Eigenvalue bounds for the singular Sturm–Liouville problem with a complex potential

2003 J. Phys. A: Math. Gen. 36 3773

(http://iopscience.iop.org/0305-4470/36/13/310)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) 3773–3787 PII: S0305-4470(03)57450-9

Eigenvalue bounds for the singular Sturm–Liouville problem with a complex potential*

B M Brown[1], **M Langer**[2,4], **M Marletta**[3,4], **C Tretter**[2,4] **and M Wagenhofer**[2]

[1] Department of Computer Science, Cardiff University, PO Box 916, Cardiff CF24 3XF, UK
[2] FB 3-Mathematik, University of Bremen, Bibliothekstr. 1, 28359 Bremen, Germany
[3] School of Mathematics, Cardiff University, PO Box 926, Cardiff CF24 4YH, UK

E-mail: Malcolm.Brown@cs.cf.ac.uk

Received 12 December 2002
Published 19 March 2003
Online at stacks.iop.org/JPhysA/36/3773

Abstract
The main objective of this paper is to report on a recent algorithm to enclose the eigenvalues of non-selfadjoint singular Sturm–Liouville problems.

PACS numbers: 02.60.−x, 02.30.Tb
Mathematics Subject Classification: 34L16, 65L15

1. Introduction

Recently there has been much interest [1, 8, 9, 21] in investigating the spectrum of the non-selfadjoint Sturm–Liouville problem

$$-y'' + qy = \lambda y \qquad \lambda \in \mathbb{C} \tag{1.1}$$

on the interval $[0, \infty)$, where q is both complex valued and bounded. For such q and functions $y \in L^2[0, \infty)$ it is well known (cf [8]) that it is sufficient to impose a boundary condition only at 0 in order to make (1.1) into a well-posed eigenvalue problem; for example

$$y(0) = 0. \tag{1.2}$$

These conditions will be assumed hereafter without further mention. Further as needed we shall assume appropriate smoothness conditions on q. We say that the endpoint 0 is a regular point and infinity a singular point of the interval.

The problem of numerically computing eigenvalues of (1.1), (1.2) when q is real valued has also received much attention. There are a number of computer codes that perform

* Dedicated to the memory of Professor Will Light, mathematician and Pro Vice Chancellor of the University of Leicester, who died while the manuscript was in preparation.
[4] Formerly of the University of Leicester.

0305-4470/03/133773+15$30.00

this task. These codes mainly work by transforming (1.1) using Prüfer variables, solving the resulting ODE in these new variables, then via a shooting method, performing a root finding operation for λ on the resulting solution until the boundary condition (1.2) is satisfied (see [4, 12, 17] for further details). A feature of these codes is that they only produce numerical estimates for eigenvalues without any absolute certainty of accuracy. In order to remedy this position Brown *et al* [7] have proposed an algorithm and a computer code that produce provably correct enclosures for λ_k, the kth eigenvalue of (1.1), with a self-adjoint boundary condition at 0 and real q. The method proposed in [7] first reduces the singular problem (1.1) on $[0, \infty)$, to a regular problem on an interval $[0, X]$, $X < \infty$, with a λ-dependent boundary condition at X. This is achieved by Eastham's diagonalization method (see [6, 10]) which replaces the solution of (1.1) in $[X, \infty)$ by its asymptotic form together with a uniform and absolute bound ε_X on the error $\varepsilon(x)$ for $x \geqslant X$. This provides a λ-dependent bound on the solution at X which provides an initial interval-value for an interval ODE solver which is used to enclose the solution of (1.1) over $[0, X]$. A shooting method is then used to find the pair λ_-, λ_+ which determine an interval $[\lambda_-, \lambda_+]$ in which λ_k must lie.

It is our intention in this paper to develop a method that will provide bounds for the eigenvalues of the non-selfadjoint problem (1.1) when q is allowed to be complex. Briefly, our approach will be to first obtain a floating point approximation to the desired eigenvalue by truncating the interval $[0, \infty)$ to $[0, X]$, for some $X < \infty$, then use a numerical procedure, for example the code [13] to obtain an estimate of the eigenvalue of the resulting regular problem. This procedure introduces errors both from the interval truncation and also from the numerical procedure inherent in solving the ODE over a finite interval. These errors must be both controlled and estimated. The goal of the procedure is to obtain a small box in the complex plane which will contain the true eigenvalue. The error estimates are computed by interval arithmetic software in which the rounding errors inherent in numerical calculations are taken into account and an interval ODE solving procedure is used to obtain an enclosure for the solution over $[0, X]$. Finally a fixed point theorem (implemented in interval arithmetic) is used to bound the truncation error.

We shall show the effectiveness of our method by computing guaranteed enclosures for the eigenvalues of Squire's problem

$$-y'' + \mathrm{i}\alpha R V y = \lambda y \qquad \text{on} \quad [0, \infty)$$

where α, R are real constants (wave number and Reynolds number) and $V \in L^\infty(0, \infty)$ is real valued. Moreover, we calculate enclosures for resonances of a particular Schrödinger operator.

For simplicity we restrict ourselves to the case of the Dirichlet boundary condition (1.2) although a more general boundary condition would be possible.

2. The operator and its spectral properties

We consider the Sturm–Liouville problem (1.1), (1.2), and we suppose that the following assumptions are satisfied:

(i) $q \in L^\infty[0, \infty)$.

(ii) The limit $\lim_{x\to\infty} q(x) =: q_\infty$ exists.

(iii) $q - q_\infty \in L^1(0, \infty)$.

Problem (1.1), (1.2) is the spectral problem for the closed linear operator T in $L^2(0,\infty)$ given by

$$D(T) = \{y \in L^2(0,\infty)\colon y', y'' \in L^2(0,\infty),\ y(0) = 0\} \tag{2.1}$$

$$Ty = -y'' + qy. \tag{2.2}$$

The essential spectrum of T is defined as $\sigma_{\mathrm{ess}}(T) := \{\lambda \in \mathbb{C} : T - \lambda \text{ is not Fredholm}\}$. Here a linear operator T is called Fredholm if the dimension of its kernel, $\mathrm{nul}(T)$, and the codimension of its range, $\mathrm{def}(T)$, are finite (the latter implying that the range is closed, see [11, I.3 and I.4]).

