Sharp eigenvalue enclosures for the perturbed angular Kerr–Newman Dirac operator

Citation for published version:
Boulton, L & Winklmeier, M 2015, 'Sharp eigenvalue enclosures for the perturbed angular Kerr–Newman Dirac operator', *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences*, vol. 471, no. 2182, 20150232. https://doi.org/10.1098/rspa.2015.0232

Digital Object Identifier (DOI):
10.1098/rspa.2015.0232

Published In:
Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences

SHARP BOUNDS FOR THE EIGENVALUES OF THE PERTURBED ANGULAR KERR-NEWMAN DIRAC OPERATOR

LYONELL BOULTON AND MONIKA WINKLMEIER

Abstract. A certified strategy for determining sharp intervals of enclosure for the eigenvalues of matrix differential operators with singular coefficients is examined. The strategy relies on computing the second order spectrum relative to subspaces of continuous piecewise linear functions. For smooth perturbations of the angular Kerr-Newman Dirac operator, explicit rates of convergence due to regularity of the eigenfunctions are established. Existing benchmarks are validated and sharpened by several orders of magnitude in the unperturbed setting.

1. Introduction

The Kerr-Newman spacetime describes a stationary electrically charged rotating black hole. In this regime the Dirac equation for an electron takes the form

$$(\widehat{\mathcal{A}} + \widehat{\mathcal{R}})\widehat{\Psi} = 0.$$

Here $\widehat{\Psi}$ is a four component spinor depending on all four spacetime variables which describes the wave function of the electron. The operators $\widehat{\mathcal{A}}$ and $\widehat{\mathcal{R}}$ have complicated 4×4 differential expressions, [Cha98]. After a suitable separation of variables, two ordinary differential equations are obtained:

$$(\mathfrak{R}_\kappa - \omega)\phi = 0 \qquad \text{and} \qquad (\mathfrak{A}_\kappa - \lambda)\psi = 0.$$

The radial part $\mathfrak{R}_\kappa$ contains only derivatives with respect to the radial coordinate and the angular part $\mathfrak{A}_\kappa$ contains only derivatives with respect to the azimuthal angular coordinate θ. The eigenvalue parameter ω in the radial equation is the energy of the electron. These two equations are not completely decoupled as they are still linked by a real parameter, usually denoted by a, corresponding to the angular momentum of the rotating black hole.

The Cauchy problem associated to the full Kerr-Newman Dirac operator has been considered in [FKSY00b, FKSY00a], [BS06] and [WY09], while the radial part of the system has been thoroughly examined in [Sch04] and [WY06]. In the present paper, we focus on the eigenvalue problem associated to the angular part which in suitable coordinates is

$$(1) \qquad \mathfrak{A}_\kappa = \begin{pmatrix} -am\cos\theta & \frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\kappa}{\sin\theta} + a\omega\sin\theta \\ -\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\kappa}{\sin\theta} + a\omega\sin\theta & am\cos\theta \end{pmatrix}, \qquad 0 < \theta < \pi.$$

Date: 21st October 2014.

2010 *Mathematics Subject Classification.* 65L15, 65L20, 65L60, 35P15, 83C57.

Key words and phrases. Numerical approximation of eigenvalues, projection methods, computation of upper and lower bounds for eigenvalues, angular Kerr-Newman Dirac operator.

The only data from the black hole in this expression is the coupling parameter a. The other physical quantities are the mass of the electron m, its energy ω and $\kappa \in \mathbb{Z} + \frac{1}{2}$ which describes its angular momentum around the axis of symmetry of the system. Here ω and κ arise from the separation process.

The operator which we will associate to (1) is self-adjoint, it has a compact resolvent and it is strongly indefinite in the sense that the spectrum accumulates at $\pm\infty$. Various attempts at computing its spectrum have been considered in the past. A series expansion for λ in terms of $a(m+\omega)$ and $a(m-\omega)$ was derived in [SFC83] by means of techniques involving continued fractions, see also [BSW05]. A further asymptotic expansion in terms of $a\omega$ and m/ω was reported in [Cha84]. In both cases however, no precise indication of the orders of magnitude of the residuals was given.

A simple explicit expression for the eigenvalues appears to be available only for the case $am = \pm a\omega$. By invoking an abstract variational principle on the corresponding operator pencil, coarse analytic enclosures for the eigenvalues in the case $am \neq \pm a\omega$ were found in [Win05] and [Win08]. Our aim below is to sharpen these enclosures by several orders of magnitude via a projection method.

Techniques for determining bounds for eigenvalues of indefinite operator matrices via variational formulations have been examined by many authors in the past, see for example [GLS99], [DES00], [LLT02], [KLT04], [LT06], [Tre08], and [BS12]. These are strongly linked with the classical complementary bounds for eigenvalues by Temple and Lehmann [Dav95, Theorem 4.6.3], which played a prominent role in the early days of quantum mechanics. See [ZM95, DP04]. The so-called quadratic method, developed by Davies [Dav98], Shargorodsky [Sha00] and others [LS04, Bou06], is an alternative to these approaches. As we shall demonstrate below, an application of this method leads to sharp eigenvalue bounds. Further recent implementations include the contexts of crystalline Schrödinger operators [BL07], the hydrogenic Dirac operator [BB09] and models from magnetohydrodynamics [Str11].

Our concrete purpose in this paper is to address the numerical calculation of intervals of enclosure for the eigenvalues of $\mathfrak{A}_\kappa$ with the possible addition of a smooth perturbation. We formulate an approach which is certified up to machine precision. We also find explicit rates for its convergence in terms of the regularity of the eigenfunctions. In the case of the unperturbed $\mathfrak{A}_\kappa$, we perform various numerical tests which validate and sharpen existing benchmarks by several orders of magnitude.

In the next section we present the operator theoretical setting of the eigenvalue problem. Lemmas 3 and 4, respectively, are devoted to explicit smoothness properties and boundary behaviour of the eigenfunctions. We include complete proofs of these statements in the appendices A and B.

In Section 3 we formulate the quadratic method on trial subspaces of piecewise linear functions. Theorem 9 establishes concrete rates of convergence for the numerical approximation of eigenvalues. A proof of this crucial statement is deferred to Section 4. The main ingredients of this proof are the explicit error estimates for the approximation of eigenfunctions by continuous piecewise linear functions in the graph norm which are established in Theorem 13.

Our numerical findings are reported in Section 5. We begin that section by describing details of [Cha84] and [SFC83]. We then report on concrete tests addressing the following.

a) Validity of the numerical values reported in [Cha84] and [SFC83].
b) Sharpening of the eigenvalue bounds in the context of the quadratic method.
c) Dependence of the ground eigenvalues on $a\omega$ and am.
d) Optimal order of convergence.

These tests were performed by implementing in a suitable manner the computer code written in Comsol LiveLink which is included in the Appendix C.

Basic notation and definitions. Below we employ calligraphic letters to refer to operator matrices. We denote by $\mathrm{dom}(A)$ the domain of the linear operator A. The Hilbert space $L_2(0,\pi)$ is that consisting of two-component vector-valued functions $u : (0,\pi) \longrightarrow \mathbb{C}^2$ such that

$$\|u\| = \left(\int_0^\pi |u(x)|^2 \mathrm{d}\theta\right)^{\frac{1}{2}} = \left(\int_0^\pi |u_1(x)|^2 + |u_2(x)|^2 \,\mathrm{d}\theta\right)^{\frac{1}{2}} < \infty.$$

Let $u \in L_2(0,\pi)$ and denote its Fourier coefficients by

$$\widehat{u}_n = \sqrt{\frac{2}{\pi}}\int_0^\pi u(t)\sin(nt)\,\mathrm{d}t \in \mathbb{C}^2, \qquad n \in \mathbb{N}.$$

Let $\langle n\rangle = (1+n^2)^{\frac{1}{2}}$. For $r > 0$ let

$$\widehat{H}^r(0,\pi) = \left\{(x_n)_{n\in\mathbb{N}} : \sum_{n\in\mathbb{N}} \langle n\rangle^{2r}|x_n|^2 < \infty\right\}.$$

The fractional Sobolev spaces $H^r(0,\pi)$ will be, by definition, the Hilbert space

$$H^r(0,\pi) = \left\{u \in L_2(0,\pi) : (\widehat{u}_n)_{n\in\mathbb{N}} \in \widehat{H}^r(0,\pi)\right\}$$

with the norm inherited from $\widehat{H}^r(0,\pi)$. If $r \in \mathbb{N}$, we recover the classical Sobolev spaces, where the norm is

$$\|u\|_r = \left(\sum_{j=0}^r \|u^{(j)}\|^2\right)^{\frac{1}{2}}.$$

We set $H_0^1(0,\pi)$ to be the completion of $[C_0^\infty(0,\pi)]^2$ in the norm of $H^1(0,\pi)$.

2. A concrete self-adjoint realisation and regularity of the eigenfunctions

Here and everywhere below κ will be a real parameter satisfying $|\kappa| \geq \frac{1}{2}$ and $V = [v_{ij}]_{ij=1}^2$ will be a hermitian matrix potential with all its entries complex analytic functions on a suitable neighbourhood of $[0,\pi]$. The operator theoretical framework of the spectral problem associated to matrices of the form

$$\mathfrak{A}_\kappa = \begin{pmatrix} 0 & \frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\pi\kappa}{\theta(\pi-\theta)} \\ -\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\pi\kappa}{\theta(\pi-\theta)} & 0 \end{pmatrix} + V \tag{2}$$

can be set by means of well establish techniques, [Wei87]. Our first goal is to identify a concrete self-adjoint realisation of (2) acting on $L_2(0,\pi)$.

Remark 1. *The spectral problem associated to the angular Kerr-Newman Dirac operator* (1) *fits into the present framework by taking*

$$V(\theta)=\kappa\left(\frac{1}{\sin(\theta)}-\frac{\pi}{\theta(\pi-\theta)}\right)\begin{pmatrix}0&1\\1&0\end{pmatrix}+\begin{pmatrix}-am\cos(\theta)&a\omega\sin(\theta)\\a\omega\sin(\theta)&am\cos(\theta)\end{pmatrix}$$

in the physically relevant regime $\kappa\in\mathbb{Z}+\frac{1}{2}$.

Let $V=0$. In this case the fundamental solutions of $\mathfrak{A}_\kappa\Psi=0$ can be found explicitly. The differential expression $\mathfrak{A}_\kappa$ is in the limit point case for $|\kappa|\geq\frac{1}{2}$ (see Appendix B) and in the limit circle case for $|\kappa|<\frac{1}{2}$ (not considered presently). Thus, for $|\kappa|\geq\frac{1}{2}$, the maximal operator

$$\mathcal{A}_\kappa=\mathfrak{A}_\kappa|_{\mathrm{dom}(\mathcal{A}_\kappa)},\quad \mathrm{dom}(\mathcal{A}_\kappa)=\left\{\Psi\in[\mathrm{AC}_{\mathrm{loc}}(0,\pi)]^2\ :\ \mathfrak{A}_\kappa\Psi\in L_2(0,\pi)\right\}\tag{3}$$

is self-adjoint in $L_2(0,\pi)$.

By virtue of the particular block operator structure of the matrix in (2), $\mathrm{dom}(\mathcal{A}_\kappa)=\mathcal{D}_1\oplus\mathcal{D}_2$, where

$$\mathcal{D}_1=\left\{f\in\mathrm{AC}_{\mathrm{loc}}(0,\pi)\ :\ \int_0^\pi\left|\left(-\frac{\mathrm{d}}{\mathrm{d}\theta}+\frac{\pi\kappa}{\theta(\pi-\theta)}\right)f(\theta)\right|^2\mathrm{d}\theta<\infty\right\}\quad\text{and}$$

$$\mathcal{D}_2=\left\{f\in\mathrm{AC}_{\mathrm{loc}}(0,\pi)\ :\ \int_0^\pi\left|\left(\frac{\mathrm{d}}{\mathrm{d}\theta}+\frac{\pi\kappa}{\theta(\pi-\theta)}\right)f(\theta)\right|^2\mathrm{d}\theta<\infty\right\}.$$

Thus, the operators

$$B_\kappa=\frac{\mathrm{d}}{\mathrm{d}\theta}+\frac{\pi\kappa}{\theta(\pi-\theta)},\qquad \mathrm{dom}(B_\kappa)=\mathcal{D}_2,$$
$$B_\kappa^\dagger=-\frac{\mathrm{d}}{\mathrm{d}\theta}+\frac{\pi\kappa}{\theta(\pi-\theta)},\qquad \mathrm{dom}(B_\kappa^\dagger)=\mathcal{D}_1,$$

are adjoint to one another and

$$\mathcal{A}_\kappa=\begin{pmatrix}0&B_\kappa\\B_\kappa^*&0\end{pmatrix}.$$

Both B_κ and B_κ^* have empty spectrum. The resolvent kernel of these expressions is square integrable, so they have compact resolvent. See (39)-(40) in Appendix B. Therefore also $\mathcal{A}_\kappa$ has a compact resolvent.

