal{D}} u,$$

where $A_{\mathcal{D}}$ is the matrix corresponding to the main part of the problem, $V_{\mathcal{D}}$ is a positive diagonal matrix corresponding to the potential, and $M_{\mathcal{D}}$ is the positive diagonal "mass matrix" corresponding to the volume weights. $A_{\mathcal{D}}$ has positive diagonal, non-positive off diagonal entries, and nonnegative row sums. Furthermore, the graph of the matrix is connected, and due to the conditions on the potential V, all values of V_K are nonnegative, and for at least one K, V_K is positive. Thus, $A_{\mathcal{D}} + M_{\mathcal{D}} V_{\mathcal{D}}$ is weakly diagonally dominant and therefore has the M-property [**10**]. As a consequence, it is non-degenerate, and by setting $\mu = \frac{1}{\lambda}$, we can rewrite our eigenvalue problem as

$$(A_{\mathcal{D}} + M_{\mathcal{D}} V_{\mathcal{D}})^{-1} M_{\mathcal{D}} u = \mu u.$$

By definition of the M-property, $T_{\mathcal{D}} = (A_{\mathcal{D}} + M_{\mathcal{D}} V_{\mathcal{D}})^{-1} M_{\mathcal{D}}$ has positive entries. By the Perron-Frobenius theorem [**10**], it has a single, positive maximum eigenvalue equal to its spectral radius. The corresponding eigenvector has a constant sign.

As a consequence, we obtain the positivity of the lowest eigenvalue of our original discretized problem and the constant signature of the corresponding discrete eigenfunction. □

4.4. Finite volume discretization of the Hamiltonian in the anisotropic case. We define the discrete Hamiltonian for the case of an anisotropic effective mass. Let $\mathcal{D} = (\mathcal{T}, \mathcal{E}, \mathcal{P})$ be an admissible discretization of Ω in the sense of definition 4.1. Based on [**7**], we give the following definition of an approximate gradient of the piecewise constant functions $\nabla_{\mathcal{D}} : H^{\mathcal{D}} \to (H^{\mathcal{D}})^d$:

$$m_K(\nabla_{\mathcal{D}} u)_K = \sum_{L \in N_K} \tau_{KL}(u_L - u_K)(x_{K|L} - x_K), \ \forall K \in \mathcal{T}. \tag{4.15}$$

Following [**7**], we define the Hermitian form

$$\langle u, v \rangle^a_{\mathcal{D}} = \int_\Omega (A(x) - \alpha I_d) \nabla_{\mathcal{D}} u(x) \cdot \nabla_{\mathcal{D}} \bar{v}(x) dx + \alpha [u, v]_{\mathcal{D},1} + \int_\Omega V(x) u(x) \bar{v}(x) dx, \ \forall u, v \in H_0^{\mathcal{D}}, \tag{4.16}$$

where α is the ellipticity constant from assumption 1.1. The role of the isotropic part is essential to get the expected coercivity, as in [**7**].

4.15. Lemma (Relative compactness in $L^2(\Omega)$). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$. Let $(\mathcal{D}_n, u_n)_{n \in \mathbb{N}}$ be a sequence such that for $n \in \mathbb{N}$, $\mathcal{D}_n$ is an admissible finite volume discretization of Ω and $u_n \in H_0^{\mathcal{D}_n}$. Assume that $\lim_{n \longrightarrow \infty} h_{\mathcal{D}_n} = 0$, and that there exists $C > 0$ such that, for all $n \in \mathbb{N}$, $\langle u_n, u_n \rangle^a_{\mathcal{D}_n} \leq C$.*

Then there exist a subsequence of $(\mathcal{D}_n, u_n)_{n \in \mathbb{N}}$, again denoted $(\mathcal{D}_n, u_n)_{n \in \mathbb{N}}$, and $\hat{u} \in H_0^1(\Omega)$ such that $\lim_{n \longrightarrow \infty} u_n = \hat{u}$ in $L^2(\Omega)$.

Proof. Due to assumption 1.1, we obtain

$$\alpha [u, v]_{\mathcal{D},1} \leq \langle u_n, u_n \rangle^a_{\mathcal{D}_n} \leq C$$

which allows to apply lemma 4.4 to obtain the existence of a subsequence of (u_n) converging to certain $\hat{u} \in H_0^1(\Omega)$. □

4.16. Lemma (Consistency). *Let Ω be an open bounded polygonal subset of $\mathbb{R}^d$. Let $(\mathcal{D}_n, u_n)_{n \in \mathbb{N}}$ be a sequence such that for $n \in \mathbb{N}$, $\mathcal{D}_n$ is an admissible finite volume discretization of Ω and $u_n \in H_0^{\mathcal{D}_n}$. Assume that $\lim_{n \longrightarrow \infty} h_{\mathcal{D}_n} = 0$, and that there exists $\hat{u} \in H_0^1(\Omega)$ such that $\lim_{n \longrightarrow \infty} u_n = \hat{u}$. Then, $\forall \varphi \in C_c^\infty(\Omega)$,*

$$\lim_{n \longrightarrow \infty} \langle u_n, P_{\mathcal{D}_n} \varphi \rangle^a_{\mathcal{D}} = \langle \hat{u}, \varphi \rangle \tag{4.17}$$

The statement follows from the strong convergence of the discrete gradient ([**7**], lemma 2.6) and the consistency estimate ([**7**], lemma 2.5).

4.17. Lemma (Finite volume schemes are admissible schemes). *Under the assumptions 1.1 and 1.2, consider a family $\mathcal{F}$ of admissible finite volume discretizations of Ω in the sense of definition 4.1 such that $\inf_{\mathcal{D} \in \mathcal{F}} h_{\mathcal{D}} = 0$. Then the family of spaces $H_0^{\mathcal{D}}$ with the inner product $\langle \cdot, \cdot \rangle^i_{\mathcal{D}}$ defined in* (4.9) *is an admissible family of finite dimensional approximations to the inner product $\langle \cdot, \cdot \rangle$ defined in* (1.4).

Proof. The compactness (i) of definition 3.1 results from lemma 4.15, and the consistency (ii) is due to (4.17). □

Now, we regard the following discrete eigenvalue problem:

4.18. Problem. *Given assumption 1.1, let $\mathcal{D}$ be an admissible finite volume discretization. Then, find $u \in H_0^{\mathcal{D}}, \lambda \in \mathbb{C}$ such that*

$$\langle u, v\rangle_{\mathcal{D}}^{a} = \lambda \int_{\Omega} u\bar{v}dx \;\forall v \in H_0^{\mathcal{D}}. \tag{4.18}$$

4.19. Theorem. *Under the assumptions 1.1 and consider a family $\mathcal{F}$ of admissible finite volume discretizations of Ω in the sense of definition 4.1 such that $\inf_{\mathcal{D}\in\mathcal{F}} h_{\mathcal{D}} = 0$. Then, the eigenvalues of problem 4.18 converge to those of 1.3 in the following sense: for each eigenvalue λ of problem 1.3 with multiplicity m, for any sequence $(\mathcal{D}_n) \subset \mathcal{F}$ such that $\lim_{n\to\infty} h_{\mathcal{D}_n} = 0$, for n large enough, there are m eigenvalues $\lambda_{\mathcal{D}_n,1} \dots \lambda_{\mathcal{D}_n,m}$ of problem 4.7 converging to λ as $n \to \infty$.*

Proof. The conclusion about convergence follows from lemma 4.17 and theorems 3.3 and 2.2. □

In order to obtain error estimates, we provide the following result.

