Error Estimation for Eigenvalues of Unbounded Linear Operators and an Application to Energy Levels in Graphene Quantum Dots

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Abstract

The eigenvalue problem for linear differential operators is important since eigenvalues correspond to the possible energy levels of a physical system. It is also important to have good estimates of the error in the computed eigenvalues. In this work we use spline interpolation to construct approximate eigenfunctions of a linear operator by using the corresponding eigenvectors of a discretized approximation of the operator. We show that an error estimate for the approximate eigenvalues can be obtained by evaluating the residual for an approximate eigenpair. The interpolation scheme is selected in such a way that the residual can be evaluated analytically. In order to demonstrate that the method gives useful error bounds we apply it to a problem originating from the study of graphene quantum dots where the goal was to investigate the change in the spectrum from incorporating electron-electron interactions in the potential.

1 Introduction

Let T be a linear operator mapping a Hilbert space H into itself. The eigenvalue problem consists of finding a $\lambda \in \mathbb{C}$ and an $u \in H$ such that

$$Tu = \lambda u, \tag{1}$$

where λ is the *eigenvalue* and x is the *eigenfunction*. The eigenvalue problem is of importance in physics as eigenvalues often correspond to the possible energy levels of a system [2, 4, 3]. For example, when designing a new electronic device, the analysis of electron dynamics in the underlying material is required. It is especially important to investigate the possibility of electron localisation and its energy spectrum by solving the eigenvalue problem within the used model [6, 9, 10, 11, 13, 14, 18]. Knowledge of the accuracy in the computed eigenvalues allows us to draw conclusions about which effects to incorporate in our models and which effects that can safely be neglected.

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In the finite dimensional case, the linear operator T is replaced by a matrix $A \in \mathbb{C}^{n\times n}$ and the eigenvalue problem becomes: Find $\lambda \in \mathbb{C}$ and $x \in \mathbb{C}^n$ such that

$$Ax = \lambda x. \tag{2}$$

The matrix eigenvalue problem has been studied extensively and efficient methods for solving it exists [5]. In the case of large sparse matrices, Krylov subspace methods [17] computes good approximate eigenvalues. Also, suppose an approximate eigenpair $(\widehat{\lambda}, \widehat{x})$ has been obtained. Then, if the matrix A is non-defective, there is an exact eigenpair (λ, x) such that

$$|\widehat{\lambda} - \lambda| \leq \kappa_2(X)\|A\widehat{x} - \widehat{\lambda}\widehat{x}\|_2, \tag{3}$$

where $\kappa_2(X)$ is the condition number of the eigenvector matrix X. This result is known as the Bauer-Fike theorem [5] and provides an estimate of the error in an approximate eigenvalue obtained by, e.g., a Krylov subspace method. The theorem is of particular importance if the matrix A is Hermitean, or symmetric in the real case, as in that case X is orthogonal and $\kappa_2(X) = 1$.

Returning to the case when T is a linear operator, eigenvalues are typically computed by discretization, i.e. approximating (1) by a matrix problem (2), and computing the eigenvalues of the discrete problem. By using this approach we have essentially two sources of error: the discretization error and the error when computing the eigenvalues of the resulting matrix. These two errors are conflicting in the sense that a more accurate discretization tends to increase the condition number of the resulting matrix, which in turn makes the matrix eigenvalue problem more difficult to solve using Krylov subspace methods. In order to balance these two sources of error and also judge the accuracy of the computed eigenvalue $\widehat{\lambda}$, we generalize the error estimate (3) to cover the case of unbounded linear operators acting on a Hilbert space.

Further, by solving the discrete problem (2) we obtain both eigenvalues $\widehat{\lambda}$ and eigenvectors $\widehat{x}$. The eigenvector is a discrete approximation of the corresponding eigenfunction u of the continuous problem (1). Thus we propose to use a suitable interpolation scheme to create an approximate eigenfunction $\widehat{u} \in H$. The interpolation problem has been studied extensively and efficient and accurate methods exists. For our purposes it is important that the interpolation scheme allows the residual $\|T\widehat{u} - \widehat{\lambda}\widehat{u}\|_H$ to be evaluated analytically. Note that if the eigenvalue problem is discretized using the finite element method [1], then an interpolation scheme is built into the numerical method.

The outline of this paper is as follows: In Section 2, we give a background on spectral theory for linear operators, and formulate our residual based error estimate. We also illustrate our result by using a simple linear differential operator with a known spectrum. In Section 3 we apply our theory and obtain error estimates for an eigenvalue calculation from an application. Finally, in Section 4, we discuss our results and point out possible directions for future research.