Theorem 2.1. *Under the assumptions* (i), (ii) *denote*

$$q_{\mathrm{r,min}} := \inf\{\mathrm{Re}\, q(x)\colon x \in [0,\infty)\},$$
$$q_{\mathrm{i,min}} := \inf\{\mathrm{Im}\, q(x)\colon x \in [0,\infty)\}, \quad q_{\mathrm{i,max}} := \sup\{\mathrm{Im}\, q(x)\colon x \in [0,\infty)\}.$$

Then

$$\sigma_{\mathrm{ess}}(T) = \{\lambda \in \mathbb{C}\colon \lambda = t + q_\infty,\ t \geqslant 0\}$$

and

$$\sigma(T) \subset \{\lambda \in \mathbb{C}\colon \mathrm{Re}\,\lambda \geqslant q_{\mathrm{r,min}},\ q_{\mathrm{i,min}} \leqslant \mathrm{Im}\,\lambda \leqslant q_{\mathrm{i,max}}\}. \tag{2.3}$$

Proof. The proof is almost the same as in the well-known self-adjoint case; however, for the convenience of the reader we present it here. Let T_∞ and T_N, $N \in \mathbb{N}$, be the operators with domain (2.1) and $T_\infty y = -y'' + q_\infty y$ and $T_N y = -y'' + q_N y$, respectively, where

$$q_N(x) = \begin{cases} q(x) & \text{for} \quad 0 \leqslant x \leqslant N \\ q_\infty & \text{for} \quad N < x < \infty. \end{cases}$$

The operator $(T_N - T_\infty)(T_\infty - (q_\infty - 1))^{-1}$ is compact since it is an integral operator with kernel

$$K(x,t) = \tfrac{1}{2}(\exp(-|x-t|) - \exp(-x-t))(q_N(x) - q_\infty)$$

which is square integrable on $[0,\infty) \times [0,\infty)$ since $q_N - q_\infty$ has compact support. The sequence $(T_N - T_\infty)(T_\infty - (q_\infty - 1))^{-1}$ converges to $(T - T_\infty)(T_\infty - (q_\infty - 1))^{-1}$ uniformly if $N \to \infty$, which implies that $T - T_\infty$ is relatively compact with respect to T_∞. Hence $\sigma_{\mathrm{ess}}(T) = \sigma_{\mathrm{ess}}(T_\infty) = \{\lambda \in \mathbb{C}\colon \lambda = t + q_\infty, t \geqslant 0\}$ and for λ outside this set we have $\mathrm{ind}(T - \lambda) := \mathrm{nul}(T - \lambda) - \mathrm{def}(T - \lambda) = 0$.

Because of

$$(Ty, y) = \int_0^\infty |y'(x)|^2\,\mathrm{d}x + \int_0^\infty q(x)|y(x)|^2\,\mathrm{d}x \qquad y \in D(T) \quad \|y\| = 1$$

the numerical range $W(T)$ is contained in the right-hand side of (2.3). For λ outside this set we have $\mathrm{nul}(T - \lambda) = 0$ and because of $\mathrm{ind}(T - \lambda) = 0$ also $\mathrm{def}(T - \lambda) = 0$. Hence λ lies in the resolvent set of T, i.e., $\lambda \in \rho(T)$. □

As a consequence, outside the horizontal ray $\{\lambda \in \mathbb{C}\colon \lambda = t + q_\infty, t \geqslant 0\}$, the spectrum of T consists only of isolated eigenvalues with finite algebraic multiplicity. Because the problem is non-selfadjoint and $q(x)$ is not assumed to decay at least as fast as $\exp(-c\sqrt{x})$ for large x ($c > 0$ constant), the essential spectrum may contain spectral singularities [20]; however, we do not consider these here, but restrict our attention to the isolated eigenvalues outside the essential spectrum.

The method which we describe in the next section is applicable whenever one is able to apply Levinson asymptotics [10, 14] to the problem, in particular, under the assumption (iii), i.e., $q - q_\infty \in L^1(0,\infty)$. A number of transformations exist to deal with the case where $q - q_\infty \notin L^1(0,\infty)$ such as the so-called repeated diagonalization technique [5]. One can even deal with some cases in which q_∞ does not exist. However, in this paper, we do not consider such situations.

By a shift of the spectral parameter we can assume without loss of generality that $q_\infty = 0$. So we assume for the rest of the paper that

$$\lim_{x\to\infty} q(x) = 0 \qquad \text{and} \quad q \in L^1(0,\infty). \tag{2.4}$$

In this case the essential spectrum is the positive real axis.

3. Eigenvalue approximation: theory behind the guaranteed error bounds

In this section we describe our approach to get guaranteed error bounds for approximations of the eigenvalues of the non-selfadjoint Sturm–Liouville problem (1.1), (1.2). To this end we replace the function q by a function Q having compact support:

$$Q(x) := \begin{cases} q(x) & \text{for} \quad 0 \leqslant x \leqslant X \\ 0 & \text{for} \quad X < x < \infty \end{cases} \tag{3.1}$$

where $X > 0$ is fixed, and consider the auxiliary problem

$$-Y'' + QY = \Lambda Y \qquad \text{on} \quad [0,\infty) \tag{3.2}$$

$$Y(0) = 0. \tag{3.3}$$

Observe that for $x > X$ we can solve the differential equation $-Y'' + QY = \Lambda Y$ exactly, and identify the unique (up to scalar multiplication) L^2 solution as the function

$$\exp(-\sqrt{-\Lambda}x) \quad x \geqslant X \qquad \operatorname{Re}\sqrt{-\Lambda} > 0.$$

Thus the eigenvalues of the problem (3.2), (3.3) are precisely the values $\Lambda \in \mathbb{C}\backslash[0,\infty)$ for which there exists a non-trivial solution of the differential equation

$$-Y'' + QY = \Lambda Y \qquad \text{on} \quad [0, X] \tag{3.4}$$

satisfying the Λ-dependent boundary conditions

$$Y(0) = 0 \qquad Y'(X) = -\sqrt{-\Lambda}Y(X) \qquad \operatorname{Re}\sqrt{-\Lambda} > 0. \tag{3.5}$$

In order to obtain guaranteed error bounds for the eigenvalues of (1.1), (1.2), two steps are necessary:

Step A: Solving the truncated problem with guaranteed error bounds. We must find the eigenvalues of (3.4), (3.5) with guaranteed error bounds. We accomplish this by calculating, with guaranteed error bounds, an analytic function whose zeros are the eigenvalues of (3.4), (3.5); and we find these zeros using an algorithm based on Rouché's Theorem, again implemented with guaranteed error bounds.