4.20. Lemma (Error estimate). *Under the assumptions 1.1 let $\mathcal{D}$ be an admissible finite volume discretization of Ω in the sense of definition 4.1. Assume that $\mathcal{D}$ is regular in the sense that $\exists\zeta_{\mathcal{D}} > 0$ such that $\operatorname{dist}(x_K, \sigma) \geq \zeta_{\mathcal{D}} \operatorname{diam}(K)$ for all $K \in \mathcal{T}$ and $\sigma \in \mathcal{E}_{int}$. Furthermore, assume $d = 2, 3$, $A \in C^1(\bar{\Omega})$ and $V(x) = 0$.*

Let μ be an eigenvalue of the inverse operator T such that $E_\mu \subset H^2(\Omega)$. Then there exists a constant C, depending on $\Omega, \zeta_{\mathcal{D}}, d, A, \alpha, E_\mu$, such that

$$\|(T_{\mathcal{D}} - T)|_{E_\mu}\|_{E_\mu \to L^2(\Omega)} \leq Ch_{\mathcal{D}}. \tag{4.19}$$

Proof. Let $u \in E_\mu$ such that $\|u\|_{L^2(\Omega)} = 1$. From the proof of [**7**], theorem 3.3 (H^2 regularity with homogeneous Dirichlet BC), we have

$$\|T_{\mathcal{D}}u - Tu\|_{L^2(\Omega)} \leq C_{EGH}h_{\mathcal{D}}\|u\|_{H^2(\Omega)}$$

where C_{GHV} depends on $\Omega, \zeta_{\mathcal{D}}, d, A, \alpha$, but not on $u, h_{\mathcal{D}}$. Based on this estimate, we conclude as in the proof of lemma 4.9. □

4.21. Corollary. *Under the conditions of theorem 4.19 and lemma 4.20 for the anisotropic case, one can prove the same error estimates as in corollaries 4.11,4.12.*

4.22. Remark. *According to remark 1.1 in* [**7**]*, the case $V(x) \neq 0$ can be treated in a similar fashion as in* [**8**].

5. Numerical results

5.1. Delaunay-Voronoï construction of admissible meshes. Let $\Omega \subset \mathbb{R}^d$ be a polygonal domain. Let $\mathcal{P} \subset \overline{\Omega}$ be a finite set of points. The *Voronoï box* ω_K around the point $x_K \in \mathcal{P}$ is defined as the set of points $x \in \mathbb{R}^d$ which are closer to x_K than to any other point x_L of $\mathcal{P}$. The set $K = \Omega \cap \omega_K$ is called *Voronoï box with respect to* Ω. The set of Voronoï boxes with respect to Ω, also called Voronoï diagram, together with the points of $\mathcal{P}$ is an admissible finite volume partition of Ω where the Voronoï boxes are used as control volumes. The application of this approach to the discretization of partial differential equations is known since at least [**11**].

What follows, is a constructive method of obtaining these Voronoï boxes. A set $\mathcal{S}$ of d-dimensional nonempty, non-overlapping simplexes such that $\overline{\Omega} = \cup_{s\in\mathcal{S}}\overline{s}$ is called simplicial partition of Ω if any face of a simplex s_1 is either a subset of the boundary $\partial\Omega$, or it is the face of another simplex s_2 of the triangulation [**12**].

Let $\mathcal{S}$ a simplicial partition of Ω. Let $\mathcal{P}$ be the set of vertices of the simplexes in $\mathcal{S}$. A simplex $s \in \mathcal{S}$ is called *Delaunay* if the interior of its circumball does not contain

any point of $\mathcal{P}$. The simplicial partition $\mathcal{S}$ is called Delaunay if all simplexes in $\mathcal{S}$ are Delaunay. The simplicial partition $\mathcal{S}$ is said to have the *boundary conforming Delaunay property* if the circumcenters of all simplexes of S are in $\overline{\Omega}$ [**13**].

Assume that $\overline{\Omega} = \cup_{m=1}^{M} \overline{\Omega}_m$ is the union of bounded polygonal subdomains Ω_m. For each Ω_m, let $\mathcal{S}_m$ be a boundary conforming Delaunay simplicial partition. If $\mathcal{S} = \cup_{m=1}^{M} \mathcal{S}_m$ is a simplicial partition of Ω then we say that $\mathcal{S}$ has the Delaunay property conforming to interior and exterior boundaries. This definition addresses the case of a discontinuous reciprocal effective mass along the interior boundaries.

For a simplicial partition possessing the boundary conforming Delaunay property, the Voronoï diagram with respect to Ω of the set of vertices of $\mathcal{S}$ can be obtained by joining the circumcenters and edge midpoints of the simplexes of the partition.

In two space dimensions, we can rely on a proven algorithm which generates this type of grids which is implemented in triangle [**14, 15**].

In three space dimensions, the generation of boundary conforming Delaunay still remains a challenge [**13**]. The development of the mesh generator TetGen [**16, 17**] is aimed at the creation of external and internal boundary conforming Delaunay meshes in three space dimensions.

The simplex based construction of the Voronoï diagram allows to implement an assembly scheme for the discrete operator defined in (4.9) which is similar to that of the finite element method in the sense that all the necessary geometrical data can be computed and assembled simplex by simplex, with no need to construct the Voronoï boxes explicitely [**18**].

5.2. Numerical solution of the discrete eigenvalue problem. As an eigenvalue solver, we use ARPACK [**19**] in the shift-invert mode with zero shift. For the one- and two-dimensional examples, the solution of the linear systems has been obtained by PARDISO [**20, 21, 22**]. In the three-dimensional case, a parallel Jacobi preconditioned conjugated gradient method [**23**] has been used. The implementation uses the toolbox pdelib2 for the numerical solution of partial differential equations developed at WIAS Berlin.

5.3. Examples. Most of the following numerical examples correspond to isotropic model configurations of quantum wells where exact solutions can be given. These exact solutions are defined in $\mathbb{R}^d$. For our computations, they are cut off at the boundary of the computational domain by homogeneous Dirichlet boundary conditions. The boundary is placed "far away" from the quantum well. Furthermore, in all the examples we assume $\hbar = 1$.