2 Spectral Theory for Linear Differential Operators

In order to explain the concepts, we begin by introducing a simple eigenvalue problem. Find $u \in C^2([0,1])$ such that

$$\begin{cases} -u'' + \lambda u = 0, & 0 < x < 1, \\ u(0) = 0, & u'(1) + u(1) = 0. \end{cases} \tag{4}$$

If a solution $u \neq 0$ exists for a certain scalar λ then (λ, u) is an eigenpair. In the formulation of the problem we consider $C^2([0,1])$ to be a subset of the Hilbert space $L^2([0,1])$. The underlying Hilbert space structure is nessecary for the theoretical analysis of the problem.

In order to reformulate the above problem in the form (1) we introduce a space

$$V = \{u \in C^2([0,1]) \text{ such that } u(0) = 0 \text{ and } u'(1) + u(1) = 0\}, \tag{5}$$

and a linear operator

$$T : V \to L^2([0,1]), \qquad (Tu)(x) = \partial_x^2 u(x). \tag{6}$$

Note that in this case V is dense in $L^2([0,1])$. The above problem has a simple analytic solution: The eigenfunctions are $u_n = \sin(\sqrt{\lambda_n} x)$, where the eigenvalues λ_n are the positive roots of the equation $\sqrt{\lambda} + \tan(\sqrt{\lambda}) = 0$. Having an analytic solution is convinient as errors in approximate solutions are explicitly known.

2.1 Unbounded Linear Operators

In this section we give the proper definitions of the concepts needed to understand eigenvalue calculations for linear differential operators. The presentation is a summary of standard theory as preseneted in e.g. Rudin or Kreyzig[16, 7].

Throughout this section we assume that H is a separable Hilbert space equipped with a scalar product (u, v) and norm $\|u\| = \sqrt{(u,u)}$, and complete in the topology inferred by its norm. By an *operator on* H we mean a linear mapping $T : \mathcal{D}(T) \to \mathcal{R}(T)$, where both the *domain* $\mathcal{D}(T)$ and the *range* $\mathcal{R}(T)$ are subsets of the space H. Furthermore, an operator is *densely defined* if its domain $\mathcal{D}(T)$ is dense in H. We tacitly assume that an operator is densely defined unless otherwise stated.

To a linear operator T we associate an *adjoint* T^*. This is done as follows:

Definition 2.1. *The* adjoint T^* *is the unique linear operator defined by the relation,*

$$(Tu, v) = (u, T^* v),$$

for all u *in* $\mathcal{D}(T)$ *and* $v \in \mathcal{D}(T^*)$*, where*

$$\mathcal{D}(T^*) = \{v \in H \text{ such that the functional } u \mapsto (Tu, v) \text{ is continuous}\}.$$

Definition 2.2. *An operator* T *on* H *is* symmetric *if*

$$(Tu, v) = (u, Tv), \quad u, v \in \mathcal{D}(T).$$

If in addition $T = T^*$ *the operator is said to be* self-adjoint*.*

Both of these are generalizations of symmetric for matrices. If T is bounded then self-adjoint and symmetric is the same. Differential operators are usually unbounded and thus the distinction is important.

In order to demonstrate that the linear mapping (6) is self-adjoint we use integeration by parts twice, and recall that $u(0)=0$ for $u\in\mathcal{D}(T)=V$, to obtain

$$(Tu,v)=\int_0^1 u''(x)v(x)dx=u'(1)v(1)-u'(0)v(0)-u(1)v'(1)+(u,Tv). \quad (7)$$

Here we have to restrict $v(0)=0$ and since $u(1)=-u'(1)$ we obtain

$$(Tu,v)=u'(1)(v(1)+v'(1))+(u,Tv). \quad (8)$$

Thus if $v\in V$, so that $v'(1)+v(1)=0$, then $(Tu,v)=(u,Tv)$ so the operator is symmetric. Furthermore, for T to be defined the function v has to be twice differentiable, so $\mathcal{D}(T^*)=V$ and T is self-adjoint.