Now consider $V\neq0$. We define the corresponding operator associated with (2) also by means of (3). As V is bounded, it yields a bounded self-adjoint matrix multiplication operator in $L_2(0,\pi)$. Routine perturbation arguments show that also in this case $\mathcal{A}_\kappa$ is a self-adjoint operator with compact resolvent. Note that $\mathrm{dom}(\mathcal{A}_\kappa)$ is independent of V.

Remark 2. *The spectrum of* $\mathcal{A}_\kappa$ *consists of two sequences of eigenvalues. One non-negative, accumulating at* $+\infty$*, and the other one negative accumulating at* $-\infty$*. An explicit analysis involving the Frobenius method (see Remark 16) shows that no eigenvalue of* $\mathcal{A}_\kappa$ *has multiplicity greater than one.*

As we shall see next, any eigenfunction of $\mathcal{A}_\kappa$ is regular in the interior of $[0,\pi]$ and has a boundary behaviour explicitly controlled by $|\kappa|$. Identity (4) below will play a crucial role later on.

Lemma 3. *Let* $|\kappa| \geq \frac{1}{2}$. *Let* $u \neq 0$ *be an eigenfunction of* $\mathcal{A}_\kappa$. *There exists a unique vector-valued function* q *which is complex analytic in a suitable neighbourhood of* $[0, \pi]$, *such that*

$$u(\theta) = \theta^{|\kappa|}(\pi - \theta)^{|\kappa|} q(\theta). \tag{4}$$

Proof. Included in Appendix A. □

A precise global bound on the rate of decay at the boundary, for all the vectors in the domains of B_κ and B_κ^*, is established in the next lemma. The part *a)* ensures that, for $|\kappa| > \frac{1}{2}$, $\mathcal{A}_\kappa$ can be written as the operator sum

$$\mathcal{A}_\kappa = \mathcal{D} + \mathcal{S}_\kappa + V \tag{5}$$

where

$$\mathcal{D} = \begin{pmatrix} 0 & \frac{\mathrm{d}}{\mathrm{d}\theta} \\ -\frac{\mathrm{d}}{\mathrm{d}\theta} & 0 \end{pmatrix}, \qquad \mathcal{S}_\kappa = \begin{pmatrix} 0 & \frac{\pi\kappa}{\theta(\pi-\theta)} \\ \frac{\pi\kappa}{\theta(\pi-\theta)} & 0 \end{pmatrix} \tag{6}$$

and $\mathrm{dom}(\mathcal{A}_\kappa) = \mathrm{dom}(\mathcal{D}) \cap \mathrm{dom}(\mathcal{S}_\kappa)$. Note that $[C_0^\infty(0, \pi)]^2$ is a core for $\mathcal{A}_\kappa$ in the full regime $|\kappa| \geq \frac{1}{2}$.

Lemma 4.

a) For $|\kappa| > \frac{1}{2}$, *every* $f \in \mathrm{dom}(B_\kappa^*)$ *and* $g \in \mathrm{dom}(B_\kappa)$ *satisfies*

$$\left.\begin{aligned} |f(\theta)| &\leq \sqrt{\frac{2}{\pi}}\, \|B_\kappa^* f\| \sqrt{\theta(\pi - \theta)}, \\ |g(\theta)| &\leq \sqrt{\frac{2}{\pi}}\, \|B_\kappa g\| \sqrt{\theta(\pi - \theta)}, \end{aligned}\right. \qquad 0 < \theta < \pi.$$

b) Let $\epsilon > 0$,

$$C(\epsilon) = \sup_{0<\theta<\pi} \left\{ \frac{\theta^{2\epsilon}[\pi(\ln(\pi) - \ln(\theta)) - (\pi - \theta)]}{(\pi - \theta)^2} \right\}^{\frac{1}{2}} < \infty,$$

$$D(\epsilon) = \sup_{0<\theta<\pi} \left\{ \frac{(\pi - \theta)^{2\epsilon}[\pi(\ln(\pi) - \ln(\theta)) - \theta]}{\theta^2} \right\}^{\frac{1}{2}} < \infty.$$

Every $f_\pm \in \mathrm{dom}(B_{\pm\frac{1}{2}}^*)$ *and* $g_\pm \in \mathrm{dom}(B_{\pm\frac{1}{2}})$ *satisfies*

$$\left.\begin{aligned} |f_+(\theta)| &\leq C(\epsilon) \|B_{\frac{1}{2}}^* f_+\| \sqrt{\pi - \theta}\, \theta^{\frac{1}{2}-\epsilon}, \\ |g_+(\theta)| &\leq D(\epsilon) \|B_{\frac{1}{2}} g_+\| \sqrt{\theta}\, (\pi - \theta)^{\frac{1}{2}-\epsilon}, \\ |f_-(\theta)| &\leq D(\epsilon) \|B_{-\frac{1}{2}}^* f_-\| \sqrt{\theta}\, (\pi - \theta)^{\frac{1}{2}-\epsilon}, \\ |g_-(\theta)| &\leq C(\epsilon) \|B_{-\frac{1}{2}} g_-\| \sqrt{\pi - \theta}\, \theta^{\frac{1}{2}-\epsilon}, \end{aligned}\right. \qquad 0 < \theta < \pi.$$

Proof. Included in Appendix B. □

By virtue of this lemma, any $v \in \mathrm{dom}(\mathcal{A}_\kappa)$ satisfies Dirichlet boundary conditions at 0 and π. We now summarise three key properties of regularity for eigenvectors and arbitrary vectors in the domain, which will be important below.

Corollary 5.

a) If $|\kappa| > \frac{1}{2}$, *then* $\mathrm{dom}(\mathcal{A}_\kappa) \subset H_0^1(0, \pi)$.

b) *Every eigenfunction of $\mathcal{A}_\kappa$ has a bounded rth derivative for every $r \in \mathbb{N}$ satisfying $1 \le r \le |\kappa|$.*
c) *Let $|\kappa| > \frac{1}{2}$. Let $\epsilon \in (0, 1]$ be such that $|\kappa| = \ell + \frac{1}{2} + \epsilon$ for $\ell \in \mathbb{N} \cup \{0\}$. Then every eigenfunction of $\mathcal{A}_\kappa$ lies in $H^r(0, \pi)$ for $r < \ell + \frac{3}{2}$.*

Proof.
Statement a). According to Lemma 4*a)*, any $u \in \mathrm{dom}(\mathcal{A}_\kappa)$ lies in $H^1(0, \pi)$ and $|u(0)| = |u(\pi)| = 0$ for $|\kappa| \ge \frac{1}{2}$.
Statement b). It is a direct consequence of Lemma 3.
Statement c). Let u be an eigenfunction of $\mathcal{A}_\kappa$ and let q be as in (4). The Fourier coefficients of u are

$$\widehat{u}_n = \sqrt{\frac{2}{\pi}} \int_0^\pi \theta^{|\kappa|} (\pi - \theta)^{|\kappa|} q(\theta) \sin(n\theta)\, \mathrm{d}\theta, \qquad n \in \mathbb{N}.$$

Integrating by parts $\ell + 1$ times gives

$$\begin{aligned}\widehat{u}_n &= \frac{1}{n}\sqrt{\frac{2}{\pi}} \int_0^\pi \theta^{|\kappa|-1} (\pi - \theta)^{|\kappa|-1} q_1(\theta) \cos(n\theta)\, \mathrm{d}\theta \\ &= \ldots = \frac{1}{n^{\ell+1}} \sqrt{\frac{2}{\pi}} \int_0^\pi \theta^{-\frac{1}{2}+\epsilon} (\pi - \theta)^{-\frac{1}{2}+\epsilon} q_{\ell+1}(\theta)\, \tau(n\theta)\, \mathrm{d}\theta,\end{aligned}$$

where q_j are analytic functions and

$$\tau = \begin{cases} \cos, & \ell \equiv_4 0, \\ -\sin, & \ell \equiv_4 1, \\ -\cos, & \ell \equiv_4 2, \\ \sin, & \ell \equiv_4 3. \end{cases}$$

Hence

$$\widehat{u}_n = \frac{1}{n^{\ell+1}} \widehat{w}_n$$

where $\widehat{w}_n$ are the Fourier-τ coefficients of a square integrable function. As the latter decay faster than n^{-1}, we have $\widehat{u}_n = o(n^{-\ell-2})$. Thus, for any $r < \ell + \frac{3}{2}$,

$$\sum_{n=1}^{\infty} \langle n \rangle^{2r} |\widehat{u}_n|^2 < \infty,$$

so u indeed lies in $H^r(0, \pi)$. ☐

Remark 6. *We believe that, whenever $|\kappa| > \frac{1}{2}$ is not an integer, an optimal threshold for regularity is $u \in H^r(0, \pi)$ for all $r < |\kappa| + 1$. The proof of the latter may be achieved by interpolating the spectral projections of the operator $\mathcal{A}_\kappa$ between suitable Sobolev spaces for κ in an appropriate segment of the real line. However, for the purpose of the linear interpolation setting presented below, this refinement is not essential.*

3. The second order spectrum and eigenvalue approximation

The self-adjoint operator $\mathcal{A}_\kappa$ is strongly indefinite. Therefore, due to variational collapse, standard techniques such as the classical Galerkin method for the numerical estimation of bounds for the eigenvalues are not directly applicable. As we shall see below, the computation of two-sided bounds for individual eigenvalues can be achieved by means of the quadratic method [Dav98, Sha00, LS04], which is convergent [Bou06, Bou07, BS11] and is known to avoid spectral pollution completely.

Everywhere below we consider the simplest possible trial subspaces, so the discretisation of $\mathcal{A}_\kappa$ is achievable in a few lines of computer code. The various benchmark experiments reported in Section 5 indicate that, remarkably, this simple choice already provides a high degree of accuracy for the angular Kerr-Newman Dirac operator whenever $|\kappa| > \frac{1}{2}$.

Set $n \in \mathbb{N}$, $h = \pi/n$ and $\theta_j = j\pi/n$ for $j = 0, \dots, n$. Here and elsewhere below $\mathcal{L}_h$ denotes the trial subspace of continuous piecewise linear functions on $[0, \pi]$ with values in $\mathbb{C}^2$, vanishing at 0 and π, such that their restrictions to the segments $[\theta_j, \theta_{j+1}]$ is affine. Without further mention we will always assume that $n \geq 4$, so that $0 < h < 1$.

It is readily seen that $\mathcal{L}_h$ is a linear subspace of $\mathrm{dom}(\mathcal{A}_\kappa)$ of dimension $2(n-1)$ and that

$$\mathcal{L}_h = \mathrm{Span}\left\{ \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ b_j \end{bmatrix} \right\}_{j=1}^{n-1}$$

where

$$b_j(\theta) = \begin{cases} \frac{\theta - \theta_{j-1}}{\theta_j - \theta_{j-1}}, & \theta_{j-1} \leq \theta \leq \theta_j, \\ \frac{\theta_{j+1} - \theta}{\theta_{j+1} - \theta_j}, & \theta_j \leq \theta \leq \theta_{j+1}, \\ 0, & \text{otherwise}, \end{cases} \qquad j = 1, \dots, n-1.$$

For any given $u \in H^1(0, \pi)$, $u_h \in \mathcal{L}_h$ will be the unique (nodal) interpolant which satisfies

$$u_h(\theta_j) = u(\theta_j), \qquad j = 1, \dots, n-1,$$

that is

$$u_h(\theta) = \sum_{j=1}^{n-1} b_j(\theta) \begin{bmatrix} u_1(\theta_j) \\ u_2(\theta_j) \end{bmatrix}.$$

Set

$$Q^h = [Q^h_{jk}]_{jk=1}^{n-1}, \qquad Q^h_{jk} = \begin{bmatrix} \left\langle \mathcal{A}_\kappa \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \mathcal{A}_\kappa \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \mathcal{A}_\kappa \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \\ \left\langle \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \mathcal{A}_\kappa \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \end{bmatrix},$$

$$R^h = [R^h_{jk}]_{jk=1}^{n-1}, \qquad R^h_{jk} = \begin{bmatrix} \left\langle \mathcal{A}_\kappa \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \mathcal{A}_\kappa \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \\ \left\langle \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \mathcal{A}_\kappa \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \end{bmatrix},$$

$$S^h = [S^h_{jk}]_{jk=1}^{n-1}, \qquad S^h_{jk} = \begin{bmatrix} \left\langle \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \begin{bmatrix} b_j \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \\ \left\langle \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \begin{bmatrix} b_k \\ 0 \end{bmatrix} \right\rangle & \left\langle \begin{bmatrix} 0 \\ b_j \end{bmatrix}, \begin{bmatrix} 0 \\ b_k \end{bmatrix} \right\rangle \end{bmatrix}.$$

These are the $2(n-1)\times 2(n-1)$ bending, stiffness and mass matrices, associated to $\mathcal{A}_\kappa$ for the trial subspace $\mathcal{L}_h$. A complex number z is said to belong to the second order spectrum of $\mathcal{A}_\kappa$ relative to $\mathcal{L}_h$, $\mathrm{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h)$, if and only if there exists a non-zero $\underline{u}\in\mathbb{C}^{2(n-1)}$ such that

$$(Q^h - 2zR^h + z^2 S^h)\underline{u} = 0.$$

All the matrix coefficients of this quadratic matrix polynomial are hermitian, therefore the non-real points in $\mathrm{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h)$ always form conjugate pairs.