In order to keep the number of unknowns under control, we use a mesh which is a priori refined in the confinement region near to the quantum well. To obtain data about the convergence of the method, we performed calculations for varying grid sizes. In order to reveal the convergence order, we use isotropically triangulated domains. The number of points in the grids mainly was influenced using the simplex volume constraint which can be set to control the grid generators. An exception is example 5.3.5 where the description of the input geometry has been refined as well. As a result, for a d dimensional grid, the mesh size $h_{\mathcal{D}}$ can be assumed to be proportional to $N^{-1/d}$ where N is the number of unknowns. For this reason, in order to visualize the estimate of the convergence order, we have chosen to plot error logarithms versus N where the N axis is scaled logarithmically. The "raw data" behind the plots the reader finds in appendix A. All two-dimensional meshes have been generated by triangle [**14, 15**], the three-dimensional meshes have been generated by TetGen [**16, 17**].

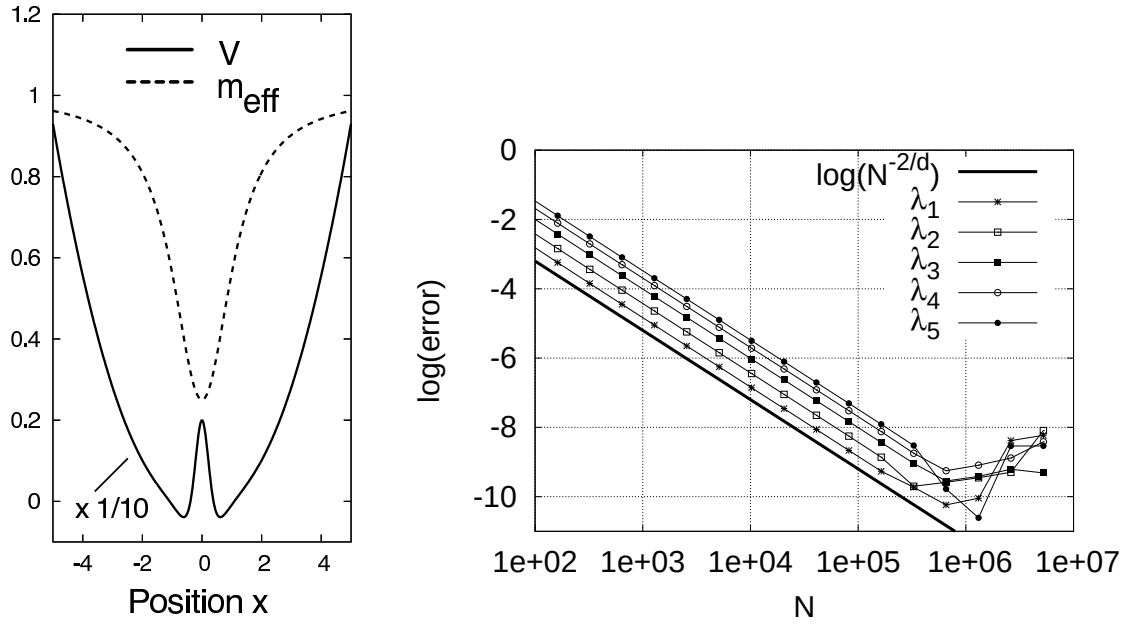

FIGURE 5.1. 1D anharmonic double well: effective mass and potential (left), h^2-convergence of the five lowest eigenvalues (right)

5.3.1. *1D anharmonic double well with position-dependent effective mass.* The first example [**24**] describes a graded heterostructure with an anharmonic double well potential. The position-dependent effective mass in one space dimension is given by

$$m(x) = \Big(\frac{\alpha + x^2}{1 + x^2}\Big)^2,$$

and the potential is defined as

$$V(x) = \frac{1}{2}\big(x + (\alpha - 1)\arctan x\big)^2 + \Big(\frac{\alpha - 1}{2}\Big)\frac{3x^4 + (4 - 2\alpha)x^2 - \alpha}{(\alpha + x^2)^4}.$$

The corresponding Hamiltonian belongs to the iso-spectral family of the harmonic oscillator with eigenvalues $\lambda_n = n - 1/2$ $(n = 1, 2 \dots)$. Our calculations have been performed for $\alpha = 0.5$. For the variation of the potential and the position dependent effective mass, see see figure 5.1 (left). Figure 5.1 (right) demonstrates second order convergence of the five lowest eigenvalues. The deviation from this behavior at large N can be attributed to roundoff errors. The obtained eigenvalues are presented in table A.1.

5.3.2. *1D quantum well with discontinuous coefficients.* A semiconductor quantum well is a layered nanostructure which consists of a layer of a well material sandwiched between two barrier materials. The different values of the band edges in both materials define a potential well for the carriers as depicted in figure 5.2. Additionally, the effective masses for both materials may be different, leading to a coefficient discontinuity at the interfaces between the two materials.

The effective mass and potential are given by

$$m(x) = \begin{cases} m_w, & |x| < L/2 \\ m_b, & |x| \geq L/2, \end{cases} \qquad V(x) = V_{\mathrm{qw}}(x) = \begin{cases} 0, & |x| < L/2 \\ V_0, & |x| \geq L/2, \end{cases} \tag{5.1}$$

see also figure 5.2 (left). These coefficients define a quantum well with thickness L, barrier height V_0. The effective mass in the well region is m_w, and in the barrier regions it is m_b.

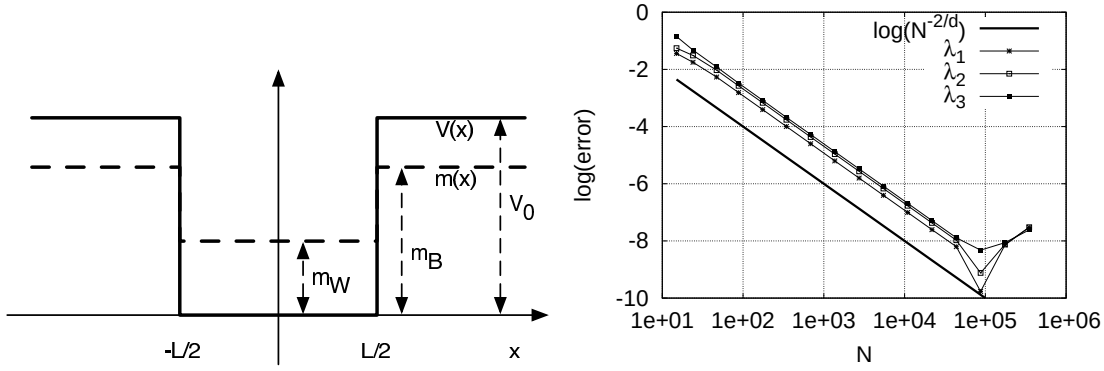

FIGURE 5.2. Effective mass and potential in a 1D quantum well (left), h^2-convergence of the 3 bounded states (right).