Definition 2.3. *The* resolvent set *for a linear operator T consists of all points $\lambda\in\mathbb{C}$ for which $T-\lambda I$ has a bounded inverse defined on $\mathcal{R}(T)\subset H$. The* spectrum $\sigma(T)$ *is the complement of the resolvent set.*

The spectrum can further be decomposed in three parts: the point spectrum, the continuous spectrum, and the residual spectrum. The point spectrum consists of those $\lambda\in\sigma(T)$ for which $T-\lambda I$ is not injective. This is the "usual" type of eigenvalues (with corresponding eigenfunctions). The continuous spectrum consists of those $\lambda\in\sigma(T)$ for which $T-\lambda I$ is injective, but the range $\mathcal{R}(T)$ is a dense proper subset of H. For λ in the residual spectrum, $T-\lambda I$ is injective but $\mathcal{R}(T)$ is not dense in H.

Note here that points in the point spectrum of T are isolated.

Definition 2.4. *The graph $\Gamma(T)$ of an operator $T\colon\mathcal{D}(T)\to H$ is defined as*

$$\Gamma(T)=\{(u,Tu):u\in\mathcal{D}(T)\}.$$

If $\Gamma(T)$ is a closed subspace of $H\times H$, the operator T is called closed.

Definition 2.5. *An operator $T\colon\mathcal{D}(T)\to H$ is called closable if there is a closed extension, that is, an operator $\overline{T}\colon\overline{\mathcal{D}(T)}\to H$ such that $\Gamma(T)\subset\Gamma(\overline{T})$.*

It is worth noting that every symmetric operator is closable. Moreover, note that the closure $\overline{\mathcal{D}(T)}$ is with respect to the norm $u\mapsto\|u\|+\|Tu\|$.

Definition 2.6. *An operator $T\colon\mathcal{D}(T)\to H$ is called essentially self-adjoint if it is symmetric and the closure $\overline{T}\colon\overline{\mathcal{D}(T)}\to H$ is self-adjoint.*

Note that the self-adjoint extension for an essentially self-adjoint operator is unique. It is also worth noting that, by the closed graph theorem, if T is self-adjoint and defined everywhere, then T must be bounded (a result known as the Hellinger-Toeplitz theorem).

We now present a version of the spectral theorem (using multipliers). The proof can be found in, for example, Reed and Simon[15, Theorem VIII.4]

Theorem 2.7. *If $T\colon\mathcal{D}(T)\to H$ is a self-adjoint operator on a separable Hilbert space H, then there is a finite measure space (X,μ), a unitary operator $U\colon H\to L^2(X,\mu)$, and a function $f\in L^\infty(X,\mu)$ so that*

1. *$\psi \in \mathcal{D}(T)$ if and only if $f(\,\cdot\,)\big(U\psi\big)(\,\cdot\,) \in L^2(X,\mu)$.*

2. *If $\varphi \in U(\mathcal{D}(T))$, then $UTU^{-1}\varphi(x) = f(x)\varphi(x)$ for almost every $x \in X$.*

The spectrum of a multiplication operator m_f with $f \in L^\infty(X,\mu)$ can be characterized as the essential range of f, that is

$$\sigma(m_f) = \{\, z \in \mathbb{C} \text{ such that for every } \epsilon > 0,\ \mu(f^{-1}(B(z\,;\epsilon))) > 0 \,\},$$

where $B(z\,;\epsilon)$ is the open ball with center z and radius ϵ. Moreover, for an operator T satisfying Theorem 2.7, it is true that the operators T and m_f share the same spectrum: $\sigma(T) = \sigma(m_f)$.

Theorem 2.8 below is stated for self-adjoint operators. If T is only essentially self-adjoint, the theorem should be applied to the self-adjoint closure $\overline{T}$. The reason for this is that if T is not closed, then $\sigma(T) = \mathbb{C}$, which renders the result uninteresting.

Theorem 2.8. *Let $(\widehat{\lambda}, v)$ be an approximate eigenvalue-eigenfunction pair for a self-adjoint operator T. If $\|v\| = 1$ and $r = Tv - \widehat{\lambda}v$, then*

$$\inf_{\lambda \in \sigma(T)} |\lambda - \widehat{\lambda}| \le \|r\|.$$

Proof. If $\widehat{\lambda} \in \sigma(T)$, the result is immediate. Suppose that $\widehat{\lambda} \notin \sigma(T)$. Using Theorem 2.7, we obtain that $UTU^{-1} = m_f$ on $L^2(X,\mu)$, so $(m_f - \widehat{\lambda}I)^{-1}$ exists and is a bounded operator in H with

$$\mathcal{D}((m_f - \widehat{\lambda}I)^{-1}) = \{\, \psi \in L^2(X,\mu) : (f - \widehat{\lambda})^{-1}\psi \in L^2(X,\mu) \,\}.$$