For $a<b$ denote by

$$\mathbb{D}(a,b) = \left\{ z\in\mathbb{C} : \left| z - \frac{a+b}{2}\right| < \frac{b-a}{2} \right\}$$

the open disk with diameter the segment (a,b). The following crucial connection between the second order spectra and the spectrum allows computation of numerical bounds for the eigenvalues of $\mathcal{A}_\kappa$. See [Sha00] or [LS04], also [BS11, Lemma 2.3].

Lemma 7. *If $(a,b)\cap\mathrm{spec}(\mathcal{A}_\kappa)=\varnothing$, then $\mathbb{D}(a,b)\cap\mathrm{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h)=\varnothing$.*

A first crucial consequence of this lemma is that

$$z\in\mathrm{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h) \quad\Longrightarrow\quad [\mathrm{Re}(z)-|\,\mathrm{Im}(z)|,\ \mathrm{Re}(z)+|\,\mathrm{Im}(z)|]\cap\mathrm{spec}(\mathcal{A}_\kappa)\neq\varnothing. \tag{7}$$

That is, segments centred at the real part of conjugate pairs in the second order spectrum are guaranteed intervals of enclosure for the eigenvalues of $\mathcal{A}_\kappa$.

A second important consequence of Lemma 7 is in place, if we possess rough *a priori* certified information about the position of the eigenvalues of $\mathcal{A}_\kappa$ [BL07, Str11].

$$\left.\begin{array}{r} (a,b)\cap\mathrm{spec}(\mathcal{A}_\kappa)=\{\lambda\} \\ z\in\mathbb{D}(a,b) \end{array}\right\} \quad\Longrightarrow\quad \mathrm{Re}(z)-\frac{|\,\mathrm{Im}(z)|^2}{b-\mathrm{Re}(z)} < \lambda < \mathrm{Re}(z)+\frac{|\,\mathrm{Im}(z)|^2}{\mathrm{Re}(z)-a}. \tag{8}$$

Both (7) and (8) will be employed for concrete calculations in Section 5. The segment in (8) will have a smaller length than that in (7) only if $z\in\mathrm{spec}(\mathcal{A}_\kappa,\mathcal{L}_h)$ is very close to the real line. As we shall see next, this will be ensured if the angle between $\ker(\mathcal{A}_\kappa-\lambda)$ and $\mathcal{L}_h$ is small. For a proof of this technical statement see [BH14, Corollary 3.2] and [Hob14]. See also [BS11]. Recall that all the eigenvalues are simple, Remark 2.

Lemma 8. *Let $u\in\ker(\mathcal{A}_\kappa-\lambda)$ be such that $\|u\|=1$. There exist constants $K>0$ and $\epsilon_0>0$ ensuring the following. If*

$$\min_{v\in\mathcal{L}_h}\left(\|u-v\|+\|\mathcal{A}_\kappa(u-v)\|\right)<\epsilon \tag{9}$$

for $\epsilon\le\epsilon_0$, then we can always find $\lambda_h\in\mathrm{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h)$ such that

$$|\lambda_h-\lambda| < K\epsilon^{1/2}. \tag{10}$$

A concrete estimate on the convergence of the second order spectra to the real line, and hence the spectrum, follows.

Theorem 9. *Let* $|\kappa| > 1/2$. *Fix* $0 < r < \frac{1}{2}$ *and let*

$$p(\kappa) = \begin{cases} |\kappa| - \frac{1}{2}, & \frac{1}{2} < |\kappa| < 1, \\ 1, & |\kappa| = 1, \\ r, & 1 < |\kappa| < \frac{3}{2}, \\ 1, & |\kappa| \geq \frac{3}{2}. \end{cases}$$

Let $\lambda \in \operatorname{spec}(\mathcal{A}_\kappa)$. *There exist constants* $h_0 > 0$ *and* $K > 0$ *such that*

$$|\lambda_h - \lambda| < K h^{\frac{1}{2} p(\kappa)}, \qquad 0 < h < h_0, \tag{11}$$

for some $\lambda_h \in \operatorname{spec}_2(\mathcal{A}_\kappa, \mathcal{L}_h)$.

The proof of this statement is presented separately in the next section. Roughly speaking it reduces to finding suitable estimates for the left hand side of (9) from specific estimates on the residual in the piecewise linear interpolation of the eigenfunctions of $\mathcal{A}_\kappa$. These estimates are of the order $h^{p(\kappa)}$, so that a direct application of Lemma 8 will lead to the desired conclusion. See Section 5.4.

Remark 10. *An explicit expression for* K *can be determined by examining closely the proof of* [BH14, Corollary 3.2] *and following track of the different constants from Section 4. A concrete determination of this constant is left to future work.*

4. The proof of Theorem 9

The following inequalities are standard in the theory of piecewise linear interpolation of functions in one dimension, [EG04, Remark 1.6 and Proposition 1.5]:

$$\|u - u_h\| \leq h\|u'\| \qquad \text{for } u \in H^1(0, \pi), \tag{12}$$

$$\|u - u_h\| \leq h^2\|u''\| \qquad \text{for } u \in H^2(0, \pi), \tag{13}$$

$$\|(u - u_h)'\| \leq h\|u''\| \qquad \text{for } u \in H^2(0, \pi). \tag{14}$$

We will employ these identities below, as well as the related inequality:

$$\|(u - u_h)'\| \leq 2\|u'\| \qquad \text{for } u \in H^1(0, \pi). \tag{15}$$

The proof of (15) can be achieved as follows. Let $u \in H^1(0, \pi)$. Since $(u_h)'$ is constant along (θ_j, θ_{j+1}) and $u'(\theta) = \frac{1}{h}(u(\theta_{j+1}) - u(\theta_j))$ for every $\theta \in (\theta_j, \theta_{j+1})$, then

$$\begin{aligned} \int_{\theta_j}^{\theta_{j+1}} |(u_h)'(\theta)|^2 \, \mathrm{d}\theta &= h^{-1} |u_h(\theta_{j+1}) - u_h(\theta_j)|^2 = h^{-1} |u(\theta_{j+1}) - u(\theta_j)|^2 \\ &= h^{-1} \left| \int_{\theta_j}^{\theta_{j+1}} u'(\theta) \, \mathrm{d}\theta \right|^2 \leq \int_{\theta_j}^{\theta_{j+1}} |u'(\theta)|^2 \, \mathrm{d}\theta. \end{aligned}$$

In the last step we invoke Hölder's inequality. Summing each side for j from 1 to $n-1$ and then taking the square root gives

$$\|(u_h)'\| \leq \|u'\|.$$

By virtue of the triangle inequality, (15) follows.

Lemma 11. *Let* $\mathcal{D}$ *be as in* (6). *Let* $\alpha \in [0, 1]$. *If* $u \in H^{1+\alpha}(0, \pi)$ *and* u_h *is its nodal interpolant, then*

$$\|\mathcal{D}(u - u_h)\| \leq 2^{1-\alpha} h^\alpha \|u\|_{1+\alpha}. \tag{16}$$

Proof. By virtue of (15), for all $u \in H^1(0,\pi)$ we have

$$\|\mathcal{D}(u-u_h)\| = \left\| \begin{pmatrix} 0 & \frac{\mathrm{d}}{\mathrm{d}\theta} \\ -\frac{\mathrm{d}}{\mathrm{d}\theta} & 0 \end{pmatrix} (u-u_h) \right\| \leq \left\| \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\| \|(u-u_h)'\| \leq 2\|u'\|. \tag{17}$$

If additionally $u \in H^2(0,\pi)$, then the same argument combined with (14) yields

$$\|\mathcal{D}(u-u_h)\| \leq h\|u''\|. \tag{18}$$

Define the linear operators

$$T_1 : H^1(0,\pi) \to L_2(0,\pi), \quad u \mapsto \mathcal{D}(u-u_h),$$
$$T_2 : H^2(0,\pi) \to L_2(0,\pi), \quad u \mapsto \mathcal{D}(u-u_h).$$

From (17) and (18), it follows that $\|T_1\| \leq 2$ and $\|T_2\| \leq h$. Hence, by complex interpolation, for every $0 \leq \alpha \leq 1$

$$T_{1+\alpha} : H^{1+\alpha}(0,1) \to L_2(0,1), \quad u \mapsto \mathcal{D}(u-u_h)$$

is a bounded operator with norm $\|T_{1+\alpha}\| \leq 2^{1-\alpha}h^\alpha$. See [RS80, Appendix to IX.4]. □

Recall the decomposition of $\mathcal{A}_\kappa$ given in (6) and the representation of the eigenfunctions in (4).

Lemma 12. *Let $|\kappa| > \frac{1}{2}$. Let u be any eigenfunction of $\mathcal{A}_\kappa$ and let q be as in (4). Set*

$$d_1(u) = \sqrt{2}|\kappa| \left[4\pi^{2|\kappa|} \frac{2|\kappa|}{2|\kappa|-1} \max_{0\leq\theta\leq\pi} |q(\theta)|^2 + \frac{1}{4} \max_{0\leq\theta\leq\pi} |u''|^2 \right]^{\frac{1}{2}},$$

$$d_2(u) = \sqrt{2}|\kappa| \left[4\pi^{2|\kappa|} \frac{2|\kappa|}{2|\kappa|-1} \max_{0\leq\theta\leq\pi} |q(\theta)|^2 + \frac{b(u)^2(6-2|\kappa|)}{4(5-2|\kappa|)} \right]^{\frac{1}{2}},$$

$$b(u) = \max_{0\leq\theta\leq\pi/2} \frac{|u''(\theta)|}{\theta^{|\kappa|-2}} + \max_{\pi/2\leq\theta\leq\pi} \frac{|u''(\theta)|}{(\pi-\theta)^{|\kappa|-2}}.$$

Then

$$\|\mathcal{S}_\kappa(u-u_h)\| \leq d_1(u)h^{\frac{3}{2}}, \qquad |\kappa| \geq 2 \quad \text{or} \quad |\kappa| = 1, \tag{19}$$

$$\|\mathcal{S}_\kappa(u-u_h)\| \leq d_2(u)h^{|\kappa|-\frac{1}{2}}, \qquad \frac{1}{2} < |\kappa| \leq 2. \tag{20}$$

Proof. Firstly observe that

$$\begin{aligned} \|\mathcal{S}_\kappa(u-u_h)\|^2 &= \int_0^\pi \left(\frac{\pi\kappa}{\theta(\pi-\theta)} \right)^2 \left| \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (u-u_h)(\theta) \right|^2 \mathrm{d}\theta \\ &\leq \pi^2\kappa^2 \int_0^\pi (\theta(\pi-\theta))^{-2} |(u-u_h)(\theta)|^2 \,\mathrm{d}\theta \\ &= \pi^2\kappa^2 \left(\mathrm{J}_1 + \mathrm{J}_2 + \mathrm{J}_3 + \mathrm{J}_4 \right) \end{aligned} \tag{21}$$

where

$$\mathrm{J}_\ell = \int_{\alpha_\ell}^{\alpha_{\ell+1}} (\theta(\pi-\theta))^{-2} |(u-u_h)(\theta)|^2 \,\mathrm{d}\theta$$

for $(\alpha_\ell)_{\ell=0}^4 = (0,\, h,\, \frac{\pi}{2},\, \pi-h, \pi)$.