The eigenvalues for the bounded states of this quantum well are given by

$$\lambda_n = \frac{\hbar^2}{2m_w}\frac{4}{L^2}\xi_n^2$$

where ξ_n are the real positive solutions of

$$\xi \tan \xi = \sqrt{\frac{m_w}{m_b}}\sqrt{\xi_0^2 - \xi^2} \quad \text{(even states)}$$

$$\xi \cot \xi = -\sqrt{\frac{m_w}{m_b}}\sqrt{\xi_0^2 - \xi^2} \quad \text{(odd states)}$$

where

$$\xi_0 = \frac{L}{2}\sqrt{\frac{2m_w}{\hbar^2}V_0}.$$

These equations have been derived by obtaining the fundamental solutions in both barrier and well regions separately. They are of the form

$$u_{\text{left}} = e^{\alpha(E)x} \quad u_{\text{well}} = ae^{ik(E)x} + be^{ik(E)x} \quad u_{\text{right}} = e^{-\alpha(E)x}$$

The four parameters $a, b, \alpha(E), k(E)$ are obtained by matching the eigenfunctions at the interfaces at $-L/2, L/2$ using continuity of the eigenfunctions u and of the their fluxes $\frac{1}{m(x)}\nabla u$ [**1**].

Figure 5.2 (right) demonstrates the quadratic convergence of the three bounded states in the case m_w=1, $m_b = 2$, $V_0 = 2$, $L = 10$. Further, we notice the deviation from the asymptotic which can be attributed to roundoff errors. For the obtained values, see table A.2.

5.3.3. *2D quantum well with in-plane harmonic confinement.* For this structure, effective mass and potential are given by

$$m(x,y) = m(x) = \begin{cases} m_w, & |x| < L/2 \\ m_b, & |x| \geq L/2, \end{cases} \qquad V(x,y) = V_{\text{qw}}(x) + \frac{m_w^2}{2m(x)}\omega_0^2 y^2.$$

Here, V_{qw} is the potential of the quantum well as defined in (5.1), see also figure 5.3 (left), and ω_0 defines the strength of the harmonic confinement in the y-direction.

Eigenfunctions and eigenvalues for this structure can be obtained by generalizing the matching approach mentioned in 5.3.3. In this case, the eigenfunctions are of product type, but the x and y eigenmodes are coupled if $m_b \neq m_w$. They follow the general ansatz

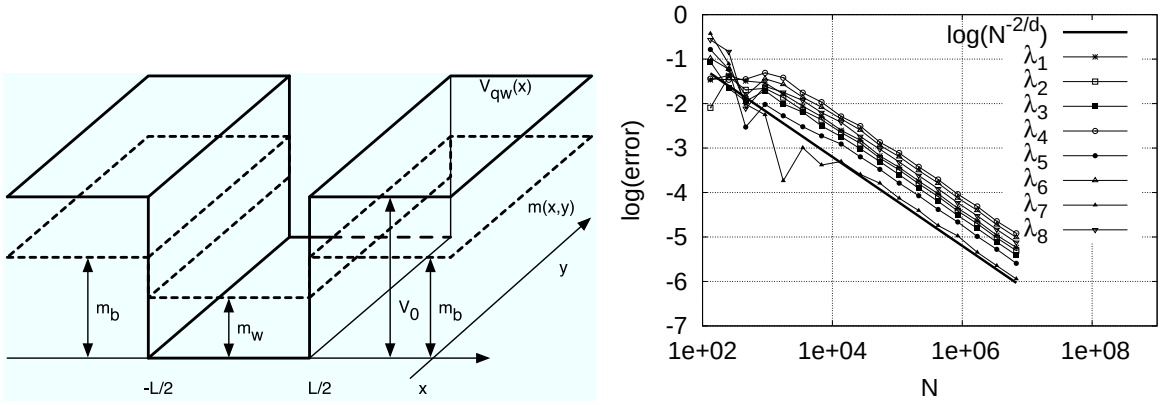

FIGURE 5.3. Effective mass and potential in 2D quantum well (without in-plane harmonic confinement) (left), h^2-convergence of the first eight lowest eigenvalues.

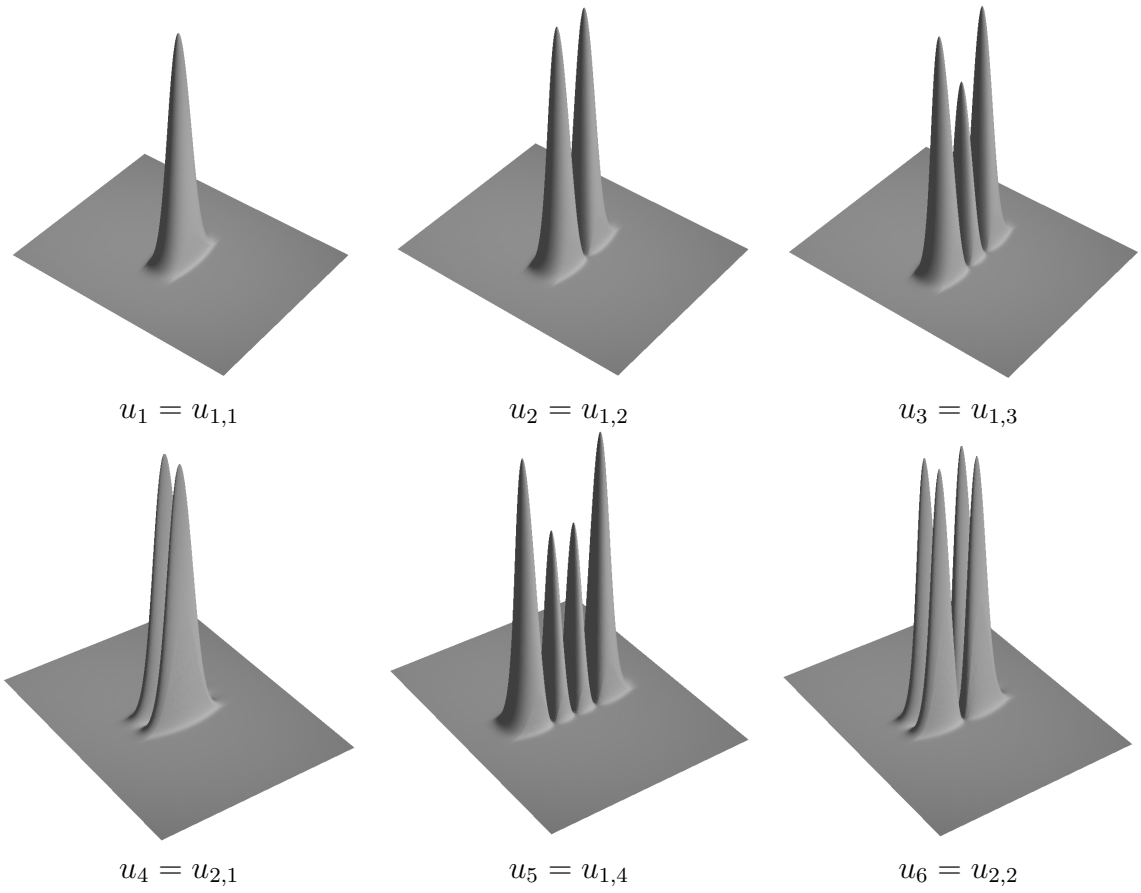

FIGURE 5.4. Eigenmodes in 2D quantum well with in-plane harmonic confinement

$u_{n,m}(x,y) = F_{n,m}(x)G_m(y)$ for $n, m = 1, 2 \ldots$. For the corresponding eigenvalues we have that

$$\lambda_{n,m} = \lambda^y_m + \lambda^x_{m,n}$$

where

$$\lambda^y_m = \hbar\omega_0(m - \frac{1}{2}), \quad \lambda^x_{m,n} = \frac{\hbar^2}{2m_w}\frac{4}{L^2}\xi^2_{m,n}.$$