Moreover, $(m_f - \widehat{\lambda}I)^{-1}$ is a multiplication operator on $L^2(X,\mu)$ with multiplier $x \mapsto (f(x) - \widehat{\lambda})^{-1}$. Note that this multiplier also belongs to $L^\infty(X,\mu)$ since $\widehat{\lambda} \notin \sigma(m_f)$. Using the spectral decomposition, it is clear that

$$v = (T - \widehat{\lambda}I)^{-1}r = (U^{-1}m_fU - \widehat{\lambda})^{-1}r = U^{-1}(m_f - \widehat{\lambda}I)^{-1}Ur,$$

so

$$\begin{aligned}\|v\| &\le \|U^{-1}\|\|(m_f - \widehat{\lambda}I)^{-1}\|\|U\|\|r\| \le \operatorname*{ess\,sup}_{x\in X} \frac{1}{|f(x) - \widehat{\lambda}|}\,\|r\| \\ &= \frac{1}{\operatorname{ess\,inf}_{x\in X}|f(x) - \widehat{\lambda}|}\,\|r\|,\end{aligned}$$

which in turn implies that

$$\inf_{\lambda \in \sigma(T)} |\lambda - \widehat{\lambda}| \le \operatorname*{ess\,inf}_{x\in X} |f(x) - \widehat{\lambda}| \le \|r\|. \quad \square$$

Observe that the infimum in the theorem is with respect to all of $\sigma(T)$. Since T is self-adjoint, there is no residual spectrum, but $\sigma(T)$ can consist of both a point spectrum and a continuous spectrum. Thus it is necessary to be careful since the infimum can be attained for λ which belongs to the continuous spectrum and not necessarily the point spectrum of T.

2.2 A Numerical Example

In order to discretize the eigenvalue problem $Tu = \lambda u$, where T is defined as in (6), we first introduce an equidistant grid $\{x_k\}_0^{n+1}$, such that $x_0 = 0$ and $x_{n+1} = 1$. In order to discretize the space V we use a one sided finite difference approximation at the grid point x_{n+1}

$$u'(x_{n+1}) = \frac{1}{2h}(3u(x_{n+1}) - 4u(x_n) + u(x_{n-1})) + \mathcal{O}(h^2), \qquad h = \frac{1}{n+1}, \quad (9)$$

so the space V is replaced by

$$V_h = \{u \in \mathbb{R}^{n+1} \text{ such that } u_0 = 0 \text{ and } (3+2h)u_{n+1} - 4u_n + u_{n-1} = 0\}, \quad (10)$$

where $\dim(V_h) = n$. Note that T maps V onto $\mathcal{R}(T) \subset L^2([0,1])$. Thus it would be natural for the discrete approximation A to map V_h into $\mathbb{R}^{n+2}$, $(Au)_k \approx u''(x_k)$, $k = 0, 1, \ldots, n+1$. However, a matrix eigenvalue problems needs to be quadratic. Thus we set $x = (u_1, u_2, \ldots, u_n)^T$ and define $A \in \mathbb{R}^{n\times n}$ by using the central difference approximation,

$$u''(x_k) = \frac{1}{h^2}(u_{k-1} - 2u_k + u_{k+1}) + \mathcal{O}(h^2), \quad k = 1, 2, \ldots, n, \qquad (11)$$

where $u_0 = 0$ in the first relation, and we use $(3+2h)u_{n+1} - 4u_n + u_{n-1} = 0$ to eliminate u_{n+1} from the last relation to obtain,

$$u''(x_n) = \frac{2}{h^2(3+2h)}((1+h)u_{n-1} - (1+2h)u_n) + \mathcal{O}(h^2). \qquad (12)$$

The above approximations results in a matrix $A \in \mathbb{R}^{n\times n}$ that represents an $\mathcal{O}(h^2)$ accurate discretization of T considered as a mapping of $V \to V$. By computing the eigenvalues of the matrix A we obtain approximate eigenvalues for T.