The interpolant u_h has the form $u_h(\theta) = \frac{\theta}{h}u(h) = \theta h^{|\kappa|-1}(\pi-h)^{|\kappa|}q(h)$ for $\theta \in [0,h]$. Then

$$\begin{aligned}
\mathrm{J}_1 &= \int_0^h \theta^{-2}(\pi-\theta)^{-2}\left|\theta^{|\kappa|}(\pi-\theta)^{|\kappa|}q(\theta) - \theta h^{|\kappa|-1}(\pi-h)^{|\kappa|}q(h)\right|^2 \mathrm{d}\theta \\
&\le 2\int_0^h \theta^{2|\kappa|-2}(\pi-\theta)^{2|\kappa|-2}|q(\theta)|^2 + h^{2|\kappa|-2}(\pi-h)^{2|\kappa|}(\pi-\theta)^{-2}|q(h)|^2\,\mathrm{d}\theta \\
&\le \frac{2h^{2|\kappa|-1}}{2|\kappa|-1}\max_{0\le\theta\le h}\left\{(\pi-\theta)^{2|\kappa|-2}|q(\theta)|^2\right\} + 2h^{2|\kappa|-1}(\pi-h)^{2|\kappa|-2}|q(h)|^2 \\
&\le 2h^{2|\kappa|-1}\max_{0\le\theta\le\pi/2}\left\{(\pi-\theta)^{2|\kappa|-2}|q(\theta)|^2\right\}\left(\frac{1}{2|\kappa|-1}+1\right).
\end{aligned}$$

Now

$$(\pi-\theta)^{2|\kappa|-2} = (\pi-\theta)^{2|\kappa|-1}(\pi-\theta)^{-1} \le \pi^{2|\kappa|-1}\frac{2}{\pi} = 2\pi^{2|\kappa|-2} \quad \text{for any} \quad 0\le\theta\le\pi/2.$$

Thus, setting

$$c_1(u) = 4\pi^{2|\kappa|-2}\left(\frac{2|\kappa|}{2|\kappa|-1}\right)\max_{0\le\theta\le\pi}\left\{|q(\theta)|^2\right\}, \tag{22}$$

gives

$$\mathrm{J}_1 \le h^{2|\kappa|-1}c_1(u). \tag{23}$$

Analogously one can show

$$\mathrm{J}_4 \le h^{2|\kappa|-1}c_1(u). \tag{24}$$

Now we estimate J_2 and J_3. Note that u is smooth in the open interval $(0,\pi)$ and for $1\le j<k\le n/2$ we have

$$|u(\theta)-u_h(\theta)| \le \frac{\sqrt{2}\,h^2}{8}\max\Big\{|u''(\theta)| : \theta\in[\theta_j,\,\theta_k]\Big\}, \quad \theta\in[\theta_j,\,\theta_k]. \tag{25}$$

First assume that $|\kappa|\ge 2$ (or $|\kappa|=1$). According to Corollary 5*b)* (or Lemma 3), u has a bounded second derivative and therefore (25) yields $|u(\theta)-u_h(\theta)| \le \frac{\sqrt{2}h^2}{8}\max_{\theta\in[0,\pi]}|u''|$ on $[0,\pi]$. So

$$\begin{aligned}
\mathrm{J}_2 &\le \frac{h^4}{32}\max_{\theta\in[0,\pi]}|u''|^2\int_h^{\frac{\pi}{2}}(\theta(\pi-\theta))^{-2}\,\mathrm{d}\theta \\
&\le \frac{h^4}{8\pi^2}\max_{\theta\in[0,\pi]}|u''|^2\int_h^{\frac{\pi}{2}}\theta^{-2}\,\mathrm{d}\theta \le \frac{h^3}{8\pi^2}\max_{\theta\in[0,\pi]}|u''|^2.
\end{aligned}$$

If we perform the analogous calculations for J_3, we conclude

$$\mathrm{J}_2 \le c_2(u)h^3, \qquad \mathrm{J}_3 \le c_2(u)h^3 \qquad\qquad \text{for } \ |\kappa|>2 \tag{26}$$

where $c_2(u) = \frac{1}{8\pi^2}\max_{\theta\in[0,\pi]}|u''|^2$.

For $\frac{1}{2}\le|\kappa|<2$ (except for the case $|\kappa|=1$), the second derivative of u diverges as $\theta\to 0$ of order $|\kappa|-2$ and the calculations above can not be performed. However, u'' is analytic in $(0,\pi)$ since

$$u''(\theta) = \theta^{|\kappa|-2}\left[|\kappa|(|\kappa|-1)(\pi-\theta)^{|\kappa|}q(\theta) + 2|\kappa|\theta[(\pi-\theta)^{|\kappa|}q(\theta)]' + \theta^2[(\pi-\theta)^{|\kappa|}q(\theta)]''\right].$$

Hence

$$|u''(\theta)| \le b(u)\theta^{|\kappa|-2}, \qquad \theta\in[0,\tfrac{\pi}{2}].$$

By assumption, $|\kappa|-2\le 0$, so $\theta\mapsto\theta^{2|\kappa|-4}$ is a positive non-increasing function on $[h,\,\frac{\pi}{2}]$. Therefore, from (25) we estimate J_2 as follows.

$$\begin{aligned}
\mathrm{J}_2 &= \sum_{j=1}^{n/2-1}\int_{\theta_j}^{\theta_{j+1}} \theta^{-2}(\pi-\theta)^{-2}|(u-u_h)(\theta)|^2\,\mathrm{d}\theta \\
&\le \frac{h^4}{32}\sum_{j=1}^{n/2-1}\int_{\theta_j}^{\theta_{j+1}} (\theta(\pi-\theta))^{-2}\max_{\theta\in[\theta_j,\,\theta_{j+1}]}\left\{|u''(\theta)|^2\right\}\,\mathrm{d}\theta \\
&\le \frac{b(u)^2h^4}{32}\quad\sum_{j=1}^{n/2-1}\max_{\theta\in[\theta_j,\,\theta_{j+1}]}\left\{\theta^{2|\kappa|-4}\right\}\int_{\theta_j}^{\theta_{j+1}}\theta^{-2}(\pi-\theta)^{-2}\,\mathrm{d}\theta \\
&\le \frac{b(u)^2h^4}{8\pi^2}\quad\sum_{j=1}^{n/2-1}\theta_j^{2|\kappa|-4}\left(\theta_j^{-1}-\theta_{j+1}^{-1}\right) \\
&= \frac{b(u)^2h^4}{8\pi^2}\quad\sum_{j=1}^{n/2-1}(jh)^{2|\kappa|-4}\frac{1}{hj(j+1)} \\
&\le \frac{b(u)^2h^{2|\kappa|-1}}{8\pi^2}\quad\sum_{j=1}^{n/2-1}j^{2|\kappa|-6}\le\frac{b(u)^2h^{2|\kappa|-1}}{8\pi^2}\quad\left[1+\int_1^\infty t^{2|\kappa|-6}\,\mathrm{d}t\right] \\
&= \frac{b(u)^2h^{2|\kappa|-1}}{8\pi^2}\left[1+\frac{1}{5-2|\kappa|}\right].
\end{aligned}$$

Set $\widetilde{c}_2(u)=\frac{b(u)^2}{8\pi^2}\left[1+\frac{1}{5-2|\kappa|}\right]$. Then, performing similar computations for J_3, we obtain

$$\mathrm{J}_2\le\widetilde{c}_2(u)h^{2|\kappa|-1},\qquad \mathrm{J}_3\le\widetilde{c}_2(u)h^{2|\kappa|-1}\qquad\qquad \text{for }\ \frac{1}{2}<|\kappa|\le 2. \tag{27}$$

Inserting (23), (24), (26) and (27) respectively into (21) yields

$$\|\mathcal{S}_\kappa(u-u_h)\|\le\pi^2\kappa^2\sqrt{2c_1(u)h^{2|\kappa|-1}+2\widetilde{c}_2(u)h^{2|\kappa|-1}}\le d_1(u)h^{|\kappa|-1/2}$$

for $\frac{1}{2}<|\kappa|\le 2$, and

$$\|\mathcal{S}_\kappa(u-u_h)\|\le\pi^2\kappa^2\sqrt{2c_1(u)h^{2|\kappa|-1}+2c_2(u)h^3}\le d_2(u)h^{3/2}$$

for $|\kappa|>2$ or $|\kappa|=1$. □

The next statement ensures the validity of Theorem 9.

Theorem 13. *Let $|\kappa|>\frac{1}{2}$. Let $\lambda\in\operatorname{spec}(\mathcal{A}_\kappa)$ and $u\in\operatorname{dom}(\mathcal{A}_\kappa)$ be an eigenpair for $\mathcal{A}_\kappa$. Assume that $\|u\|=1$. Then there exists a constant $c>0$ ensuring the following. For every $h>0$,*

$$\|u-u_h\|+\|\mathcal{A}_\kappa u-\mathcal{A}_\kappa u_h\|\le ch,\qquad\qquad |\kappa|>\frac{3}{2}\quad\textit{or}\quad|\kappa|=1, \tag{28}$$

$$\|u-u_h\|+\|\mathcal{A}_\kappa u-\mathcal{A}_\kappa u_h\|\le ch^r,\qquad\qquad 1<|\kappa|\le\frac{3}{2},\ r<\frac{1}{2}, \tag{29}$$

$$\|u-u_h\|+\|\mathcal{A}_\kappa u-\mathcal{A}_\kappa u_h\|\le ch^{|\kappa|-\frac{1}{2}},\qquad\qquad \frac{1}{2}<|\kappa|<1. \tag{30}$$

	$\frac{1}{2} < \lvert\kappa\rvert < 1$	1	$1 < \lvert\kappa\rvert \le \frac{3}{2}$	$\frac{3}{2} < \lvert\kappa\rvert \le 2$	$\lvert\kappa\rvert > 2$
$\lVert(u-u_h)\rVert$	1	2	1	2	2
$\lVert\mathcal{S}_\kappa(u-u_h)\rVert$	$\lvert\kappa\rvert - \frac{1}{2}$	$\frac{3}{2}$	$\lvert\kappa\rvert - \frac{1}{2}$	$\lvert\kappa\rvert - \frac{1}{2}$	$\frac{3}{2}$
$\lVert\mathcal{D}_\kappa(u-u_h)\rVert$	$r < \frac{1}{2}$	1	$r < \frac{1}{2}$	1	1

TABLE 1. A summary of the different estimates employed in the proof of Theorem 13. See (12), (13), (16), (19) and (20). Also Corollary 5. The term of lowest order is shaded.

Proof. Recall that $u \in \mathrm{dom}(\mathcal{D}) \cap \mathrm{dom}(\mathcal{S}_\kappa)$ since $|\kappa| > \frac{1}{2}$. Decompose the operator $\mathcal{A}_\kappa$ as in (5). Then

$$\|u - u_h\| + \|\mathcal{A}_\kappa u - \mathcal{A}_\kappa u_h\| \le (1 + \|V\|)\|u - u_h\| + \|\mathcal{D}(u - u_h)\| + \|\mathcal{S}_\kappa(u - u_h)\|.$$

Part *c)* of Corollary 5 shows that $u \in H^2(0, \pi)$ if $|\kappa| > \frac{3}{2}$, and $u \in H^r(0, \pi)$ for any $r < \frac{3}{2}$ if $\frac{1}{2} < |\kappa| \le \frac{3}{2}$. The statements (28), (29) and (30) follow from (12), (13), Lemma 11 and Lemma 12. See Table 1. □

5. NUMERICAL BENCHMARKS

We now determine various numerical approximations of intervals of enclosure for eigenvalues of the angular Kerr-Newman Dirac operator (1) by means of suitable combinations of (7) and (8). In order to implement the latter, we employ the analytic enclosures derived in [Win05] and [Win08]. Our purpose here is twofold. On the one hand we verify the numerical quantities reported in [SFC83] and [Cha84]. On the other hand we establish new sharp benchmarks for the eigenvalues of $\mathcal{A}_\kappa$.

Denote the eigenvalues of the angular operator by $\lambda_n \equiv \lambda_n(\kappa; am, a\omega)$ where

$$-\infty < \cdots < \lambda_{-n} < \ldots < \lambda_{-1} < 0 \le \lambda_1 < \ldots < \lambda_n < \cdots < \infty.$$

Explicit expressions for these eigenvalues are known only if $am = \pm a\omega$. In this case,

$$\lambda_n(\kappa; am, \pm am) = \pm\frac{1}{2} + \mathrm{sign}(n)\sqrt{\left(\lambda_n(\kappa, 0, 0) \mp \frac{1}{2}\right)^2 \pm 2\kappa am + (am)^2} \tag{31}$$

where

$$\lambda_n(\kappa; 0, 0) = \mathrm{sign}(n)\Big(|\kappa| - \frac{1}{2} + |n|\Big), \qquad n \in \mathbb{Z} \setminus \{0\}.$$

See [BSW05, Formula (45)]. For $am \ne \pm a\omega$, the two canonical references on numerical approximations of $\lambda_n(\kappa; am, a\omega)$ are [SFC83] and [Cha84].

Suffern *et al* derived in [SFC83] an asymptotic expansion of the form

$$\lambda_n = \sum_{r,s} C^n_{r,s} (m - \omega)^r (m + \omega)^s.$$

The coefficients $C^n_{r,s}$ can be determined from a suitable series expansion of the eigenfunctions in terms of hypergeometric functions. On the other hand, Chakrabarti [Cha84] expressed the eigenfunctions in terms of spin weighted spherical harmonics and wrote the squares of the eigenvalues in terms of $a\omega$ and ω/m. The tables reported in [Cha84, Tables 1-3] includes predictions for the values of λ_{-1}^2 and λ_{-2}^2 for various ranges of κ, $a\omega$ and am. It has been shown ([BSW05, Formula (45) and Remark 2]) that [Cha84, Formula (54)] and (31) differ in the case $a\omega = am$, and that the correct expression turns out to be the latter. See tables 2 and 3 below.

In both [SFC83] and [Cha84], the numerical estimation of λ_n depends on series expansions in terms of certain expressions of $a\omega$ and am. No guaranteed error bounds are given, and they are quite difficult to derive. It is to be expected, and confirmed by our numerical calculations, that the approximations in both cases become less accurate as $|a\omega|$ and $|am|$ increase.

A computer code written in Comsol LiveLink v4.3b, which we developed in order to produce all the computations reported here, is available in Appendix C. The relative tolerance of the eigenvalue solver and integrators was set to 10^{-12}, therefore all the numerical quantities reported in the tables below are correct to the number of digits shown.

5.1. **The paper [Cha84].** Our first experiment consists in assessing the quality of the numerical approximations in [Cha84, Table 2b] for $a\omega \neq am$, by means of a direct application of (7). For this purpose we fix $h = 0.001$.