The values $\xi_{m,n}$ are positive real solutions of

$$\xi \tan \xi = \sqrt{\frac{m_w}{m_b}} \sqrt{\xi_{m,0}^2 - \xi^2}, \ n \text{ odd}$$

$$\xi \cot \xi = \sqrt{\frac{m_w}{m_b}} \sqrt{\xi_{m,0}^2 - \xi^2}, \ n \text{ even}$$

where

$$\xi_{m,0} = \frac{L}{2\hbar} \sqrt{2m_w \big(V_0 - (1 - \frac{m_w}{m_b})\lambda_m^y\big)}. \tag{5.2}$$

For our calculations we used the values $m_w = 1$, $m_b = 2$, $V_0 = 2$, $L = 10$, $\omega_0 = 0.2$, The first six eigenmodes are plotted in figure 5.4. Figure 5.3 (right) confirms the quadratic convergence of the six lowest eigenvalues. The obtained values are given in table A.3.

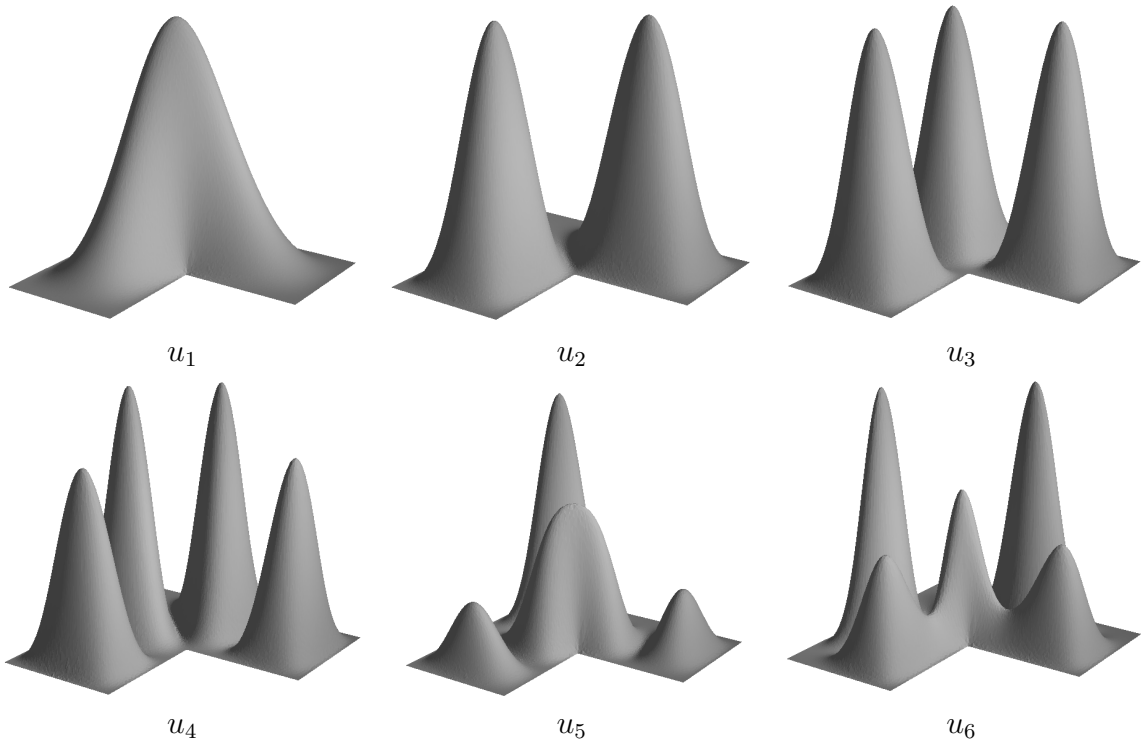

FIGURE 5.5. First six eigenmodes (squared) of the L-shape domain. Please note the higher regularity of u_2, u_3, u_4 in comparison to that of u_1, u_5, u_6.

5.3.4. *Eigenvalues of the L-shape domain.* The L-shape example is relevant in the theory of quantum transistors as it is the half of the domain of a T-stub structure [**26**].

We compare the eigenvalues obtained by our method with the high accuracy eigenvalues published in [**25**] (see table A.4) for the unit L-shape domain. Please note that in difference to all other examples in this paper, where we have at least piecewise H^2-regularity, this domain has eigenmodes with singularities at the re-entrant corner. The convergence result 2.2 claims the dependence of the approximation of the eigenvalue on the quality of approximation of the corresponding eigenmodes. This behavior is clearly seen in figure 5.6 where $\lambda_1, \lambda_5, \lambda_6$ asymptotically converge worse than $\lambda_2, \lambda_3, \lambda_4$ which show $O(h^2)$ convergence. In figure 5.5 one can see that the former eigenfunctions are affected by the re-entrant corner singularity while due to the symmetry of the domain the later have crossing nodelines at the corner point, leading to H^2-regularity.

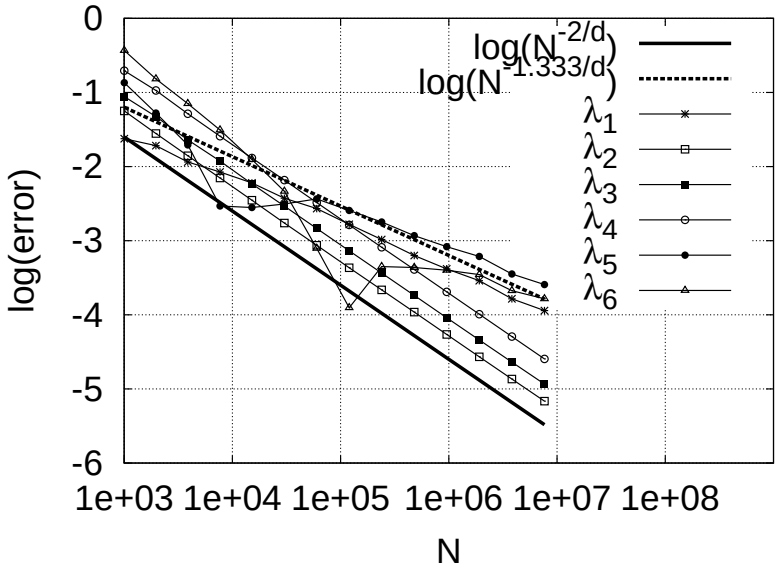

FIGURE 5.6. Convergence of the first six eigenvalues of the Laplacian in the L-shape domain to the values published in [**25**]. Please note the better convergence of $\lambda_2, \lambda_3, \lambda_4$ in comparison to that of $\lambda_1, \lambda_5, \lambda_6$

This example reveals the fact that the lowest eigenmode may converge worse than some of the higher ones.