In order to obtain approximate eigenfunctions of the operator T we recall that by solving the matrix eigenvalue problem $Ax = \lambda x$, we obtain eigenpairs $(\hat{x}, \hat{\lambda})$. In order to obtain an approximate eigenpair for the operator T we need an interpolation scheme that given the discrete function values $\widehat{x} = (u(x_1), \ldots, u(x_n))^T$ finds a suitable twice differentiable function $\widehat{u}(x)$ to serve as the approximate eigenfunction. The simplest approach is to use cubic splines, i.e. find a piecewise cubic polynomial that interpolates the discrete function values and that also satisfies the boundary conditions. Once such a cubic spline $\hat{u}$ has been found, the residual

$$\|T\widehat{u} - \widehat{\lambda}\widehat{u}\|_{L^2([0,1])}, \qquad (13)$$

can be calculated analytically.

The condition $u(0)=0$ simply means $u(x_0)=0$. The requirement that $u'(1)+u(1)=0$ needs a bit of caution. The simplest approach is to calculate $u(x_{n+1})$ using the discretized version included in the definition of V_h. This ensures that $u'(1) + u(1) = 0$ is satisfied to order $\mathcal{O}(h^2)$. Two additional constraints are needed to make the cubic spline unique. For simplicity we use the not-a-knot conditions, i.e. continuous third derivative at the points x_1 and x_n. In Figure 1 we show the results. The calculated residuals are a close match to the

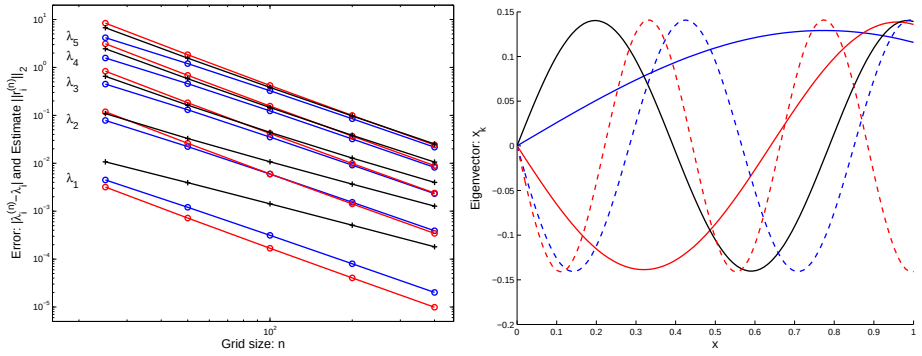

Figure 1: To the left we display both the errors $|\widehat{\lambda}_k - \lambda_k|$ (blue,rings) for the first five eigenvalues as a function of the grid size n, for $n = 25, 50, 100, \ldots, 400$. We also display the error estimates $\|r\|_{L^2([0,1])}$ for the case when the spline $\widehat{u}$ only satisfies the condition $\widehat{u}'(1) + \widehat{u}(1) = 0$ approximatey (red,rings) and for the case when the condition is satisfied exactly so $\widehat{u} \in V$ (black,plus). To the right we display the first five eigenvectors for the discretized problem using the grid size $n = 100$.

actual errors $|\lambda_k - \widehat{\lambda}|$ for the first 5 eigenvalues of T and a variety of grid sizes. Note however that strictly the approximate eigenfunctions $\widehat{u}$ do not belong to $V = \mathcal{D}(T)$, as the constraint $u'(1) + u(1) = 0$ is only satisfied with accuracy $\mathcal{O}(h^2)$. This means that in a few cases the actual error might be slightly larger than the estimate provided by the residual.

In order to obtain valid estimates it is essential that the suggested eigenfunctions $\widehat{u}$ belongs to the correct space. We achieve this by first computing an initial guess for $u(x_{n+1})$ using the above discrete approximation of $u'(1) + u(1) = 0$. Second, we find the smallest number α so that the cubic spline $\widehat{u}$ obtained by interpolating $(0\,,\, u(x_1)\,, \ldots,\, u(x_n)\,,\, u(x_{n+1}) + \alpha)^T$, using not-a-knot conditions, satisfies $\widehat{u}'(1) + \widehat{u}(1) = 0$. Finding the appropriate value α is formulated as a non-linear equation that is solved using a standard equation solver. The results are again shown in Figure 1. Now since the approximate eigenfunctions do belong to the correct space the error estimate holds. The estimate is not very sharp for the first eigenvalue λ_1. The required modification to the function value $u(x_{n+1})$ was large in comparison to the discretization parameter h. This has the effect that the second derivative $\widehat{u}''(x)$ becomes very large in the last interval $x_{n-1} < x < x_n$) and thus the residual is also large. The error estimate behaves roughly as $\mathcal{O}(h)$ while the actual error $|\widehat{\lambda}_1 - \lambda_1|$ behaves as $\mathcal{O}(h^2)$.