The tables 2 and 3 include computations of $|\lambda_{-1}(\pm 3/2, am, a\omega)|$ for the range

$$a\omega \in \{0.1, 0.2, \dots, 1.0\}, \qquad \omega/m \in \{0,\, 0.1,\, \dots,\, 1.0\}.$$

On the top of each row we have reproduced the positive square root of the original numbers from [Cha84, Table 2b]. On the bottom of each row, we show the corresponding correct eigenvalue enclosures with upper and lower bounds displayed in small font. These bounds were obtained from (7), by computing the conjugate pairs $z, \overline{z} \in \operatorname{spec}_2(\mathcal{A}_\kappa, \mathcal{L}_{0.001})$ near the segment $(-3, 3)$.

Only for $a\omega = 0.1,\ 0.2,\ 0.3$ (and the pair $(a\omega, m/\omega) = (0.4, 0)$ when $\kappa = -3/2$), the predictions made in [Cha84] are inside the certified enclosures. We have highlighted the relative degree of disagreement with the other quantities in different shades of colour. For $\kappa = 3/2$ the latter are always above the corresponding enclosure and for $\kappa = -3/2$ they are always below it.

5.2. **The paper [SFC83] and sharp eigenvalue enclosures.** In this next experiment we validate the numbers reported in [SFC83] by means of sharpened eigenvalue enclosures determined from (8). This requires knowing beforehand some rough information about the position of the eigenvalues and the neighbouring spectrum. In the present context, we have employed a combination of the analytical inclusions found in [Win05] and [Win08], and numerically calculated inclusions determined from (7). This technique allows reducing by roughly two orders of magnitude the length of the segments of eigenvalue inclusion.

The columns in Table 4 marked as “A” are analytic upper and lower bounds for the eigenvalues calculated following [Win08, Theorem 4.5] and [Win05, Remarks 6.4 and 6.5]. For our choices of the physical parameters, we always find that the upper bound for the nth eigenvalue is less than the lower bound for the $(n+1)$th eigenvalue, so each one of these segments contains a single non-degenerate eigenvalue of $\mathcal{A}_\kappa$. The columns marked as “N” were determined by fixing $h = 0.001$ and applying directly (7) in a similar fashion as for the previous experiment. When these are contained in the former, which is not always the case (see the rows corresponding to $\kappa = \pm\frac{1}{2}$ for $am = 0.005$ and $aw = 0.015$), it is guaranteed that there is exactly one eigenvalue in each one of these smaller segments.

Remark 14. *The approach employed in* [Win05] *and* [Win08] *involves a perturbation from the case* $am = aw = 0$*. We expect that for* $am = 0.005$*,* $aw = 0.015$ *and the critical cases* $\kappa = \pm\frac{1}{2}$*, where convergence of the numerical method seems to be lost (see Section 5.4), the analytical bounds are sharper than the numerically computed bounds.*

From the data reported in Table 4, we can implement (8) and compute sharper intervals of enclosure for λ_1 and λ_2. Note that we always need information on adjacent eigenvalues: an upper bound for the one below and a lower bound for the one above. In order for the enclosures on the right side of (8) to be certified, we also need to ensure that the condition on the left hand side there holds true. For the data reported in Table 5, this is always the case.

In Table 5 we show the improved inclusions, computed independently from the analytical bound and from the numerical bound. Some of these improved inclusions do not differ significantly, even when the quality of one of the *a priori* bounds from Table 4 appears to be far lower than the other. See for example the rows corresponding to $|\kappa| \geq \frac{3}{2}$. In these cases the factor $|\operatorname{Im}(z)|^{-2}$ turns out to be far smaller than the coefficient corresponding to the distance to the adjacent points in the spectrum. By contrast, for the case $|\kappa| = \frac{1}{2}$, a sharp *a priori* localisation of the adjacent eigenvalues (such as $\kappa = -\frac{1}{2}$, $am = 0.25$ and $a\omega = 0.75$) is critical, because $|\operatorname{Im}(z)|$ is not very small.

5.3. **Global behaviour of the eigenvalues in** aw **and** am**.** Figure 1 shows $\lambda_{\pm 1}(\frac{3}{2}, am, aw)$ for a square mesh of 100 equally spaced $(a\omega, am) \in [-1,1] \times [0,2]$. The surfaces depicted correspond to an average of the upper and lower bounds for $\lambda_{\pm 1}$ computed directly from (7), fixing $h = 0.1$. They show the local behaviour of the eigenvalues as functions of am and $a\omega$. On top of the surfaces we also depict the curve (in red) corresponding to the known analytical values for $am = \pm a\omega$ from (31).

5.4. **Optimality of the exponent in Theorem 9.** We now test optimality of the leading order of convergence $p(\kappa)$ given in Theorem 9.

For this purpose we compute a numerical approximation of the slope of lines of the form

$$l(h) = \log\left|\lambda_1\left(\kappa, \frac{1}{4}, \frac{1}{4}\right) - \tilde{\lambda}_h\right|$$

by interpolating values for $h \in \{10^{-3}, 10^{-2.8}, \ldots, 10^{-2}\}$. Here $\tilde{\lambda}_h$ is the nearest point (conjugate pair) in $\operatorname{spec}_2(\mathcal{A}_\kappa, \mathcal{L}_h)$ to $\lambda_1(\kappa, \frac{1}{4}, \frac{1}{4})$. According to (31),

$$\lambda_1\left(\kappa, \frac{1}{4}, \frac{1}{4}\right) = \frac{1}{2} + \sqrt{|\kappa|^2 + 2\kappa\frac{1}{4} + \frac{1}{16}}.$$

In Figure 2 we have depicted the interpolated slopes of these lines, for 49 equally spaced $\kappa \in (\frac{1}{2}, 3)$. Various conclusions about Theorem 9 can be derived from this figure. Taking into account Remark 6 it appears that an optimal version of (11) for $|\kappa| \neq 1$ is

$$|\lambda_h - \lambda| = \mathcal{O}(h^{\min\{1, |\kappa| - \frac{1}{2}\}}), \qquad h \to 0.$$

As it has been observed in [BS11] and [Bou06], most likely the term $\epsilon^{1/2}$ (10) can be improved to ϵ^1. In such a case, the above conjectured exponent appears to be optimal, at least in the range $|\kappa| \notin [1, 3/2]$. See Theorem 13.

Appendix A. Proof of Lemma 3

According to [CL55, Theorem 4.1 in Cap. 4], the following holds true.

Theorem 15. *Let $z_0 \in \mathbb{C}$ and V be a complex analytic matrix valued function in a neighbourhood of z_0. If W is a constant 2×2 matrix with eigenvalues μ and ν such that $|\mu-\nu| \notin \mathbb{N}$, then the differential equation*

$$\left(\frac{\mathrm{d}}{\mathrm{d}z} + (z-z_0)^{-1}W + V\right)u = 0$$

has a fundamental system of the form

$$U(z) = (z-z_0)^{-W}P(z)$$

where P is complex analytic in a neighbourhood of z_0 and $P(z_0) = I_{2\times 2} = \begin{pmatrix} 1 & 0 \\ 0 & 1\end{pmatrix}$.

of Lemma 3. Without loss of generality we can assume that $\kappa \geq 1/2$, as the proof of the complementary case $\kappa \leq -1/2$ is analogous.

Firstly suppose that $2\kappa \notin \mathbb{N}$. Let λ be an eigenvalue of $\mathcal{A}_\kappa$ and U be a fundamental system of

$$(\mathfrak{A}_\kappa - \lambda)U = 0. \tag{32}$$

Multiplying (32) on the left by $\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0\end{smallmatrix}\right)$ gives

$$\left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \left(\frac{1}{\theta} + \frac{1}{\pi-\theta}\right)\begin{pmatrix} -\kappa & 0 \\ 0 & \kappa\end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0\end{pmatrix}(V-\lambda)\right]U = 0, \qquad \theta \in (0,\pi). \tag{33}$$

By Theorem 15, (33) has fundamental systems

$$U_0(\theta) = \begin{pmatrix} \theta^{-\kappa} & 0 \\ 0 & \theta^{\kappa}\end{pmatrix}P_0(\theta), \qquad U_\pi(\theta) = \begin{pmatrix} (\pi-\theta)^{-\kappa} & 0 \\ 0 & (\pi-\theta)^{\kappa}\end{pmatrix}P_\pi(\theta) \tag{34}$$

where P_0 is analytic in $[0,\pi)$, P_π is analytic in $(0,\pi]$ and $P_0(0) = P_\pi(\pi) = I_{2\times 2}$.

Let u be an eigenfunction. As $u \in L_2(0,\pi)$, it follows that there are constants $c_{0,\pi}$ such that

$$u(\theta) = \begin{pmatrix} \theta^{-\kappa} & 0 \\ 0 & \theta^{\kappa}\end{pmatrix}P_0(\theta)\begin{pmatrix} 0 \\ c_0\end{pmatrix} = \begin{pmatrix} (\pi-\theta)^{-\kappa} & 0 \\ 0 & (\pi-\theta)^{\kappa}\end{pmatrix}P_\pi(\theta)\begin{pmatrix} 0 \\ c_\pi\end{pmatrix}, \quad \theta \in (0,\pi).$$

This gives (4) under the assumption that $2\kappa \notin \mathbb{N}$.

Now assume that $2\kappa \in \mathbb{N}$. We follow a recursive argument. Set

$$W_0(\theta) = \begin{pmatrix} a_0(\theta) & b_0(\theta) \\ c_0(\theta) & d_0(\theta)\end{pmatrix} = \frac{1}{\pi-\theta}\begin{pmatrix} -\kappa & 0 \\ 0 & \kappa\end{pmatrix} + \begin{pmatrix} 0 & -1 \\ 1 & 0\end{pmatrix}(V(\theta)-\lambda).$$

Then a_0, b_0, c_0, d_0 are analytic functions in $[0,\pi)$. Let

$$S(\theta) = \begin{pmatrix} \theta & 0 \\ 0 & 1\end{pmatrix} \quad \text{so that} \quad S^{-1}(\theta)S'(\theta) = \begin{pmatrix} \frac{1}{\theta} & 0 \\ 0 & 0\end{pmatrix}, \qquad \theta \in (0,\pi). \tag{35}$$

The equation (33) can be transformed into

$$
\begin{aligned}
0 &= S^{-1}\left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} -\kappa & 0 \\ 0 & \kappa \end{pmatrix} + W_0\right] S S^{-1} U \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + S^{-1}S' + \frac{1}{\theta}\begin{pmatrix} -\kappa & 0 \\ 0 & \kappa \end{pmatrix} + S^{-1}W_0 S\right] S^{-1} U \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} -\kappa+1 & 0 \\ 0 & \kappa \end{pmatrix} + \begin{pmatrix} a_0 & \theta^{-1} b_0 \\ \theta c_0 & d_0 \end{pmatrix}\right] S^{-1} U \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\underbrace{\begin{pmatrix} -\kappa+1 & b_0(0) \\ 0 & \kappa \end{pmatrix}}_{W_1} + \begin{pmatrix} a_0 & \beta_0 \\ \theta c_0 & d_0 \end{pmatrix}\right] S^{-1} U \qquad (36)
\end{aligned}
$$

where $\beta_0(\theta) = \theta^{-1}(b_0(\theta) - b_0(0))$ is analytic in $[0, \pi)$. In order to diagonalise W_1, let $T_1 = \begin{pmatrix} 1 & b_0(0) \\ 0 & 2\kappa - 1 \end{pmatrix}$. A further transformation of (36) gives

$$
\begin{aligned}
0 &= T_1^{-1}\left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} -\kappa+1 & b_0(0) \\ 0 & \kappa \end{pmatrix} + \begin{pmatrix} a_0 & \beta_0 \\ \theta c_0 & d_0 \end{pmatrix}\right] T_1 T_1^{-1} S^{-1} U \\
&= \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} -\kappa+1 & 0 \\ 0 & \kappa \end{pmatrix} + \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}\right] T_1^{-1} S^{-1} U
\end{aligned}
$$

where a_1, b_1, c_1, d_1 are analytic. By repeating this process $2\kappa - 1$ times we get

$$
0 = \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} \kappa-1 & 0 \\ 0 & \kappa \end{pmatrix} + \begin{pmatrix} a_{2\kappa-1} & b_{2\kappa-1} \\ c_{2\kappa-1} & d_{2\kappa-1} \end{pmatrix}\right] T_{2\kappa-1}^{-1} S^{-1} \dots T_1^{-1} S^{-1} U \qquad (37)
$$

where $a_{2\kappa-1}, b_{2\kappa-1}, c_{2\kappa-1}, d_{2\kappa-1}$ are analytic in $[0, \pi)$ and

$$
T_j = \begin{pmatrix} 1 & b_{j-1}(0) \\ 0 & 2\kappa - j \end{pmatrix}.
$$

A final transformation of (37) with S yields

$$
0 = \left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\underbrace{\begin{pmatrix} \kappa & b_{2\kappa-1}(0) \\ 0 & \kappa \end{pmatrix}}_{W_{2\kappa}} + \begin{pmatrix} a_{2\kappa-1} & \beta_{2\kappa-1} \\ \theta c_{2\kappa-1} & d_{2\kappa-1} \end{pmatrix}\right] S^{-1} T_{2\kappa-1}^{-1} S^{-1} \dots T_1^{-1} S^{-1} U.
$$

The eigenvalues of $W_{2\kappa}$ do not differ by a positive integer, therefore the differential equation $\left[\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{1}{\theta}\begin{pmatrix} \kappa & b_{2\kappa-1}(0) \\ 0 & \kappa \end{pmatrix} + \begin{pmatrix} a_{2\kappa-1} & \beta_{2\kappa-1} \\ \theta c_{2\kappa-1} & d_{2\kappa-1} \end{pmatrix}\right] Y = 0$ has a fundamental system of the form $Y(\theta) = \theta^{-\kappa} P_0(\theta)$ for P_0 analytic in $[0, \pi)$ and $P_0(0) = I_{2\times 2}$. Hence a fundamental system of (33) is given by

$$
\begin{aligned}
U_0(\theta) &= S T_1 S T_2 \dots S T_{2\kappa-1} S Y \\
&= \theta^{-\kappa}\begin{pmatrix} \theta & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & b_0(0) \\ 0 & 2\kappa-1 \end{pmatrix}\begin{pmatrix} \theta & 0 \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & b_{2\kappa-2}(0) \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \theta & 0 \\ 0 & 1 \end{pmatrix} P_0(\theta) \\
&= \theta^{-\kappa}\begin{pmatrix} \theta^{2\kappa} & p_0(\theta) \\ 0 & (2\kappa-1)! \end{pmatrix} P_0(\theta) = \begin{pmatrix} \theta^{\kappa} & \theta^{-\kappa} p_0(\theta) \\ 0 & \theta^{-\kappa}(2\kappa-1)! \end{pmatrix} P_0(\theta), \qquad (38)
\end{aligned}
$$

where p_0 is a polynomial of degree $\leq 2\kappa - 1$.