5.3.5. *3D embedded spherical quantum dot of radius R.* A three dimensional quantum dot can be described by a radially symmetric effective mass and potential functions

$$V(r) = \begin{cases} 0, & r < R \\ V_0 & R \le r \end{cases} \quad m_{\text{eff}}(r) = \begin{cases} m_{dot}, & r < R \\ m_{barrier} & R \le r. \end{cases}$$

We use the general ansatz for the eigenfunctions in spherical coordinates

$$u_{l,m} = P_l(r) Y_{lm}(\theta, \phi)$$

where Y_{lm} are the spherical harmonics. To match the radial basis function $P_l(r)$ in the quantum dot, we use the spherical Bessel functions $J_l(kr)$. In the bulk, we use the modified spherical Bessel functions of second kind $K_{1,l}(qr)$ [**27**].

Extending the matching approach described in 5.3.2, we obtain the eigenvalue of the fundamental mode (figure 5.7, left) corresponding to the 1s orbital with $l = 0, m = 0$ by

$$\lambda_{1s} = \frac{\hbar^2}{2m_w R^2} \xi_{1s}^2$$

with ξ_{1s} being the lowest positive solution of

$$\xi \cot \xi = -\sqrt{\frac{m_{dot}}{m_{barrier}}} \sqrt{\xi_0^2 - \xi^2} + \left(1 - \frac{m_{dot}}{m_{barrier}}\right)$$

where

$$\xi_0 = \sqrt{\frac{2m_{dot}}{\hbar^2} V_0 R^2}.$$

For the 1p orbital with $l = 1, m = -1, 0, 1$, we get the eigenvalues

$$\lambda_{1p} = \frac{\hbar^2}{2m_{dot} R^2} \xi_{1p}^2. \tag{5.3}$$

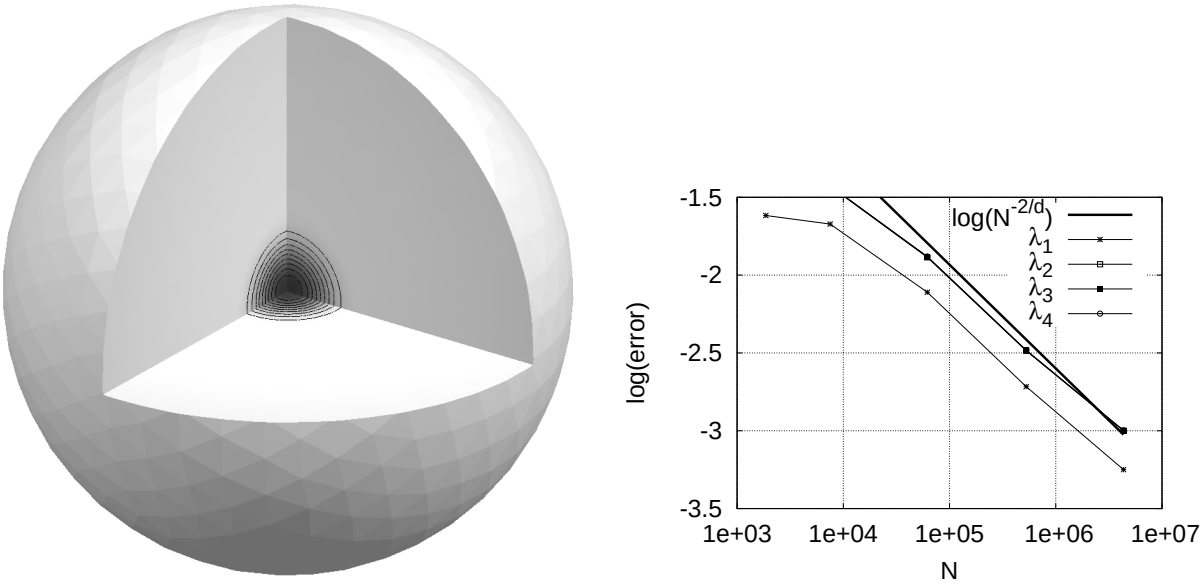

FIGURE 5.7. Fundamental eigenmode for quantum dot (left), convergence of the 1s and 1p eigenmodes (right)

Here ξ_{1p} is the lowest positive zero of

$$\frac{\xi^2}{1-\xi\cot\xi} = -\frac{{\xi_0}^2-\xi^2}{1+\sqrt{\frac{m_{barrier}}{m_{dot}}}\cdot\sqrt{{\xi_0}^2-\xi^2}} + 2\Big(1-\frac{m_{dot}}{m_{barrier}}\Big) \tag{5.4}$$

For $m_{dot}=1, m_{barrier}=2, R=4, V_0=2$, the fundamental eigenmode is depicted in 5.7 (left).

Fig. 5.7 (right) demonstrates second order convergence for the fundamental eigenmode. Please note that in this case, the asymptotic region is reached for a similar values of h as in the 2D case, however, the corresponding number of unknowns was approximately 600000.

We see the same convergence order for the next group of eigenvalues, however, the constant is worse. This seems to be due to the fact that the discretization grids have been designed such that the fundamental eigenmode is well represented already on coarser grids. At the same time, the grids were suboptimal for the next three modes.

Please note that from table A.3 we establish that it is not possible to conclude from the closeness of the three approximate 1p eigenvalues one to each other to their closeness to the exact eigenvalue.

6. Conclusions

In order to prove the convergence of the finite volume method for the solution of the eigenvalue problem 1.3, we introduced the framework of admissible finite dimensional approximations in subspaces of $L^2(\Omega)$ to a given inner product in $H_0^1(\Omega)$. This notion allows to establish the convergence in norm of the discrete solution operators obtained by the to their continuous counterpart from compactness and consistency statements for the discrete approximations.

Based on the construction of an admissible finite volume mesh, these two properties are proven for two variants of the finite volume discretization. One is derived from the classical approach using two point fluxes for the case of an isotropic effective mass. The other one is derived from the discrete gradient introduced in [**7**]. In both cases, the convergence of

eigenvalues and eigenvectors can be obtained from classical spectral approximation results reviewed in [**3**].

In both the isotropic and anisotropic case, with certain restrictions on the coefficients of the problem, for two- and three-dimensional domains, first order error estimates have been obtained in the case of H^2 regular eigenfunctions.