Step B: Guaranteed error bounds for the truncation error. For each eigenvalue Λ of (3.4), (3.5), step A yields a set $\mathcal{R} \subset \mathbb{C}$ containing Λ. The aim is to find a neighbourhood $\mathcal{C}$ of the origin in $\mathbb{C}$, controlling the error due to the truncation of the interval, so that

$$\mathcal{R} + \mathcal{C} := \{r + c\colon r \in \mathcal{R}, c \in \mathcal{C}\}$$

contains an eigenvalue of (1.1), (1.2). This is achieved by showing that $\mathcal{C}$ contains a fixed point of a certain function, cf theorem 3.1 below.

In the remainder of this section we give a more detailed description of the mathematics behind steps A and B, starting with step B in section 3.1, followed by step A in section 3.2.

Since in the following we shall rely heavily on (complex) interval arithmetic, we have summarized the most important features found in a typical software package such as AWA [15] and VNODE [19] in the appendix. Such packages integrate initial value problems numerically, starting from interval valued initial conditions, satisfying interval valued differential equations, and returning interval valued results.

3.1. Guaranteed error bounds for the truncation error (step B)

Let us first assume that an eigenvalue Λ_0 and an eigenfunction Y_0 of the problem (3.2), (3.3) are known exactly. In section 3.1.1 we establish the equivalence of the original eigenvalue problem to a fixed point problem of a certain function Φ_{Λ_0}. Then in section 3.1.2 we show how this equivalence can be used to obtain an enclosure of an eigenvalue of the original problem even if an eigenvalue of the truncated problem is not known exactly.

3.1.1. Equivalence to a fixed point problem. Let Λ_0 and Y_0 be an eigenvalue and an eigenfunction of the problem (3.2), (3.3). Suppose that $\lambda \in \mathbb{C}\backslash[0,\infty)$ and let $y_2(\cdot,\lambda)$ denote the unique (up to scalar multiplication) L^2 solution of (1.1). Then λ is an eigenvalue of the original problem (1.1), (1.2) if and only if $y_2(0,\lambda) = 0$. Multiplying (1.1) (with $y = y_2$) by Y_0, then multiplying (3.2) by y_2, and subtracting, we obtain

$$(\lambda - \Lambda_0) y_2 Y_0 = (q - Q) y_2 Y_0 + y_2 Y_0'' - y_2'' Y_0.$$

Integration by parts now yields

$$(\lambda - \Lambda_0) \int_0^\infty y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x = \int_X^\infty q(x) y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x - y_2(0,\lambda) Y_0'(0,\Lambda_0)$$

where we have exploited the facts that $Y_0(0,\Lambda_0) = 0$ and $q(x) - Q(x) = 0$ for $0 \leqslant x \leqslant X$. Thus

$$\lambda - \Lambda_0 = \frac{\int_X^\infty q(x) y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x - y_2(0,\lambda) Y_0'(0,\Lambda_0)}{\int_0^\infty y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x} \tag{3.6}$$

provided the integral appearing in the denominator of the right-hand side is non-zero. We know that $y_2(0,\lambda) = 0$ if and only if λ is an eigenvalue of the original problem (1.1), (1.2), and in this case we have

$$\lambda - \Lambda_0 = \frac{\int_X^\infty q(x) y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x}{\int_0^\infty y_2(x,\lambda) Y_0(x,\Lambda_0)\,\mathrm{d}x}. \tag{3.7}$$

Let $\Lambda \in \mathbb{C}\backslash[0,\infty)$ and let $Y_2(\cdot,\Lambda)$ be an L^2 solution of (3.2). Then we define the following function:

$$\Phi_\Lambda(\varepsilon) := \frac{\int_X^\infty q(x) y_2(x,\Lambda+\varepsilon) Y_2(x,\Lambda)\,\mathrm{d}x}{\int_0^\infty y_2(x,\Lambda+\varepsilon) Y_2(x,\Lambda)\,\mathrm{d}x} \tag{3.8}$$

which is continuous on the domain

$$\mathcal{D}(\Phi_\Lambda) = \left\{ \varepsilon \in \mathbb{C}\colon \Lambda + \varepsilon \notin [0,\infty), \int_0^\infty y_2(x,\Lambda+\varepsilon) Y_2(x,\Lambda)\,\mathrm{d}x \neq 0 \right\}.$$

With this function we can prove the following fixed point theorem.

Theorem 3.1. *Suppose that* $\Lambda_0 \in \mathbb{C}\backslash[0,\infty)$ *is an eigenvalue of* (3.2), (3.3) *and let* $\varepsilon \in \mathcal{D}\big(\Phi_{\Lambda_0}\big)$. *Then* $\Lambda_0 + \varepsilon$ *is an eigenvalue of the original problem* (1.1), (1.2) *if and only if* ε *is a fixed point of* Φ_{Λ_0}.