Now, we can repeat a similar argument at $\theta = \pi$ instead, and find another fundamental system of (33) for the segment $(0, \pi]$ of the form

$$U_\pi(\theta) = \begin{pmatrix} (\pi-\theta)^{-\kappa}(2\kappa-1)! & 0 \\ (\pi-\theta)^{-\kappa} p_\pi(\theta) & (\pi-\theta)^{\kappa} \end{pmatrix} P_\pi(\theta),$$

where p_π is a suitable polynomial in $(\pi - \theta)$ of degree $\le 2\kappa - 1$ and P_π is analytic in $(0, \pi]$. If u is an eigenfunction of $\mathcal{A}_\kappa$, then there are constants c_1, c_2, d_1, d_2 such that

$$u = U_0 \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = U_\pi \begin{pmatrix} d_1 \\ d_2 \end{pmatrix}.$$

By (38), and the analogous equation at π, it follows that, for u to be square integrable, it is necessary that $c_2 = d_1 = 0$. □

Remark 16. *In this proof it becomes clear that all eigenvalues of $\mathcal{A}_\kappa$ are simple. Any other solution of $(\mathcal{A}_\kappa - \lambda)u = 0$ would diverges of order $-|\kappa|$ for $\theta \to 0$ and $\theta \to \pi$.*

Appendix B. Proof of Lemma 4

Up to a constant factor, the solutions of the differential equations

$$(B_\kappa - \lambda)\,\phi_{\lambda,\kappa} = 0 \qquad \text{and} \qquad (B_\kappa^* - \lambda)\,\psi_{\lambda,\kappa} = 0,$$

on $(0, \theta)$ are

$$\phi_{\lambda,\kappa}(\theta) = \mathrm{e}^{\lambda\theta}\left(\frac{\pi-\theta}{\theta}\right)^{\kappa} \qquad \text{and} \qquad \psi_{\lambda,\kappa}(\theta) = \mathrm{e}^{-\lambda\theta}\left(\frac{\theta}{\pi-\theta}\right)^{\kappa}.$$

Since none of these turns out to be square integrable in $(0, \pi)$, neither B_κ nor B_κ^* have eigenvalues. Recall that $B_\kappa = \frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\pi\kappa}{\theta(\pi-\theta)}$ and $B_\kappa^* = -\frac{\mathrm{d}}{\mathrm{d}\theta} + \frac{\pi\kappa}{\theta(\pi-\theta)}$.

For every square integrable g,

$$(B_\kappa - \lambda)^{-1} g(\theta) = \phi_{\lambda,\kappa}(\theta) \cdot \begin{cases} \int_0^\theta \psi_{\lambda,\kappa}(t) g(t)\,\mathrm{d}t, & \kappa \ge \frac{1}{2}, \\ \int_\pi^\theta \psi_{\lambda,\kappa}(t) g(t)\,\mathrm{d}t, & \kappa \le -\frac{1}{2}, \end{cases} \tag{39}$$

$$(B_\kappa^* - \lambda)^{-1} g(\theta) = \psi_{\lambda,\kappa}(\theta) \cdot \begin{cases} \int_\theta^\pi \phi_{\lambda,\kappa}(t) g(t)\,\mathrm{d}t, & \kappa \ge \frac{1}{2}, \\ \int_\theta^0 \phi_{\lambda,\kappa}(t) g(t)\,\mathrm{d}t, & \kappa \le -\frac{1}{2}. \end{cases} \tag{40}$$

These two expressions are employed below in order to estimate the decay of the functions in the domain of B_κ and B_κ^*.

of Lemma 4. Statement a). Fix $\kappa > \frac{1}{2}$ and $f \in \operatorname{dom}(B_\kappa^*)$. For all $\theta \in (0, \pi)$

$$\begin{aligned} |f(\theta)| = |B_\kappa^{*-1} B_\kappa^* f(\theta)| &= \left|\psi_{\lambda,\kappa}(\theta) \int_\theta^\pi \phi_{\lambda,\kappa}(t) B_\kappa^* f(t)\,\mathrm{d}t\right| \\ &= \left| \int_\theta^\pi \left(\frac{\theta}{t}\right)^{\kappa} \left(\frac{\pi-t}{\pi-\theta}\right)^{\kappa} B_\kappa^* f(t)\,\mathrm{d}t\right| \le \|B_\kappa^* f\| \left(\int_\theta^\pi \left(\frac{\theta}{t}\right)^{2\kappa} \mathrm{d}t\right)^{1/2} \\ &= \frac{\|B_\kappa^* f\|}{\sqrt{2\kappa-1}} \sqrt{\theta} \left(1 - \left(\frac{\theta}{\pi}\right)^{2\kappa-1}\right)^{1/2} \\ &\le \frac{\sqrt{2\kappa}\|B_\kappa^* f\|}{\sqrt{\pi(2\kappa-1)}} \sqrt{\theta}\sqrt{\pi-\theta}. \end{aligned}$$

Hence f is absolutely continuous in $[0,\pi]$ and $f(0)=f(\pi)=0$. The arguments for $\kappa<-\frac{1}{2}$ and functions in $\operatorname{dom}(B_\kappa)$ are similar.

Statement b). Let $\epsilon>0$ and $f\in\operatorname{dom}(B_\kappa^*)$. In a similar way as before we obtain

$$\begin{aligned}|f(\theta)| = |B_{\frac{1}{2}}^{*-1}B_{\frac{1}{2}}^* f(\theta)| &= \Big|\int_\theta^\pi \left(\frac{\theta}{\pi-\theta}\right)^{\frac{1}{2}}\left(\frac{\pi-t}{t}\right)^{\frac{1}{2}} B_{\frac{1}{2}}^* f(t)\,\mathrm{d}t\Big| \\ &\le \|B_{\frac{1}{2}}^* f\| \left(\frac{\theta}{\pi-\theta}\int_\theta^\pi \frac{\pi-t}{t}\,\mathrm{d}t\right)^{1/2} \\ &= \|B_{\frac{1}{2}}^* f\| \left(\frac{\theta}{\pi-\theta}\left[\pi(\ln(\pi)-\ln(\theta))-(\pi-\theta)\right]\right)^{1/2} \\ &= \|B_{\frac{1}{2}}^* f\|\sqrt{\pi-\theta}\,\theta^{\frac{1}{2}-\epsilon}\,h(\theta)^{\frac{1}{2}}\end{aligned}$$

for $h(\theta)=\frac{\theta^{2\epsilon}[\pi(\ln(\pi)-\ln(\theta))-(\pi-\theta)]}{(\pi-\theta)^2}$. Now, h is continuous in $(0,\pi)$, $\lim_{\theta\to0}h(\theta)=0$ and $\lim_{\theta\to\pi}h(\theta)=\frac{\pi^{2\epsilon-1}}{2}$. Hence

$$C(\epsilon)=\sup_{\theta\in[0,\pi]}\left\{\frac{\theta^{2\epsilon}(\pi(\ln(\pi)-\ln(\theta))-(\pi-\theta))}{(\pi-\theta)^2}\right\}^{\frac{1}{2}}<\infty$$

and the corresponding estimate follows. The other cases are similar. □

Appendix C. Computer code

Complete Comsol LiveLink v4.3b code for computing $\operatorname{spec}_2(\mathcal{A}_\kappa,\mathcal{L}_h)$. See [Com13].

```
% BASIC_KND_EIGS    Computes conjugate pairs in the second order spectra
%                   of the angular Kerr-Newman Dirac operator
%                   for trial spaces made of continuous affine functions
%
% BASIC_KND_EIGS(AM,AW,KAPPA,H,NEVP,SH,RTL)
%    AM    = mass term
%    AW    = energy term
%    KAPPA = angular momentum around axis of symmetry
%    H     = element size
%    NEVP  = number of conjugate pairs
%    SH    = shift
%    RTL   = relative tolerance
%
% Example:
%      z=basic_KND_eigs(0.25,0.75,2.5,0.1,8,0,1E-12)

function z=basic_KND_eigs(am,aw,kappa,h,nevp,sh,rtl)

import com.comsol.model.*
import com.comsol.model.util.*

model = ModelUtil.create('Model');
geom1=model.geom.create('geom1', 1);
mesh1=model.mesh.create('mesh1', 'geom1');
```

```
i1=geom1.feature.create('i1', 'Interval');
i1.set('intervals', 'one');
i1.set('p1', '0');
i1.set('p2', 'pi');
geom1.run;

mesh1.automatic(false);
mesh1.feature('size').set('custom', 'on');
mesh1.feature('size').set('hmax', num2str(h));
mesh1.run;

model.param.set('am',num2str(am));
model.param.set('aw',num2str(aw));
model.param.set('kappa',num2str(kappa));
model.param.set('C','am*cos(x)');
model.param.set('S','(kappa/sin(x)+aw*sin(x))');

w=model.physics.create('w', 'WeakFormPDE', 'geom1', {'u1' 'u2'});
w.prop('ShapeProperty').set('shapeFunctionType', 'shlag');
w.prop('ShapeProperty').set('order', 1);
w.feature('wfeq1').set('weak', 1,...
   '(-C*u1+u2x+S*u2)*test(-C*u1+u2x+S*u2)-2*u1t*test(-C*u1+u2x+S*u2)+u1t*test(u1t)');
w.feature('wfeq1').set('weak', 2,...
   '(-u1x+S*u1+C*u2)*test(-u1x+S*u1+C*u2)-2*u2t*test(-u1x+S*u1+C*u2)+u2t*test(u2t)');

cons1=w.feature.create('cons1', 'Constraint',0);
cons1.selection.set([1 2]);
cons1.set('R',1, 'u1^2');
cons1.set('R',2, 'u2^2');

std1=model.study.create('std1');
std1.feature.create('eigv', 'Eigenvalue');
std1.feature('eigv').activate('w', true);

sol1=model.sol.create('sol1');
sol1.study('std1');
sol1.feature.create('st1', 'StudyStep');
sol1.feature('st1').set('study', 'std1');
sol1.feature('st1').set('studystep', 'eigv');
sol1.feature.create('v1', 'Variables');
sol1.feature.create('e1', 'Eigenvalue');
sol1.feature('e1').set('control', 'eigv');
sol1.feature('e1').set('shift', num2str(sh));
sol1.feature('e1').set('neigs', nevp);
sol1.feature('e1').set('rtol', rtl);
sol1.attach('std1');
sol1.runAll;
```

```
info= mphsolinfo(model,'soltag','sol1');
z=info.solvals;
```

Acknowledgements

The authors wish to express their gratitude to P. Chigüiro for insightful comments during the preparation of this manuscript. This research was initiated as part of the programme Spectral Theory of Relativistic Operators held at the Isaac Newton Institute for Mathematical Sciences in July 2012. Subsequent funding was provided by the British Engineering and Physical Sciences Research Council grant EP/I00761X/1, FAPA research grant No. PI160322022 of the Facultad de Ciencias de la Universidad de los Andes, the Carnegie Trust for the Universities of Scotland reference 31741, the London Mathematical Society reference 41347 and the Edinburgh Mathematical Society Research Support Fund.

References

[BB09] L. Boulton and N. Boussaid. Non-variational computation of the eigenstates of Dirac operators with radially symmetric potentials. *LMS J. Comput. Math*, pages 1–30, 2009.

[BH14] L. Boulton and A. Hobiny. On the convergence of the quadratic method. *Preprint, arXiv:1307.0313*, 2014.

[BL07] L. Boulton and M. Levitin. On approximation of the eigenvalues of perturbed periodic Schrödinger operators. *J. Phys. A*, 40(31):9319–9329, 2007.

[Bou06] L. Boulton. Limiting set of second order spectra. *Math. Comp.*, 75(255):1367–1382, 2006.