In the isotropic case, using M-matrix theory, we could prove the positivity of the lowest eigenvalue and constant sign of the corresponding discrete eigenfunction.

Admissible meshes can be constructed using the Delaunay-Voronoï method based on boundary conforming Delaunay grids. These grids can be obtained by the mesh generators triangle (2D, [**14, 15**]) and, with some restrictions, TetGen (3D, [**16, 17**]).

Based on an implementation of a finite volume eigenvalue solver within the framework of the toolbox pdelib2 for the numerical solution of partial differential equations developed at WIAS, using the direct solver PARDISO and the iterative eigenvalue solver ARPACK, we demonstrated the applicability of the described approach to test problems close to those from the theory of semiconductor nanostructures. All the examples regardless of the space dimension show quadratic convergence in the eigenvalue if at least piecewise H^2 regularity of the corresponding eigenfunctions can be expected.

Possible directions of further work are improved error estimates, more efficient eigenvalue solvers, adaptive approaches, and coupling to more complex models like the Schrödinger Poisson system.

Acknowledgements

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Appendix A. Numerical raw data

In the appendix, for reference purposes, we present the data obtained during our numerical experiments.

N	λ_1	λ_2	λ_3	λ_4	λ_5
12	0.00000000	0.00000000	0.00000000	0.00000000	0.00000000
22	0.14838846	1.42063123	2.09011487	3.01344329	3.25045474
42	0.47646180	1.47860442	2.43112511	3.37723432	4.28548542
82	0.49769193	1.49425865	2.48488564	3.46886212	4.44885523
162	0.49943133	1.49855234	2.49620424	3.49216813	4.48717041
322	0.49985777	1.49963619	2.49904690	3.49803292	4.49677965
642	0.49996438	1.49990879	2.49976109	3.49950689	4.49919284
1282	0.49999108	1.49997716	2.49994019	3.49987654	4.49979792
2562	0.49999777	1.49999429	2.49998504	3.49996911	4.49994944
5122	0.49999944	1.49999857	2.49999626	3.49999228	4.49998736
10242	0.49999986	1.49999964	2.49999906	3.49999807	4.49999684
20482	0.49999997	1.49999991	2.49999977	3.49999952	4.49999921
40962	0.49999999	1.49999998	2.49999994	3.49999988	4.49999980
81922	0.50000000	1.49999999	2.49999999	3.49999997	4.49999995
163842	0.50000000	1.50000000	2.50000000	3.49999999	4.49999999
327682	0.50000000	1.50000000	2.50000000	3.50000000	4.50000000
655362	0.50000000	1.50000000	2.50000000	3.50000000	4.50000000
1310722	0.50000000	1.50000000	2.50000000	3.50000000	4.50000000
2621442	0.50000000	1.50000000	2.50000000	3.50000000	4.50000000
5242882	0.50000001	1.49999999	2.50000000	3.50000000	4.50000000
∞	0.5	1.5	2.5	3.5	4.5

TABLE A.1. Approximate and exact eigenvalues for the 1D anharmonic double well 5.3.1

N	λ_1	λ_2	λ_3
15	0.20569282	0.74256558	1.39830263
24	0.18717801	0.71791091	1.49297382
47	0.17490300	0.69660613	1.52805675
88	0.17102931	0.68987813	1.53693778
175	0.16987820	0.68789142	1.53941252
344	0.16958615	0.68738849	1.54002864
687	0.16951090	0.68725898	1.54018646
1368	0.16949209	0.68722661	1.54022584
2735	0.16948736	0.68721847	1.54023575
5464	0.16948617	0.68721643	1.54023822
10927	0.16948588	0.68721592	1.54023884
21848	0.16948580	0.68721579	1.54023899
43695	0.16948578	0.68721576	1.54023903
87384	0.16948578	0.68721575	1.54023904
174767	0.16948577	0.68721574	1.54023904
349528	0.16948581	0.68721578	1.54023907
∞	0.16948577	0.68721575	1.54023904

TABLE A.2. Approximate and exact eigenvalues for a one-dimensional quantum well

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6	λ_7	λ_8
132	0.31224724	0.46833873	0.58766252	0.78472724	1.03715175	1.11860620	1.44505152	1.47945220
253	0.32119549	0.51671488	0.65260595	0.78657429	0.93145340	0.95479457	0.99255201	1.05967667
462	0.31031859	0.49664981	0.68588650	0.85631279	0.86962387	1.02908239	1.06084599	1.21468219
917	0.30742721	0.49834349	0.69397216	0.86998254	0.88217761	1.05014618	1.07615785	1.23129658
1751	0.29447489	0.49000308	0.68436583	0.85903269	0.87789766	1.04120560	1.07036473	1.22485258
3495	0.28688799	0.48337785	0.68095278	0.83848139	0.87561013	1.02790386	1.07156167	1.21867856
6802	0.28321580	0.48071424	0.67767495	0.83173043	0.87446723	1.02239785	1.07096324	1.21315115
13614	0.28062829	0.47861028	0.67632535	0.82606496	0.87382261	1.01861106	1.07104474	1.21070365
26871	0.27962832	0.47764863	0.67549104	0.82404867	0.87322366	1.01662608	1.07080379	1.20871676
53732	0.27879514	0.47696456	0.67502283	0.82227908	0.87292052	1.01523361	1.07071001	1.20784108
106678	0.27849682	0.47669262	0.67477811	0.82170174	0.87275124	1.01472531	1.07062201	1.20738636
213365	0.27831053	0.47652901	0.67465172	0.82130623	0.87267361	1.01439908	1.07058716	1.20714062
425311	0.27822278	0.47645214	0.67458981	0.82112416	0.87263037	1.01424732	1.07056598	1.20702055
850540	0.27817329	0.47640942	0.67455741	0.82101978	0.87261059	1.01416043	1.07055845	1.20695816
1697843	0.27815212	0.47639094	0.67454238	0.82097639	0.87259914	1.01412468	1.07055241	1.20692943
3395968	0.27813988	0.47638059	0.67453451	0.82095046	0.87259411	1.01410372	1.07055015	1.20691432
6785939	0.27813474	0.47637595	0.67453073	0.82093995	0.87259139	1.01409467	1.07054903	1.20690710
∞	0.27812894	0.47637099	0.67452682	0.82092783	0.87258883	1.01408488	1.07054789	1.20689955