Proof. It follows from the considerations above that if $\lambda := \Lambda_0 + \varepsilon$ is an eigenvalue of (1.1), (1.2), then equation (3.7) is valid, hence ε is a fixed point of Φ_{Λ_0}. Conversely, if ε is a fixed point of Φ_{Λ_0}, then (3.7) holds with $\lambda := \Lambda_0 + \varepsilon$. Since (3.6) is always true, it follows that $y_2(0,\lambda) = 0$. □

3.1.2. Localizing a fixed point. We now look for a set that contains a fixed point of Φ_{Λ_0} if Λ_0 is an eigenvalue of the truncated problem (3.4), (3.5). In practice we do not know an eigenvalue Λ_0 of the truncated problem exactly but only some set $\mathcal{R}$ which is guaranteed to contain an eigenvalue. Moreover, we cannot calculate Φ_Λ exactly. So we proceed as follows. Let $\mathcal{B}$ be a closed convex set in the complex plane with $\mathcal{B} \subset \mathcal{D}(\Phi_\Lambda)$ for all $\Lambda \in \mathcal{R}$. We will see that we can get a closed convex enclosure $\mathcal{C}$ which contains the set

$$\Phi_{\mathcal{R}}(\mathcal{B}) := \bigcup_{\Lambda\in\mathcal{R}} \Phi_\Lambda(\mathcal{B}).$$

If $\mathcal{C} \subset \mathcal{B}$ and if we know that $\mathcal{R}$ contains an eigenvalue Λ_0 of the truncated problem, then

$$\Phi_{\Lambda_0}(\mathcal{C}) \subset \Phi_{\Lambda_0}(\mathcal{B}) \subset \Phi_{\mathcal{R}}(\mathcal{B}) \subset \mathcal{C} \tag{3.9}$$

which implies that $\mathcal{C}$ contains a fixed point of Φ_{Λ_0}; by theorem 3.1 we then conclude that $\mathcal{R} + \mathcal{C}$ contains an eigenvalue of the original problem.

Remark 3.2. Of course, one must guess a suitable set $\mathcal{B}$ *a priori*. This can be done by trial and error or by making estimates based on the eigenvalue condition number, calculated in floating point arithmetic using any standard discretization method.

In order to get an enclosure $\mathcal{C}$ of $\Phi_{\mathcal{R}}(\mathcal{B})$, we estimate, for fixed Λ and ε,

$$\begin{aligned}|\Phi_\Lambda(\varepsilon)| &\leqslant \frac{\max\limits_{x\in[X,\infty)} |q(x)| \int_X^\infty |y_2(x,\Lambda+\varepsilon)Y_2(x,\Lambda)|\,\mathrm{d}x}{\left|\int_0^X y_2(x,\Lambda+\varepsilon)Y_2(x,\Lambda)\,\mathrm{d}x\right| - \int_X^\infty |y_2(x,\Lambda+\varepsilon)Y_2(x,\Lambda)|\,\mathrm{d}x} \\ &= \frac{\max\limits_{x\in[X,\infty)} |q(x)| \int_X^\infty |y_2(x,\Lambda+\varepsilon)\exp(-\sqrt{-\Lambda}x)|\,\mathrm{d}x}{\left|\int_0^X y_2(x,\Lambda+\varepsilon)Y_2(x,\Lambda)\,\mathrm{d}x\right| - \int_X^\infty |y_2(x,\Lambda+\varepsilon)\exp(-\sqrt{-\Lambda}x)|\,\mathrm{d}x}\end{aligned} \tag{3.10}$$

provided the denominator in (3.10) is positive and fixing the normalization

$$Y_2(x,\Lambda) = \exp(-\sqrt{-\Lambda}x) \qquad x \geqslant X.$$

We use Levinson asymptotics [10, 14], summarized in the following theorem, for an estimate of the solution y_2.

Theorem 3.3. *For* $\lambda \in \mathbb{C}\backslash[0,\infty)$ *the* L^2 *solution* y_2 *of* (1.1), *suitably normalized, satisfies*

$$\begin{aligned}y_2(x,\lambda) &= \exp(-\sqrt{-\lambda}x)(1+\eta_1(x)) \\ y_2'(x,\lambda) &= -\sqrt{-\lambda}\exp(-\sqrt{-\lambda}x)(1+\eta_2(x))\end{aligned} \tag{3.11}$$

in which $\mathrm{Re}\sqrt{-\lambda} > 0$ *and, for all* $x \geqslant X$,

$$|\eta_j(x)| \leqslant \frac{\alpha_X}{1-\alpha_X} \qquad j = 1,2 \quad \alpha_X := \int_X^\infty |q(s)|\,\mathrm{d}s \tag{3.12}$$

provided only that X is large enough to ensure that $\alpha_X < 1$.

This allows an immediate estimate of the integral in the numerator and the second integral in the denominator of (3.10):

$$\begin{aligned}\int_X^\infty |y_2(x,\Lambda+\varepsilon)\exp(-\sqrt{-\Lambda}x)|\,\mathrm{d}x &\leqslant \int_X^\infty \exp\left(-x\,\mathrm{Re}\left(\sqrt{-\Lambda-\varepsilon}+\sqrt{-\Lambda}\,\right)\right)\mathrm{d}x(1+|\eta_1(X)|)\\ &\leqslant \frac{\exp\left(-X\,\mathrm{Re}\left(\sqrt{-\Lambda-\varepsilon}+\sqrt{-\Lambda}\,\right)\right)}{\mathrm{Re}\left(\sqrt{-\Lambda-\varepsilon}+\sqrt{-\Lambda}\,\right)}\cdot\frac{1}{1-\alpha_X} =: M_X(\Lambda,\varepsilon). \end{aligned} \tag{3.13}$$

The integral over $[0, X]$ in the denominator in (3.10) must be estimated from below. Unlike the other integrals, this cannot be done with an explicit expression such as (3.13). The technique which is used to deal with this is as follows.