[Bou07] L. Boulton. Non-variational approximation of discrete eigenvalues of self-adjoint operators. *IMA J. Numer. Anal.*, 27(1):102–121, 2007.

[BS06] D. Batic and H. Schmid. The Dirac propagator in the Kerr-Newman metric. *Progr. Theoret. Phys.*, 116(3):517–544, 2006.

[BS11] L. Boulton and M. Strauss. On the convergence of second-order spectra and multiplicity. *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.*, 467(2125):264–284, 2011.

[BS12] L. Boulton and M. Strauss. Eigenvalue enclosures and convergence for the linearized MHD operator. *BIT*, 52(4):801–825, 2012.

[BSW05] D. Batic, H. Schmid, and M. Winklmeier. On the eigenvalues of the Chandrasekhar-Page angular equation. *J. Math. Phys.*, 46(1):012504–35, 2005.

[Cha84] S. K. Chakrabarti. On mass-dependent spheroidal harmonics of spin one-half. *Proc. Roy. Soc. London, Ser. A*, 391(1800):27–38, 1984.

[Cha98] S. Chandrasekhar. *The mathematical theory of black holes*. Oxford Classic Texts in the Physical Sciences. The Clarendon Press Oxford University Press, New York, 1998. Reprint of the 1992 edition.

[CL55] E. A. Coddington and N. Levinson. *Theory of ordinary differential equations*. McGraw-Hill Book Company, Inc., New York-Toronto-London, 1955.

[Com13] Comsol. *LiveLink for Matlab v4.3b user's guide*. Comsol, 2013.

[Dav95] E.B. Davies. *Spectral theory and differential operators*. Cambridge University Press, Cambridge, 1995.

[Dav98] E.B. Davies. Spectral enclosures and complex resonances for general self-adjoint operators. *LMS J. Comput. Math.*, 1:42–74, 1998.

[DES00] J. Dolbeault, M. J. Esteban, and E. Séré. Variational characterization for eigenvalues of Dirac operators. *Calc. Var. Partial Differential Equations*, 10(4):321–347, 2000.

[DP04] E.B. Davies and M. Plum. Spectral pollution. *IMA J. Numer. Anal.*, 24(3):417–438, 2004.

[EG04] A. Ern and J.-L. Guermond. *Theory and practice of finite elements*, volume 159 of *Applied Mathematical Sciences*. Springer-Verlag, New York, 2004.

[FKSY00a] F. Finster, N. Kamran, J. Smoller, and S.-T. Yau. Erratum: "Nonexistence of time-periodic solutions of the Dirac equation in an axisymmetric black hole geometry". *Comm. Pure Appl. Math.*, 53(9):1201, 2000.

[FKSY00b] F. Finster, N. Kamran, J. Smoller, and S.-T. Yau. Nonexistence of time-periodic solutions of the Dirac equation in an axisymmetric black hole geometry. *Comm. Pure Appl. Math.*, 53(7):902–929, 2000.

[GLS99] M. Griesemer, R. T. Lewis, and H. Siedentop. A minimax principle for eigenvalues in spectral gaps: Dirac operators with Coulomb potentials. *Doc. Math.*, 4:275–283 (electronic), 1999.

[Hob14] A. Hobiny. *Enclosures for the eigenvalues of self-adjoint operators and applications to Schrödinger operators*. PhD Thesis, Heriot-Watt University, 2014.

[KLT04] M. Kraus, M. Langer, and C. Tretter. Variational principles and eigenvalue estimates for unbounded block operator matrices and applications. *J. Comput. Appl. Math.*, 171(1-2):311–334, 2004.

[LLT02] H. Langer, M. Langer, and C. Tretter. Variational principles for eigenvalues of block operator matrices. *Indiana Univ. Math. J.*, 51(6):1427–1459, 2002.

[LS04] M. Levitin and E. Shargorodsky. Spectral pollution and second-order relative spectra for self-adjoint operators. *IMA J. Numer. Anal.*, 24(3):393–416, 2004.

[LT06] M. Langer and C. Tretter. Variational principles for eigenvalues of the Klein-Gordon equation. *J. Math. Phys.*, 47(10):103506, 18, 2006.

[RS80] M. Reed and B. Simon. *Methods of Modern Mathematical Physics*, volume II. Academic Press, San Diego, 1980.

[Sch04] H. Schmid. Bound state solutions of the Dirac equation in the extreme Kerr geometry. *Math. Nachr.*, 274/275:117–129, 2004.

[SFC83] K. G. Suffern, E. D. Fackerell, and C. M. Cosgrove. Eigenvalues of the Chandrasekhar-Page angular functions. *J. Math. Phys.*, 24(5):1350–1358, 1983.

[Sha00] E. Shargorodsky. Geometry of higher order relative spectra and projection methods. *J. Operator Theory*, 44(1):43–62, 2000.

[Str11] M. Strauss. Quadratic projection methods for approximating the spectrum of self-adjoint operators. *IMA J. Numer. Anal.*, 31(1):40–60, 2011.

[Tre08] C. Tretter. *Spectral theory of block operator matrices and applications*. Imperial College Press, London, 2008.

[Wei87] J. Weidmann. *Spectral theory of ordinary differential operators*, volume 1258 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1987.

[Win05] M. Winklmeier. *The angular part of the Dirac equation in the Kerr-Newman metric: Estimates for the eigenvalues*. PhD thesis, Universität Bremen, 2005.

[Win08] M. Winklmeier. A variational principle for block operator matrices and its application to the angular part of the Dirac operator in curved spacetime. *J. Differential Equations*, 245(8):2145–2175, 2008.

[WY06] M. Winklmeier and O. Yamada. Spectral analysis of radial Dirac operators in the Kerr-Newman metric and its applications to time-periodic solutions. *J. Math. Phys.*, 47(10):102503, 17, 2006.

[WY09] M. Winklmeier and O. Yamada. A spectral approach to the Dirac equation in the non-extreme Kerr-Newmann metric. *J. Phys. A*, 42(29):295204, 15, 2009.

[ZM95] S. Zimmermann and U. Mertins. Variational bounds to eigenvalues of self-adjoint eigenvalue problems with arbitrary spectrum. *Z. Anal. Anwendungen*, 14(2):327–345, 1995.

Lyonell Boulton
Department of Mathematics & Maxwell Institute for the Mathematical Sciences
Heriot-Watt University
Edinburgh, EH14 4AS, United Kingdom
E-mail address: l.boulton@hw.ac.uk
URL: http://www.ma.hw.ac.uk/~lyonell/

Monika Winklmeier
Departamento de Matemáticas
Universidad de Los Andes
Cra. 1a No 18A-70, Bogotá, Colombia
E-mail address: mwinklme@uniandes.edu.co
URL: http://matematicas.uniandes.edu.co/~mwinklme/

$a\omega$	$m/\omega = 0$	$m/\omega = 0.2$	$m/\omega = 0.4$	$m/\omega = 0.6$	$m/\omega = 0.8$	$m/\omega = 1.0$
0.1	2.080309	2.076445	2.072607	2.068795	2.065008	2.061246
	2.080^{500}_{123}	2.076^{638}_{260}	2.072^{800}_{423}	2.068^{988}_{610}	2.06^{5200}_{4823}	2.061^{438}_{061}
0.2	2.161189	2.153720	2.146351	2.139083	2.131917	2.124853
	2.161^{402}_{027}	2.153^{939}_{563}	2.146^{573}_{199}	2.13^{9305}_{8933}	2.13^{2137}_{1764}	2.12^{5067}_{4694}
0.3	2.242573	2.231734	2.221119	2.210730	2.200569	2.190635
	2.242^{851}_{476}	2.23^{2029}_{1655}	2.221^{425}_{049}	2.21^{1035}_{0663}	2.200^{863}_{494}	2.190^{910}_{540}
0.4	2.324395	2.310402	2.296806	2.283610	2.270815	2.258419
	2.324^{801}_{427}	2.310^{849}_{472}	2.29^{7271}_{6899}	2.28^{4073}_{3702}	2.27^{1254}_{0880}	2.258^{810}_{436}
0.5	2.406589	2.389642	2.373312	2.357605	2.342520	2.328049
	2.40^{7214}_{6840}	2.3^{90339}_{89965}	2.37^{4040}_{3672}	2.35^{8325}_{7953}	2.34^{3184}_{2810}	2.328^{615}_{239}
0.6	2.489091	2.469373	2.450543	2.432607	2.415559	2.399378
	2.4^{90049}_{89676}	2.470^{448}_{076}	2.451^{665}_{295}	2.433^{700}_{328}	2.416^{545}_{169}	$2.^{400186}_{399814}$
0.7	2.571837	2.549516	2.528407	2.508514	2.489817	2.472274
	2.57^{3273}_{2897}	2.55^{1127}_{0758}	2.5^{30079}_{29708}	2.5^{10118}_{09745}	2.49^{1231}_{0858}	2.473^{400}_{027}
0.8	2.654763	2.629996	2.606820	2.585231	2.565189	2.546616
	2.656^{846}_{473}	2.63^{2332}_{1961}	2.60^{9221}_{8852}	2.587^{503}_{129}	2.56^{7151}_{6778}	2.54^{8137}_{7763}
0.9	2.737803	2.710737	2.685697	2.662669	2.641580	2.622294
	2.740^{741}_{368}	2.71^{4015}_{3646}	2.68^{9038}_{8666}	2.665^{783}_{411}	2.64^{4218}_{3841}	2.62^{4288}_{3912}
1.0	2.820892	2.791662	2.764958	2.740745	2.718899	2.699206
	2.824^{924}_{551}	2.79^{6140}_{5767}	2.769^{476}_{101}	2.744^{894}_{523}	2.72^{2345}_{1971}	2.701^{750}_{374}

TABLE 2. Computation of $|\lambda_{-1}(3/2, am, a\omega)|$ for different $a\omega$ and ω/m, as shown. The quantities in the upper part of each row are the positive square root of those in [Cha84, Table 2b]. The quantities in the lower part of each row are the enclosures determined directly from an application of (7). Quantities on the upper rows which are not within our guaranteed error bounds are shaded.

$a\omega$	$m/\omega = 0$	$m/\omega = 0.2$	$m/\omega = 0.4$	$m/\omega = 0.6$	$m/\omega = 0.8$	$m/\omega = 1.0$
0.1	1.920331 1.920^{516}_{141}	1.924477 1.924^{659}_{287}	1.928648 1.928^{830}_{457}	1.932845 1.93^{3027}_{2653}	1.937067 1.93^{7249}_{6876}	1.941315 1.941^{497}_{125}
0.2	1.841373 1.841^{536}_{163}	1.849972 1.8^{50129}_{49755}	1.858676 1.858^{828}_{454}	1.867484 1.867^{632}_{259}	1.876395 1.876^{543}_{170}	1.885406 1.885^{559}_{185}
0.3	1.763193 1.76^{3306}_{2931}	1.776584 1.776^{673}_{299}	1.790217 1.7^{90285}_{89910}	1.804084 1.80^{4140}_{3765}	1.818181 1.81^{8236}_{7859}	1.832498 1.832^{569}_{192}
0.4	1.685863 1.685^{883}_{507}	1.704417 1.704^{377}_{002}	1.723408 1.72^{3316}_{2939}	1.742821 1.742^{693}_{314}	1.762635 1.762^{500}_{122}	1.782831 1.782^{732}_{353}
0.5	1.609449 1.60^{9331}_{8955}	1.633573 1.63^{3333}_{2955}	1.658395 1.65^{8041}_{7660}	1.683877 1.683^{441}_{060}	1.709979 1.709^{519}_{138}	1.736651 1.73^{6258}_{5878}
0.6	1.534014 1.533^{718}_{340}	1.564156 1.563^{634}_{255}	1.595324 1.594^{586}_{204}	1.627446 1.626^{545}_{163}	1.660439 1.659^{483}_{099}	1.694209 1.69^{3364}_{2979}
0.7	1.459615 1.45^{9117}_{8734}	1.496266 1.495^{386}_{003}	1.534344 1.53^{3088}_{2702}	1.573721 1.57^{2172}_{1786}	1.614248 1.612^{585}_{196}	1.655756 1.65^{4261}_{3871}
0.8	1.386295 1.385^{601}_{219}	1.429994 1.428^{695}_{310}	1.475600 1.473^{686}_{299}	1.522898 1.520^{493}_{104}	1.571636 1.56^{9022}_{8628}	1.621537 1.61^{9158}_{8766}
0.9	1.314077 1.31^{3256}_{2870}	1.365418 1.363^{678}_{289}	1.419230 1.416^{530}_{140}	1.475166 1.471^{685}_{292}	1.532828 1.528^{987}_{591}	1.591781 1.58^{8261}_{7862}
1.0	1.242955 1.24^{2165}_{1776}	1.302592 1.300^{452}_{060}	1.365353 1.361^{773}_{379}	1.430702 1.425^{926}_{528}	1.498032 1.492^{675}_{274}	1.566699 1.561^{754}_{352}

TABLE 3. Computation of $|\lambda_{-1}(-3/2, am, a\omega)|$ for different $a\omega$ and ω/m, as shown. The quantities in the upper part of each row are the positive square root of those in [Cha84, Table 2b]. The quantities in the lower part of each row are the enclosures determined directly from an application of (7). Quantities on the upper rows which are not within our guaranteed error bounds are shaded.