TABLE A.3. Approximate and exact eigenvalues of 2D quantum well 5.3.3

N	λ_1	λ_2	λ_3	λ_4	λ_5	λ_6
1002	9.66350281	15.14100689	19.65122339	29.32487860	31.77710836	41.10521569
1967	9.65891389	15.16931575	19.69200016	29.41498942	31.85986020	41.32235883
3874	9.65124522	15.18324946	19.71627895	29.46990886	31.89304626	41.40374030
7683	9.64817406	15.19022571	19.72734289	29.49577491	31.90969343	41.44333613
15162	9.64573035	15.19373524	19.73336927	29.50841414	31.91544042	41.46203557
30230	9.64346928	15.19552140	19.73628054	29.51490259	31.91576125	41.46986637
60220	9.64243805	15.19638372	19.73774815	29.51821139	31.91629888	41.47372075
120137	9.64138417	15.19682051	19.73847840	29.51984872	31.91519758	41.47463459
239543	9.64075945	15.19703515	19.73884345	29.52066509	31.91442139	41.47495788
479093	9.64035444	15.19714329	19.73902645	29.52107263	31.91380711	41.47494426
956008	9.64013950	15.19719770	19.73911759	29.52127724	31.91346584	41.47491020
1911881	9.64001276	15.19722484	19.73916323	29.52137905	31.91324881	41.47485904
3821712	9.63988842	15.19723841	19.73918600	29.52143007	31.91299147	41.47472143
7641318	9.63983796	15.19724516	19.73919740	29.52145561	31.91289147	41.47467410
∞	9.63972380	15.19725200	19.73920900	29.52148100	31.91263600	41.47451000

TABLE A.4. Approximate and high accuracy [**25**] eigenvalues of the Laplacian in the L-shape domain 5.3.4

N	λ_1	λ_2	λ_3	λ_4
1864	0.24225737	0.49861759	0.49925303	0.50071187
7512	0.23939208	0.48469811	0.48491725	0.48499876
61741	0.22587507	0.46047041	0.46056203	0.46063176
527008	0.22003405	0.45072389	0.45074423	0.45075516
4341423	0.21867613	0.44846269	0.44846386	0.44846540
∞	0.21811352	0.44746088	0.44746088	0.44746088

TABLE A.5. Approximate and exact eigenvalues for quantum dot 5.3.5

References

[1] G. Bastard. *Wave mechanics applied to semiconductor heterostructures*. Halsted Press, 1988.

[2] H. W. Alt. *Lineare Funktionalanalysis*. Springer, 1999.

[3] I. Babuška and J. Osborn. Eigenvalue problems. In Ph. Ciarlet and J.L. Lions, editors, *Handbook of Numerical Analysis II*, pages 641–787. North-Holland, 1991.

[4] W. Kolata. Approximation in variationally posed eigenproblems. *Numerische Mathematik*, 29:159–171, 1978.

[5] R. Eymard, T. Gallouët, and R. Herbin. The finite volume method. In Ph. Ciarlet and J.L. Lions, editors, *Handbook of Numerical Analysis VII*, pages 723–1020. North Holland, 2000.

[6] R. Eymard, T. Gallouët, R. Herbin, and A. Michel. Convergence of a finite volume scheme for nonlinear degenerate parabolic equations. *Numer.Math*, 92:41–82, 2002.

[7] R. Eymard, T. Gallouët, and R. Herbin. A cell-centered finite-volume approximation for anisotropic diffusion operators on unstructured meshes in any space dimension. *IMA J. Numer. Anal.*, 26(2):326–353, 2006.

[8] T. Gallouët, R. Herbin, and M.H. Vignal. Error estimate on the approximate finite volume solution of convection diffusion equations with general boundary conditions. *SIAM J. Numer. Anal.*, 37(6):1935–1972, 2000.

[9] R. Courant and D. Hilbert. *Methods of Mathematical Physics*. Wiley VCH, 1989.

[10] R. S. Varga. *Matrix iterative analysis*. Prentice-Hall, Englewood Cliffs, NJ, 1962.

[11] R. H. Macneal. An asymmetrical finite difference network. *Quart. Math. Appl.*, 11:295–310, 1953.

[12] Ph. Ciarlet. The finite element method. In Ph. Ciarlet and J.L. Lions, editors, *Handbook of Numerical Analysis II*, pages 17–351. North-Holland, 1991.

[13] H. Si. *Three-Dimensional Boundary Conforming Delaunay Mesh Generation*. PhD thesis, Technical University Berlin, 2007. In preparation.

[14] J. R. Shewchuk. Triangle: Engineering a 2D Quality Mesh Generator and Delaunay Triangulator. In M. C. Lin and D. Manocha, editors, *Applied Computational Geometry: Towards Geometric Engineering*, volume 1148 of *Lecture Notes in Computer Science*, pages 203–222. Springer-Verlag, May 1996.

[15] J. R. Shewchuk. triangle version 1.6. URL: http://www.cs.cmu.edu/˜quake/triangle.html, 2007. Retrieved 2007-09-26.

[16] H. Si and K. Gärtner. Meshing piecewise linear complexes by constrained Delaunay tetrahedralizations. In B. W. Hanks, editor, *Proc of 14th Intl. Meshing Roundtable, San Diego, CA*, pages 147–163. Springer, 2005.

[17] H. Si. TetGen version 1.4.2. URL: http://tetgen.berlios.de/, 2007. Retrieved 2007-09-26.

[18] H. Gajewski and K. Gärtner. On the discretization of van Roosbroeck's equations with magnetic field. *Z. Angew. Math. Mech.*, 76(5):247–264, 1996.

[19] R. Lehoucq, K. Maschhoff, D. Sorensen, and C. Yang. ARPACK - Arnoldi package. URL: http://www.caam.rice.edu/software/ARPACK/, 2007. Retrieved 2007-09-26.

[20] O. Schenk and K. Gärtner. Solving unsymmetric sparse systems of linear equations with PARDISO. *J. Future Gen. Comp. Sys*, 20(3):475–487, 2004.

[21] O. Schenk and K. Gärtner. On fast factorization pivoting methods for symmetric indefinite systems. *ETNA*, 23:158–179, 2006.

[22] O. Schenk, K. Gärtner, G. Karypis, S. Röllin, and M. Hagemann. PARDISO - sparse direct solver. URL: http://www.pardiso-project.org, 2007. Retrieved 2007-09-26.

[23] M. R. Hestenes and R. E Stiefel. Methods of conjugate gradients for solving linear systems. *J. Res. Nat. Bur. Standards*, 49:409–436, 1952.

[24] A. R. Plastino, A. Rigo, M. Casas, F. Garcias, and A. Plastino. Supersymmetric approach to quantum systems with position- dependent effective mass. *Phys. Rev. A*, 60(6):4318–4325, Dec 1999.

[25] L. N. Trefethen and T. Betcke. Computed eigenmodes of planar regions. In *Recent advances in differential equations and mathematical physics*, volume 412 of *Contemp. Math.*, pages 297–314, Providence, RI, 2006. Amer. Math. Soc.

[26] F. Sols, M. Macucci, U. Ravaioli, and K. Hess. Theory for a quantum modulated transistor. *Journal of Applied Physics*, 66:3892–3906, 1989.

[27] M. Abramowitz and I. Stegun, editors. *Handbook of Mathematical Functions.*, volume 55 of *Applied Mathematics Series*. National Bureau of Standards, 1972.