Observe that we have initial conditions at $x = X$ for both Y_2 and y_2:

$$Y_2(x,\Lambda) = \exp(-\sqrt{-\Lambda}X) \qquad Y_2'(x,\Lambda) = -\sqrt{-\Lambda}\exp(-\sqrt{-\Lambda}X)$$

and for y_2 we have the conditions (3.11), which can be regarded as 'interval valued' initial conditions since the parameters η_j are constrained by (3.12) to lie in bounded sets which we can compute in terms of q. Let $\tilde{y}_2(x,\Lambda,\varepsilon,\kappa_1,\kappa_2)$ be the solution of the differential equation

$$-\tilde{y}_2'' + q(x)\tilde{y}_2 = (\Lambda+\varepsilon)\tilde{y}_2 \qquad x\in[0,X] \tag{3.14}$$

satisfying the initial conditions

$$\begin{aligned}\tilde{y}_2(X,\Lambda,\varepsilon,\kappa_1,\kappa_2) &= \exp\left(-\sqrt{-\Lambda-\varepsilon}X\right)(1+\kappa_1)\\ \tilde{y}_2'(X,\Lambda,\varepsilon,\kappa_1,\kappa_2) &= -\sqrt{-\Lambda-\varepsilon}\exp\left(-\sqrt{-\Lambda-\varepsilon}X\right)(1+\kappa_2).\end{aligned}$$

For the estimate of (3.10) for $\Lambda\in\mathcal{R}$, $\varepsilon\in\mathcal{B}$ we need an enclosure of the set

$$I_X(\mathcal{R},\mathcal{B}) := \left\{\left|\int_0^X \tilde{y}_2(x,\Lambda,\varepsilon,\kappa_1,\kappa_2)Y_2(x,\Lambda)\,\mathrm{d}x\right| : \Lambda\in\mathcal{R},\varepsilon\in\mathcal{B},|\kappa_i|\leqslant\frac{\alpha_X}{1-\alpha_X}\right\}.$$

A numerical solver for ODEs based on interval arithmetic (such as VNODE [19] or AWA [15]) can recover guaranteed enclosing sets for the solutions at every $x\in[0,X]$ where the coefficients in the differential equations and the boundary conditions are interval valued; it can also compute simultaneously an enclosing set $\tilde{I}_X(\mathcal{R},\mathcal{B})\supset I_X(\mathcal{R},\mathcal{B})$.

Introducing the set

$$M_X(\mathcal{R},\mathcal{B}) := \{M_X(\Lambda,\varepsilon):\Lambda\in\mathcal{R},\varepsilon\in\mathcal{B}\}$$

which can be calculated explicitly ($M_X(\Lambda,\varepsilon)$ was defined in (3.13)), we finally get

$$|\Phi_\Lambda(\varepsilon)| \leqslant \frac{\max_{x\in[X,\infty)}|q(x)|\sup M_X(\mathcal{R},\mathcal{B})}{\inf\tilde{I}_X(\mathcal{R},\mathcal{B})-\sup M_X(\mathcal{R},\mathcal{B})} =: \delta_{X,\mathcal{R},\mathcal{B}} \qquad \Lambda\in\mathcal{R}\quad\varepsilon\in\mathcal{B} \tag{3.15}$$

which provides an enclosure $\mathcal{C}=\{z=\xi+\mathrm{i}\eta:|\xi|,|\eta|\leqslant\delta_{X,\mathcal{R},\mathcal{B}}\}$ for $\Phi_{\mathcal{R}}(\mathcal{B})$.

Altogether, if $\mathcal{R}$ contains an eigenvalue of the truncated problem (3.4), (3.5) and if $\mathcal{C}\subset\mathcal{B}$, then $\mathcal{R}+\mathcal{C}$ contains an eigenvalue of the original problem, see (3.9).

Remark 3.4. Note that the approximation to y_2 which is used to bound the denominator in (3.8) away from zero need not generally be particularly accurate. It is the numerator in (3.8), decreasing exponentially as a function of X, which generally plays the most important rôle in determining the eigenvalue error. In particular, the fact that the numerator is exponentially small as a function of X shows that the eigenvalue error will typically be much smaller than, say, the error in the computed value of $y_2(0,\lambda)$. This is why we do not try to obtain eigenvalue enclosures directly from computed enclosures for $y_2(0,\lambda)$.

3.2. Solving the truncated problem with guaranteed error bounds (step A)

For the purpose of numerical solution, we treat the approximating problem in the form (3.4), (3.5) rather than in the form (3.2), (3.3). In principle, the strategy is straightforward: let Y be the solution of (3.4) starting from the initial conditions $Y(X, \Lambda) = \exp(-\sqrt{-\Lambda}X)$, $Y'(X, \Lambda) = -\sqrt{-\Lambda}\exp(-\sqrt{-\Lambda}X)$, and let $f(\Lambda) := Y(0, \Lambda)$, $\Lambda \in \mathbb{C}$; now proceed as follows:

- The function f is analytic and the zeros of f are the eigenvalues of (3.2), (3.3). Find a box $\mathcal{R}$ guaranteed to contain a zero of f by using Rouché's theorem.
- For this, calculate the values of $f(\Lambda)$ solving the initial value problem for $Y(\cdot, \Lambda)$ starting from $x = X$ and integrating to $x = 0$, using an ODE solver capable of delivering a solution with guaranteed error bounds. We do this using the VNODE code of Nedialkov, which implements the ideas described by Nedialkov, Jackson and Pryce in [18, 19].

The second of these two steps is not different, in principle, from the approach in [7] for the self-adjoint case. We therefore examine how Rouché's theorem can be implemented numerically to give guaranteed error bounds, bearing in mind that the function f is known *numerically*, not *symbolically* as would normally be required for a guaranteed-error integration.

Suppose that an eigenvalue approximation Λ has been calculated, together with an error estimate or guess. One may then construct a rectangle $\mathcal{R}$ in the complex plane, containing Λ in its interior; one wishes to know whether or not $\mathcal{R}$ really contains an eigenvalue of the problem (3.4), (3.5). To this end, we employ the following lemma.