We remark that the boundary condition $u(0) = 0$ does not cause any issues with the spline interpolation. Similarily a boundary condition $u'(1) = 0$ can be treated without any problematic effects appearing.

3 Electron-electron interactions in graphene field-induced quantum dots in high magnetic field

The recent discovery of graphene[12] brought a new possible material for quantum dot fabrication. The confinement of electrons required for quantum dot creation is more difficult to achive in graphene than in the usual semiconductors. This is because graphene electrons behave like massless particles and undergo Klein tunneling. Graphene quantum dots have to be created by mixture of effects; e.g. by simulataneous application of a magniectic field and an electrostatic potential. In the paper [13] such a quantum dot was considered. The goal was to investigate the change in the electrons spectrum by including electron-electron interactions in the model. These interactions were incorporated using the Thomas-Fermi approximation and the mirror charge method, see [8, 19].

The electron dynamics in the considered quantum dot are described by the Dirac equation

$$H\Psi(r,\theta) = E\Psi(r,\theta) \tag{14}$$

with

$$H := \begin{pmatrix} V(r) & \gamma e^{-i\theta}(-i\partial_r - \frac{1}{r}\partial_\theta - i\frac{e}{\hbar}\frac{Br}{2}) \\ \gamma e^{i\theta}(-i\partial_r + \frac{1}{r}\partial_\theta + i\frac{e}{\hbar}\frac{Br}{2}) & V(r) \end{pmatrix}, \tag{15}$$

where E is energy level for electrons, B is the strength of the magnetic field perpendicular to the graphene surface, m is the angular momentum, $V(r)$ is the potential that includes electron-electron interactions and define the quantum dot. The potential $V(r)$ that we use was described in detail in the paper [13]. The remaining constants have the values: $\gamma = 646\, meV \cdot nm$ and $e/\hbar = 1.52 \cdot 10^{-3}\,(T \cdot nm^2)^{-1}$.

Let us introduce the domain $C_R = \{x \in \mathbb{R}^2 \,:\, |x| \leq R\}$ and the space

$$X = \{\Psi \in L^2(C_R) \times L^2(C_R) \,:\, H\Psi \in L^2(C_R) \times L^2(C_R)\}, \tag{16}$$

where $\Psi = (\Psi_1\,, \Psi_2)^T$. The space X is a natural domain of definition for the operator H. Since the problem originates from an assumption of circular symmetry of the potential $V(r)$, an appropriate scalar product is

$$\left(\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}, \begin{pmatrix}\Psi_3\\ \Psi_4\end{pmatrix}\right) = \int_0^\infty \int_0^{2\pi} \left(\overline{\Psi_1(r,\theta)}\Psi_3(r,\theta) + \overline{\Psi_2(r,\theta)}\Psi_4(r,\theta)\right) r d\theta dr. \tag{17}$$

The operator H, with the domain X, is self-adjoint, in $L^2(C_R) \times L^2(C_R)$, when the above scalar product is used [13].

Due to known properties of the wave functions, we can write

$$\Psi(r,\theta) = \begin{pmatrix} \chi_1(r)e^{i(m-1)\theta} \\ \chi_2(r)e^{im\theta} \end{pmatrix}, \tag{18}$$

which after insertion into (14) leads to the new operator L for the radial components:

$$\begin{pmatrix} e^{i(m-1)\theta} \\ e^{im\theta} \end{pmatrix} \cdot L \begin{pmatrix} \chi_1(r) \\ \chi_2(r) \end{pmatrix} = \begin{pmatrix} e^{i(m-1)\theta} \\ e^{im\theta} \end{pmatrix} \cdot E \begin{pmatrix} \chi_1(r) \\ \chi_2(r) \end{pmatrix}, \tag{19}$$

where

$$L := \begin{pmatrix} V(r) & \gamma(-i\partial_r + (-i\frac{m}{r} - i\frac{e}{\hbar}\frac{Br}{2})) \\ \gamma(-i\partial_r + (i\frac{m-1}{r} + i\frac{e}{\hbar}\frac{Br}{2})) & V(r) \end{pmatrix}. \tag{20}$$

Thus we have an eigenvalue problem

$$L \begin{pmatrix} \chi_1(r) \\ \chi_2(r) \end{pmatrix} = E \begin{pmatrix} \chi_1(r) \\ \chi_2(r) \end{pmatrix}. \tag{21}$$