$am = 0.005,\ a\omega = 0.015$

	$n=-1$		$n=1$		$n=2$		$n=3$	
	A	N	A	N	A	N	A	N
$\kappa=-4.5$	-4.9^{7997}_{9299}	-4.98^{547}_{817}	4.9^{9299}_{7997}	4.98^{727}_{456}	5.9^{9500}_{8248}	5.9^{9176}_{8497}	6.9^{9643}_{8427}	6.9^{9622}_{8395}
-3.5	-3.9^{7997}_{9374}	-3.98^{611}_{833}	3.9^{9374}_{7997}	3.98^{723}_{500}	4.9^{9600}_{8298}	4.9^{9190}_{8620}	5.9^{9750}_{8499}	5.9^{9621}_{8570}
-2.5	-2.9^{7996}_{9499}	-2.98^{698}_{874}	2.9^{9499}_{7996}	2.98^{731}_{555}	3.9^{9750}_{8373}	3.9^{9242}_{8776}	4.9^{9900}_{8599}	4.9^{9659}_{8778}
-1.5	-1.9^{7994}_{9749}	-1.98^{812}_{990}	1.9^{9749}_{7994}	1.98^{789}_{612}	${}^{3.00000}_{2.98498}$	2.9^{9404}_{8971}	${}^{4.00125}_{3.98749}$	3.9^{9808}_{9005}
-0.5	$-^{0.97988}_{1.00500}$	$-^{0.81076}_{1.17342}$	${}^{1.00500}_{0.97988}$	${}^{1.16967}_{0.80779}$	${}^{2.00500}_{1.98748}$	${}^{2.25132}_{1.74245}$	${}^{3.00500}_{2.98999}$	${}^{3.30912}_{2.68941}$
0.5	$-^{0.99500}_{1.01990}$	$-^{0.82905}_{1.18847}$	${}^{1.01990}_{0.99500}$	${}^{1.19218}_{0.83197}$	${}^{2.01249}_{1.99500}$	${}^{2.26051}_{1.75063}$	${}^{3.01000}_{2.99500}$	${}^{3.31501}_{2.69440}$
1.5	-2.0^{0248}_{1995}	-2.01^{013}_{189}	2.0^{1995}_{0248}	2.01^{389}_{212}	${}^{3.01499}_{2.99999}$	3.0^{1032}_{0600}	${}^{4.01250}_{3.99874}$	4.00^{998}_{196}
2.5	-3.0^{0498}_{1997}	-3.01^{127}_{303}	3.0^{1997}_{0498}	3.01^{446}_{270}	4.0^{1624}_{0249}	4.0^{1226}_{0760}	5.0^{1400}_{0099}	5.0^{1225}_{0343}
3.5	-4.0^{0623}_{1998}	-4.01^{167}_{389}	4.0^{1998}_{0623}	4.01^{500}_{278}	5.0^{1699}_{0399}	5.0^{1382}_{0812}	6.0^{1500}_{0249}	6.0^{1432}_{0381}
4.5	-5.0^{0698}_{1998}	-5.01^{183}_{454}	5.0^{1998}_{0698}	5.01^{545}_{274}	6.0^{1749}_{0499}	6.0^{1504}_{0825}	7.0^{1571}_{0356}	7.0^{1607}_{0379}

$am = 0.25,\ a\omega = 0.75$

	$n=-1$		$n=1$		$n=2$		$n=3$	
	A	N	A	N	A	N	A	N
$\kappa=-4.5$	$-^{3.93330}_{4.61607}$	-4.3^{4800}_{5071}	${}^{4.61607}_{3.93330}$	4.29^{891}_{622}	$5.^{73293}_{08853}$	5.4^{3238}_{2561}	$6.^{81221}_{19204}$	6.5^{2368}_{1143}
-3.5	$-^{2.91227}_{3.65037}$	-3.37^{259}_{482}	${}^{3.65037}_{2.91227}$	3.30^{981}_{759}	$4.^{78460}_{10889}$	4.4^{7115}_{6547}	$5.^{86806}_{22722}$	5.5^{7087}_{6039}
-2.5	$-^{1.87132}_{2.71222}$	-2.41^{258}_{438}	${}^{2.71222}_{1.87132}$	2.32^{746}_{570}	$3.^{86421}_{14116}$	3.5^{3220}_{2756}	$4.^{94708}_{27769}$	4.63^{890}_{012}
-1.5	$-^{0.75000}_{1.85079}$	-1.4^{8796}_{9000}	${}^{1.85079}_{0.75000}$	1.3^{6075}_{5885}	${}^{3.00000}_{2.19948}$	2.6^{4203}_{3770}	${}^{4.06609}_{3.35555}$	3.7^{4491}_{3691}
-0.5	$-^{0.25000}_{1.28078}$	$-0.^{44078}_{90569}$	${}^{1.28078}_{0.25000}$	$0.^{65248}_{22804}$	${}^{2.26557}_{1.33113}$	${}^{2.12229}_{1.65046}$	${}^{3.26040}_{2.48861}$	${}^{3.22283}_{2.62846}$
0.5	$-^{0.75000}_{1.85079}$	$-1.^{32502}_{62848}$	${}^{1.85079}_{0.75000}$	$1.^{76746}_{42913}$	${}^{2.60850}_{1.75000}$	$2.^{55401}_{02453}$	${}^{3.50000}_{2.75000}$	${}^{3.51065}_{2.87169}$
1.5	$-2.^{09520}_{90754}$	-2.57^{578}_{743}	$2.^{90754}_{09520}$	2.65^{737}_{566}	${}^{3.72312}_{2.99037}$	3.4^{4251}_{3822}	${}^{4.61607}_{3.93330}$	4.3^{3398}_{2596}
2.5	$-3.^{21410}_{93274}$	-3.62^{132}_{304}	$3.^{93274}_{21410}$	3.68^{315}_{142}	$4.^{784591}_{10889}$	4.51^{774}_{313}	$5.^{68715}_{04150}$	5.4^{1754}_{0876}
3.5	$-4.^{27769}_{94708}$	-4.64^{746}_{965}	$4.^{94708}_{27769}$	4.69^{794}_{575}	$5.^{82338}_{18139}$	5.5^{6358}_{5791}	$6.^{73557}_{11396}$	6.4^{7365}_{6318}
4.5	$-5.^{31776}_{95636}$	-5.66^{448}_{717}	$5.^{95636}_{31776}$	5.70^{757}_{488}	$6.^{85020}_{23074}$	6.5^{9460}_{8784}	$7.^{77081}_{16619}$	7.5^{1404}_{0180}

Table 4. Analytic (A) and numeric (N) bounds for the eigenvalues of $\mathcal{A}_\kappa$. The range of κ, n, am and $a\omega$ employed corresponds to analogous calculations in [SFC83, Table II]. Here the numerical bounds were determined directly from (7) and their computation does not use any input from the analytical bounds.

$am = 0.005,\ a\omega = 0.015$

	$n=1$			$n=2$		
	from A	from N	[SFC83]	from A	from N	[SFC83]
$\kappa = -4.5$	4.9859^{2}_{0}	4.9859^{2}_{0}	4.98581	5.9883^{8}_{4}	5.9883^{8}_{4}	
-3.5	3.9861^{2}_{1}	3.9861^{2}_{1}	3.98611	4.9890^{6}_{3}	4.9890^{6}_{3}	4.98905
-2.5	2.9864^{4}_{2}	2.9864^{4}_{2}	2.98643	3.990^{10}_{08}	3.990^{10}_{08}	3.99009
-1.5	1.9870^{1}_{0}	1.9870^{1}_{0}	1.98700	2.9918^{8}_{6}	2.9918^{8}_{6}	2.99187
-0.5	$^{1.00537}_{0.95595}$	$^{1.00693}_{0.94529}$	0.98843	$^{2.06215}_{1.93169}$	$^{2.07515}_{1.90340}$	1.99567
0.5	$^{1.02824}_{0.97907}$	$^{1.02970}_{0.96816}$	1.01167	$^{2.07151}_{1.93988}$	$^{2.08548}_{1.91121}$	2.00435
1.5	2.0130^{1}_{0}	2.0130^{1}_{0}	2.01300	3.0081^{7}_{5}	3.0081^{7}_{5}	3.00815
2.5	3.0135^{8}_{7}	3.0135^{8}_{7}	3.01357	4.0099^{4}_{2}	4.0099^{4}_{2}	4.00993
3.5	4.013^{90}_{88}	4.013^{90}_{88}	4.01389	5.0109^{8}_{5}	5.0109^{8}_{5}	5.01096
4.5	5.014^{10}_{08}	5.014^{10}_{08}	5.01409	6.0116^{6}_{3}	6.0116^{6}_{3}	

$am = 0.25,\ a\omega = 0.75$

	$n=1$			$n=2$		
	from A	from N	[SFC83]	from A	from N	[SFC83]
$\kappa = -4.5$	4.2975^{7}_{5}	4.2975^{7}_{6}	4.29756	5.42^{902}_{898}	5.42^{901}_{898}	
-3.5	3.308^{70}_{69}	3.308^{70}_{69}	3.30870	4.468^{32}_{29}	4.4683^{2}_{0}	4.46676
-2.5	2.3265^{8}_{7}	2.3265^{8}_{7}	2.32657	3.5298^{9}_{6}	3.5298^{9}_{7}	3.52651
-1.5	1.359^{80}_{79}	1.359^{80}_{79}	1.35984	2.6398^{7}_{5}	2.6398^{7}_{5}	2.63036
-0.5	$0.^{54256}_{38970}$	0.4^{9138}_{0304}	0.44058	1.79^{828}_{396}	$1.^{93148}_{81137}$	1.84225
0.5	$1.^{61048}_{40966}$	$1.^{60808}_{53115}$	1.59764	$2.^{44911}_{13715}$	$2.^{42358}_{16893}$	2.22587
1.5	2.6565^{1}_{0}	2.6565^{1}_{0}	2.65654	3.4403^{8}_{5}	3.4403^{7}_{5}	3.43391
2.5	3.6822^{9}_{8}	3.6822^{9}_{8}	3.68229	4.5154^{5}_{2}	4.5154^{4}_{2}	4.51300
3.5	4.6968^{5}_{4}	4.6968^{5}_{4}	4.69685	5.5607^{6}_{2}	5.5607^{5}_{3}	5.55956
4.5	5.7062^{3}_{1}	5.7062^{3}_{1}	5.70622	6.591^{24}_{19}	6.5912^{3}_{0}	

TABLE 5. Improved numerical enclosures for the eigenvalues originally reported in [SFC83, Table II]. These improved bounds were found from the data in Table 4, analytical or numerical as appropriate, and by means of an implementation of (8). Values from [SFC83] that are over or under-shot are highlighted in colour.

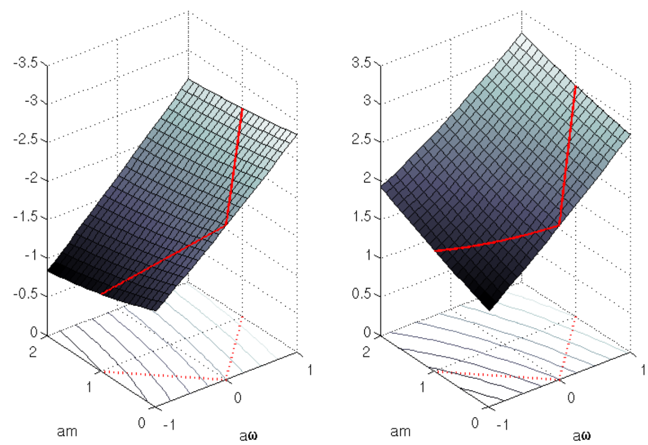

FIGURE 1. Approximation of $\lambda_{\pm 1}(\frac{3}{2}, am, a\omega)$ for 100 different $(a\omega, am)$ equally distributed in the rectangle $[-1,1] \times [0,2]$. The red curve corresponds to the exact value of $\lambda_{\pm 1}$ from (31).

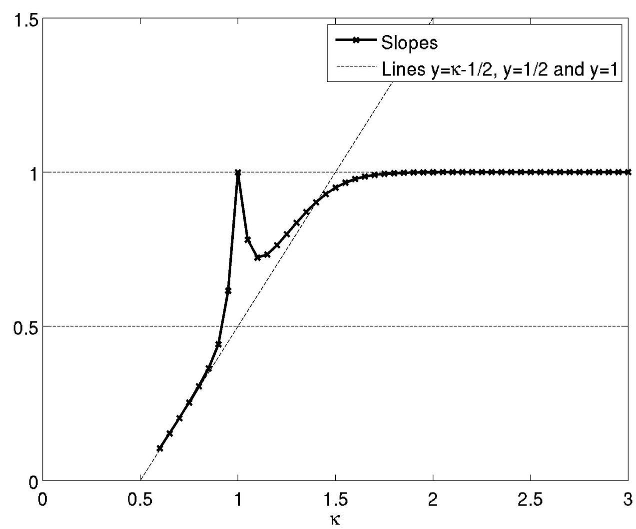

FIGURE 2. A numerical approximation of the optimal exponent in Theorem 9.