Lemma 3.5. *Let f be defined as above and $(\mu_j)_{j=0}^N$ be a sequence of points on $\partial\mathcal{R}$ with $\mu_N = \mu_0$ and containing the corners of $\mathcal{R}$, chosen so that for each $j = 1, \ldots, N$,*

$$\left|\arg\left(\frac{f([\mu_{j-1}, \mu_j])}{f(\mu_{j-1})}\right)\right| < \pi/2 \tag{3.16}$$

where by $f([\mu_{j-1}, \mu_j])$ we mean the image under f of the line segment from μ_{j-1} to μ_j, and by arg *we mean the argument such that* $\arg(z) \in (-\pi, \pi]$ *for $z \neq 0$. Then the number of eigenvalues of the problem* (3.4), (3.5) *in $\mathcal{R}$ equals*

$$\frac{1}{2\pi}\sum_{j=1}^{N}\arg\left(\frac{f(\mu_j)}{f(\mu_{j-1})}\right). \tag{3.17}$$

Proof. As f has no poles in $\mathcal{R}$, the number of eigenvalues in $\mathcal{R}$ is

$$\frac{1}{2\pi\mathrm{i}}\int_{\partial R}\frac{f'(z)}{f(z)}\,\mathrm{d}z.$$

Since the $(\mu_j)_{j=0}^N$ satisfy (3.16), they also satisfy

$$-\pi/2 < \arg\left(\frac{f(z)}{f(\mu_{j-1})}\right) < \pi/2 \qquad z \in [\mu_{j-1}, \mu_j] \quad j = 1, \ldots, N.$$

Thus $f(z)/f(\mu_{j-1})$ never crosses a cut-line of the argument function for $z \in [\mu_{j-1}, \mu_j]$, $j = 1, \ldots, N$, and so

$$\frac{1}{2\pi\mathrm{i}}\int_{\partial R}\frac{f'(z)}{f(z)}\,\mathrm{d}z = \frac{1}{2\pi}\sum_{j=1}^{N}\arg\left(\frac{f(\mu_j)}{f(\mu_{j-1})}\right).$$

This completes the proof. □

An interval enclosing the value of (3.17) can be evaluated from intervals enclosing the values of the $f(\mu_j)$, thus (3.17) can be dealt with purely numerically. If the enclosure is small

enough so that it contains only one integer, then the number of eigenvalues in $\mathcal{R}$ is known exactly.

The ability of the initial value code which computes $f(\cdot)$ to accept a complex interval valued parameter as an argument is vital for checking (3.16). The initial value code is able to accept the line segment $[\mu_{j-1}, \mu_j]$ as input in place of λ and to return a rectangle in the complex plane containing the set $f([\mu_{j-1}, \mu_j])$; thus, at least in principle, (3.16) is easy to check.

Remark 3.6. In practice, difficulties can arise if the eigenvalue is close to the boundary of the box $\mathcal{R}$, as it may then become extremely difficult to compute sets containing $f([\mu_{j-1}, \mu_j])$ which do not contain 0 at the same time. (Recall that $f(\lambda) = 0$ when λ is an eigenvalue.) If 0 is contained in any of these sets then condition (3.16) will immediately be violated. One can attempt to overcome these problems by

- choosing more points μ_j on $\partial\mathcal{R}$ to make the sets $f([\mu_{j-1}, \mu_j])$ smaller;
- choosing a bigger box $\mathcal{R}$ (but at the expense of a slacker bound on the eigenvalue error) so that ∂R is further from the eigenvalue, so that $\arg(f)$ does not vary so rapidly;
- tightening the tolerance in the numerical computation of $f([\mu_{j-1}, \mu_j])$ (at the expense of longer run-times).

For ill-conditioned problems, where f is very small over large regions, it may be numerically impossible to satisfy the conditions (3.16) with any reasonable choice of $\mathcal{R}$.

4. Description of the algorithm and numerical results

4.1. The algorithm

In this section we describe how the algorithm is implemented and present some numerical results with a discussion of the choice of the parameters. The following parameters are needed as input to the algorithm:

X	endpoint for the regular problem,
α_X	upper bound for $\int_X^\infty \lvert q(x)\rvert \,\mathrm{d}x$,
$\varepsilon_{\mathcal{B}}$	determining the (initial) set $\mathcal{B}$ by $\mathcal{B} = [-\varepsilon_{\mathcal{B}}, \varepsilon_{\mathcal{B}}] \times [-\varepsilon_{\mathcal{B}}, \varepsilon_{\mathcal{B}}]$,
ε_{Z}	desired precision for an eigenvalue box $\mathcal{R}$,
ε_{L}	lower bound for $\lvert\mu_j - \mu_{j-1}\rvert$, $j = 1, \ldots, N$, in remark 3.6,
E_a	absolute tolerance, see remark 4.1 below,
$\mathcal{R}_0$	box where eigenvalues are sought.

To get a good choice of a box $\mathcal{R}_0$, one can solve the eigenvalue problem using floating point arithmetic.

The algorithm consists of the following steps:

Step A. Find a small box $\mathcal{R}$ such that $\mathcal{R}$ contains an eigenvalue of the regular problem (3.4), (3.5). This is done with contour integration described in section 3.2.

1. Calculate the number of eigenvalues in $\mathcal{R}_0$ according to (3.17) in lemma 3.5. We consider this step failed if for the calculation of the contour integral along $\partial\mathcal{R}_0$ the condition $\lvert\mu_j - \mu_{j-1}\rvert \geqslant \varepsilon_{\mathrm{L}}$ is violated.
2. If step 1 did not fail and there are eigenvalues in $\mathcal{R}_0$, divide $\mathcal{R}_0$ into two boxes $\mathcal{R}_0'$ and $\mathcal{R}_0''$ (horizontally or vertically depending on which of width and height of $\mathcal{R}_0$ is greater) and apply step 1 to $\mathcal{R}_0 := \mathcal{R}_0'$ and $\mathcal{R}_0 := \mathcal{R}_0''$ respectively.

Continue until boxes are found which contain an eigenvalue of the problem (3.4, (3.5) and whose lengths are smaller than ε_Z.