In the previous paper [13] a numerical discretization of the eigenvalue problem (3), with an equidistant grid $\{r_i\}_{i=1}^n$, $r_1 = 0$ and $r_n = R$, was used together with the backward-forward finite difference method to find eigenenergies E and wavefunctions $\chi_1(r)$ and $\chi_2(r)$. To eliminate the singularity of $\chi_2(r)$ at $r = 0$, it was assumed that $\chi_2(0) = 0$, which is equivalent to an antisymmetry assumption. A second assumption was that $\chi_1(R) = 0$. The resulting matrix-eigenvalue problem

$$Ax = Ex, \tag{22}$$

where the matrix A is of size $2n \times 2n$, and the vector x contains the value of the functions (χ_1, χ_2) at the grid points $\{r_i\}$, with the grid parameter $h = R/n$, was be solved and we obtained approximate eigenvalues of the problem (3). The discretization was $\mathcal{O}(h)$ accurate, where h is the grid parameter.

In the numerical simulations we used $R = 600\,nm$, $B = 75\,T$, and $m = 1$. Thus the size of the physical domain under consideration is relatively large. As a result we need a large grid size n. Thus, we treat the matrix A as a sparse matrix and use a Krylov subspace method, e.g. `eigs` in Matlab, see [17], to compute a few of the lowest eigenvalues and eigenvectors of the matrix. During the iterations a Krylov subspace for A^{-1} is constructed and in each step a linear system of equations is solved using the generalized minimal residual method (GMRES). For our discretization of the operator L, cf. (20), the condition number behaves as $\kappa_2(A) = \mathcal{O}(h^{-1})$. This means for a larger n the accuracy achived by GMRES is lower and the computed eigenvalues might have a larger error.

The matrix eigenvalue problem (22) was solved for a range of grid sizes n. For each grid size we obtained approximate eigenvalues $\widehat{\lambda}$, or energy levels $\widehat{E}$, and also eigenvectors ($\widehat{\chi}_1$ and $\widehat{\chi}_2$). In Figure 2 we illustrate the first three eigenvectors.

In order to obtain appropriate eigenfunctions, and apply Theorem 2.8, we again use cubic spline interpolation. For the first component we let $\chi_1(r) = p_1(r)$, where $p_1(r)$ is a cubic spline interpolating the eigenvector $\widehat{\chi}_1$ at the grid points, using the end point conditions $p_1'(0) = 0$ and $p_1''(R) = 0$. For the second component we observe that the eigenfunction $\chi_2(r)$ should behave roughly as $\sqrt{r}$ as $r \to 0$. This has to be taken into account as otherwise we encounter a non-integrable singularity in the analytical calcuation of the residual. Thus we use $\chi_2(r) = \sqrt{r}p_2(r)$, where $p_2(r)$ is a cubic spline interpolating $\widehat{\chi}_2(r)/\sqrt{r}$ on the computational grid. Now the residual

$$\|r\|_2 = \left\| H \begin{pmatrix} \widehat{\Psi}_1(r) \\ \widehat{\Psi}_2(r) \end{pmatrix} - \widehat{E} \begin{pmatrix} \widehat{\Psi}_1(r) \\ \widehat{\Psi}_2(r) \end{pmatrix} \right\| = \left\| L \begin{pmatrix} \widehat{\chi}_1(r) \\ \widehat{\chi}_2(r) \end{pmatrix} - \widehat{E} \begin{pmatrix} \widehat{\chi}_1(r) \\ \widehat{\chi}_2(r) \end{pmatrix} \right\|$$

can be calculated analytically. The differential operator L can be applied to the interpolated wavefunctions. During the residual calculations we only need

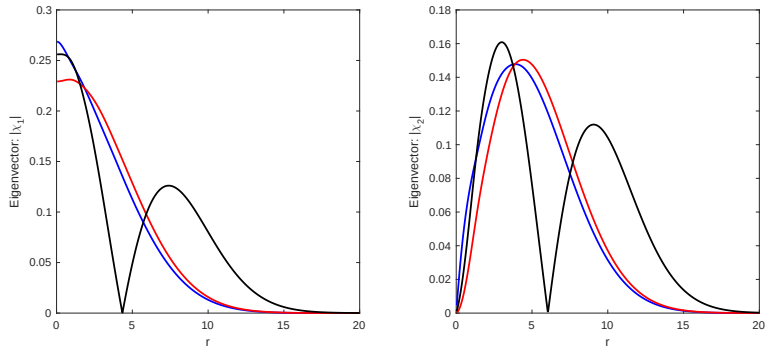

Figure 2: We show the first three eigenvectors of the matrix problem for a large grid size n. The first (blue) and the second (red) eigenvector are quite similar. The third eigenvector (black) is different. The components $|\chi_1(r)|$ (left) and $|\chi_2(r)|$ (right) are shown.

derivatives of the $\sqrt{r}$ and of the piecewise polynomials $p_1(r)$ and $p_2(r)$. In Figure 3, we present the three lowest eigenenergies, with their respective residuals, for different grid sizes n. We remark that the residuals behave as $\mathcal{O}(h)$, which is the same as the discretization error in the finite difference approximation.

4 Concluding Remarks

In this paper we have generalized the Bauer-Fike theorem to unbounded self-adjoint operators. This class of operators covers many differential operators that are intressting in applications. The main result is a way to estimate the error in an approximate eigenvalue obtained by discretizing the differential operator and solving the resulting matrix eigenvalue problem. We apply the theorem to both a simple eigenvalue problem with a known solution and also to obtain error bounds for numerically computed eigenvalues of a system describing electron-electron interactions in grahene quantum dots [13]. The results show that the method works well and gives useful error bounds.

It is worth mentioning that in this paper we work with a classic formulation of the differential operator and assume that the the operator is discretized using finite differences. A central part of our method is thus to find an interpolation scheme that takes the eigenvectors of the discrete problem and produces approximate eigenfunctions of the differential operator. In order to obtain good error estimates it is important to incorporate information about the behaviour of the wave functions, e.g. singularities, in the interpolation scheme. In our work we use cubic splines so that the eigenfunctions can be differentiated easily and the residual calculated analytically. An alternative is trigonometric interpolation that also gives eigenfunctions that can easily be differentiated analytically.

In our example (3) the operator is restricted to the domain $0 \leq r < R$. The interval length R was introduced simply because the finite difference discretization requires a finite domain, see [13]. The specific value of R was selected large enough so that the first few eigenfunctions would remain unchanged. For the

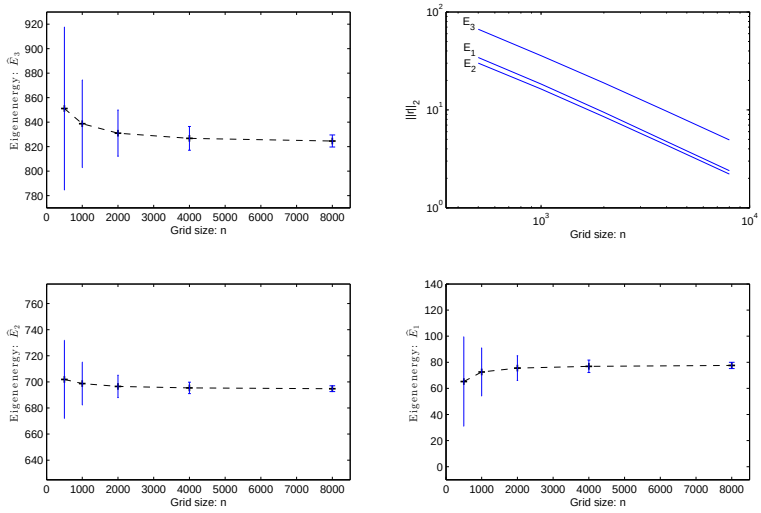

Figure 3: The approximate eigenvalues $\widehat{E}_k$, $k = 1, 2, 3$, for the discrete problem are displayed together with the error bounds provided by the residual. We also display the residual norms $\|r\|_2$.

residual calculation we can extend both $\chi_1(r)$ and $\chi_2(r)$ as zero for $r > R$ and the residual would remain the same. This means that the residual provides an error estimate also the for the case when the operator is defined for $0 \leq r < \infty$. Thus we can estimate the effect of truncating the infinite domain for the purpose of numerical computations. This means that we can lower R, while keeping the number of grid points constant in order to approximate the differential operator as accurately as possible, and be sure that the the truncation of the domain does not cause a large error.

Finally, in a future paper we intend to redo the theory and the examples in a weak setting. Instead of using finite differences we intend to discretize the operator using finite elements. Since a finite element discretzation uses a linear combination of appropriately selected basis functions we get a natural interpolation scheme for creating approximate eigenfunctions.

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