Step B. Having determined a box $\mathcal{R}$ according to step A which is guaranteed to contain an eigenvalue of the truncated problem, check whether $\mathcal{R} + \mathcal{B}$ also contains an eigenvalue of the original problem:

1. Calculate the enclosure $\tilde{I}_X(\mathcal{R}, \mathcal{B})$ as described in subsection 3.1.2. To this end, solve simultaneously the differential equations for $Y_2(\cdot, \Lambda)$ and for $\tilde{y}_2(\cdot, \Lambda, \varepsilon, \kappa_1, \kappa_2)$ with interval valued Λ, ε and κ_i, and compute the integral $\int_0^X \tilde{y}_2(x, \Lambda, \varepsilon, \kappa_1, \kappa_2) Y_2(x, \Lambda)\,\mathrm{d}x$. The latter is achieved by introducing a new variable w with $w' = -\tilde{y}_2 Y_2$ and $w(X) = 0$ and then evaluating $w(0)$.
2. Compute $M_X(\mathcal{R}, \mathcal{B})$ and $\delta_{X,\mathcal{R},\mathcal{B}}$ in (3.15) and check whether $\delta_{X,\mathcal{R},\mathcal{B}} \leqslant \varepsilon_{\mathcal{B}}$. If yes, then $\mathcal{R} + \mathcal{C}$ contains an eigenvalue of the original problem (1.1), (1.2), where $\mathcal{C}$ is the box of the form $[-\delta_{X,\mathcal{R},\mathcal{B}}, \delta_{X,\mathcal{R},\mathcal{B}}] \times [-\delta_{X,\mathcal{R},\mathcal{B}}, \delta_{X,\mathcal{R},\mathcal{B}}]$.
3. If step 2 was successful, then set $\mathcal{B} := \mathcal{C}$ and restart with step 1.

If step 2 was successful at least once, then the box $\mathcal{R} + \mathcal{C}$ is guaranteed to contain an eigenvalue of the original problem (1.1), (1.2).

Remark 4.1. To integrate the IVPs we use the class `SOLVER_2` from the VNODE package. When using this validated solver for our purpose, the absolute tolerance E_a (see [18, section 3.4]) for the variable step size control turned out to be crucial. Smaller values for E_a result in a more accurate enclosure for the solution, thus making the contour integral in step A more unlikely to fail; however, this also rapidly increases the time needed for integration. We will see its effects in the examples in the next section.

4.2. Examples

In this final section we present three examples for problem (1.1), (1.2) with different potentials q. The first has been chosen to explain the performance of the algorithm in detail, the second one is a Squire problem and the third one is a resonance problem.

4.2.1. $q(x) = 10\mathrm{i}\,\mathrm{e}^{-x}$. This example is designed to demonstrate the strategy in finding enclosures, the effects of the various parameters listed above and the performance of the code in detail. Setting the parameters

$$X := 10 \quad \varepsilon_Z := 10^{-2} \quad \varepsilon_L := 10^{-20} \quad E_a := 10^{-12} \quad \mathcal{R}_0 := [0.1, 3] \times [0.1, 3]$$

our reference machine (2 GHz Pentium IV running Linux) took more than 11 min to produce the enclosure $\mathcal{R}_1 = 2.8^{1309}_{0742} + 2.1^{7305}_{6738}\,\mathrm{i}$ for an eigenvalue of the truncated problem[5]. Thus, in general it is a good idea to use floating point methods for getting a first guess on the location of the eigenvalues. Nevertheless, we use $\mathcal{R}_0 := \mathcal{R}_1$ now for further calculations. Fixing the remaining parameters and decreasing the desired precision ε_Z, the algorithm finally fails in subdividing the rectangle $\mathcal{R}_2 = 2.812267294^{690}_{351} + 2.17223816^{519}_{484}\,\mathrm{i}$ (starting from $\mathcal{R}_0 = \mathcal{R}_1$, this took about 3 min and 40 s). Using the upper bound $\alpha_X = 4.54 \times 10^{-4}$ and an initial $\varepsilon_{\mathcal{B}} = 10^{-5}$, step B of the algorithm yields $\mathcal{R}_2 + \mathcal{C}_2 = 2.812267^{380}_{209} + 2.172238^{250}_{080}\,\mathrm{i}$ as a rectangle containing an eigenvalue of the original problem. (In fact, step B was applied three times, and the diameters of the sets $\mathcal{C}$ obtained were bounded by $8.448463695 \times 10^{-8}$, $8.435722689 \times 10^{-8}$, $8.435722523 \times 10^{-8}$, so there was no significant improvement after the first application.)

[5] The notation 2.8^{1309}_{0742} indicates the interval [2.80742, 2.81309].

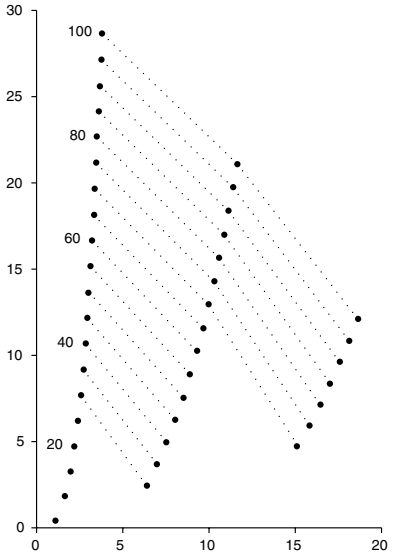

Figure 1. Eigenvalues for $q(x) = \mathrm{i}R \sin x \cdot \mathrm{e}^{-x}$, $R = 5, \ldots, 100$; dotted lines connect eigenvalues for the same R.

As stated in remark 4.1, a smaller value for E_a results in a better enclosure of eigenvalues in step A. But as we have seen above, the size of $\mathcal{C}_2$ is also rather large, so that an enlargement of the truncation interval seems appropriate. Indeed restarting the process with $\mathcal{R}_0 := \mathcal{R}_1$, $X = 11$, $\alpha_X = 6.2 \times 10^{-5}$ and $E_a := 10^{-30}$ yields the following slightly better result after about 33 min:

$$\mathcal{R}_3 = 2.81226729019^{81}_{73} + 2.172238188857^{94}_{27}\mathrm{i} \qquad \mathcal{R}_3 + \mathcal{C}_3 = 2.8122672^{92}_{89} + 2.17223818^{99}_{78}\mathrm{i}.$$

4.2.2. $q(x) = \mathrm{i}R \sin x \cdot \mathrm{e}^{-x}$. Proceeding as in the previous example, we calculated enclosures for the eigenvalues of the following (Squire's) problem

$$-y''(x) + \mathrm{i}R \sin x \cdot \mathrm{e}^{-x} y(x) = \lambda y(x) \qquad x \in [0, \infty) \tag{4.1}$$

for Reynolds numbers $R = 5, 10, \ldots, 100$, truncating at $X = 10$ in most cases. The results are shown in table 1 and figure 1. It seems that with growing Reynolds number R, more eigenvalues emerge from the essential spectrum $[0, \infty)$.

4.2.3. $q(x) = x^2 \exp(-\mathrm{e}^{\mathrm{i}\theta}\, 0.2x^2)$. Finally we considered resonances of the problem

$$(Ly)(x) := -y''(x) + x^2\, \mathrm{e}^{-0.2x^2} y(x) = \lambda y(x) \qquad x \in [0, \infty) \tag{4.2}$$

with $y(0) = 0$ using the complex scaling method, see [2, section 5]. This operator describes quantum particles trapped by a rotationally invariant barrier through which they may tunnel and escape to infinity. Let $\theta \in (0, \pi/2)$. With the formal transformation $(U_\theta y)(x) = \mathrm{e}^{\mathrm{i}\theta/2} y(\mathrm{e}^{\mathrm{i}\theta} x)$, the resonances of (4.2) are $\mathrm{e}^{-\mathrm{i}\theta}$ times the eigenvalues of the operator

$$(Ty)(x) := (U_\theta L U_\theta^{-1} y)(x) = -y''(x) + x^2 \exp(-\mathrm{e}^{\mathrm{i}\theta}\, 0.2x^2) y(x).$$

Using $\theta = 1.5$ and $X = 33$, we have found enclosures for seven resonances, which are listed in table 2; see also figure 2. The first resonance has been calculated in [2] using floating point arithmetic.

Table 1. Eigenvalues for the potential $q(x) = \mathrm{i}R\sin x \cdot \mathrm{e}^{-x}$ for $R = 5, 10, \ldots, 100$.

R	Box enclosing the eigenvalue	Error
5	$1.081984^{82}_{78} + 0.4270356^{90}_{59}\mathrm{i}$	3×10^{-8}
10	$1.6043912^{58}_{44} + 1.7978849^{81}_{67}\mathrm{i}$	2×10^{-8}
15	$1.943126968^{96}_{86} + 3.242375016^{54}_{44}\mathrm{i}$	1×10^{-10}
20	$2.19343181^{62}_{46} + 4.7140110538^{91}_{15}\mathrm{i}$	2×10^{-10}
25	$2.391580548^{89}_{28} + 6.19801886^{54}_{49}\mathrm{i}$	6×10^{-10}
30	$2.55564161^{35}_{19} + 7.688187018^{19}_{03}\mathrm{i}$	2×10^{-10}
	$6.37465^{91}_{12} + 2.4699^{55}_{46}\mathrm{i}$	8×10^{-6}
35	$2.696015918^{86}_{70} + 9.18152057^{84}_{76}\mathrm{i}$	2×10^{-10}
	$6.98512^{92}_{88} + 3.7034^{31}_{29}\mathrm{i}$	3×10^{-7}
40	$2.81926355^{96}_{83} + 10.67646671^{42}_{35}\mathrm{i}$	2×10^{-9}
	$7.531816^{95}_{89} + 4.9742698^{72}_{24}\mathrm{i}$	5×10^{-8}
45	$2.92979131^{92}_{62} + 12.17219564^{81}_{20}\mathrm{i}$	6×10^{-10}
	$8.02685004^{74}_{44} + 6.26662694^{96}_{42}\mathrm{i}$	6×10^{-9}
50	$3.030698508^{63}_{32} + 13.668268663^{89}_{28}\mathrm{i}$	6×10^{-10}
	$8.4791425^{81}_{75} + 7.5756725^{63}_{59}\mathrm{i}$	5×10^{-9}
55	$3.12424177^{60}_{29} + 15.164470189^{81}_{51}\mathrm{i}$	3×10^{-10}
	$8.89546381^{96}_{71} + 8.89787246^{95}_{70}\mathrm{i}$	3×10^{-9}
60	$3.212108659^{75}_{44} + 16.660716631^{27}_{11}\mathrm{i}$	3×10^{-10}
	$9.2810938^{74}_{64} + 10.2305645^{61}_{56}\mathrm{i}$	10^{-8}
65	$3.29558777^{52}_{45} + 18.157004321^{82}_{21}\mathrm{i}$	6×10^{-10}
	$9.64024408^{82}_{34} + 11.5716966^{63}_{58}\mathrm{i}$	5×10^{-9}
70	$3.37567926^{53}_{46} + 19.65337845^{75}_{68}\mathrm{i}$	6×10^{-10}
	$9.9763374^{33}_{13} + 12.9196564^{30}_{19}\mathrm{i}$	2×10^{-8}
	$15.16037^{63}_{56} + 4.738191^{88}_{24}\mathrm{i}$	7×10^{-7}
75	$3.453169233^{51}_{20} + 21.14991393^{21}_{14}\mathrm{i}$	6×10^{-10}
	$10.2922015^{91}_{85} + 14.27315692^{43}_{18}\mathrm{i}$	5×10^{-9}
	$15.81043^{75}_{47} + 5.93413^{74}_{47}\mathrm{i}$	3×10^{-6}
80	$3.528681406^{98}_{37} + 22.64670317^{95}_{88}\mathrm{i}$	6×10^{-10}
	$10.5902058^{80}_{41} + 15.631157^{42}_{37}\mathrm{i}$	4×10^{-8}
	$16.42798^{36}_{29} + 7.144672^{97}_{43}\mathrm{i}$	6×10^{-7}
85	$3.60271395^{75}_{68} + 24.14384827^{62}_{49}\mathrm{i}$	2×10^{-9}
	$10.872360^{31}_{28} + 16.992806^{92}_{89}\mathrm{i}$	2×10^{-8}
	$17.01603^{71}_{63} + 8.36800^{54}_{41}\mathrm{i}$	2×10^{-6}
90	$3.67566634^{96}_{89} + 25.64145570^{94}_{87}\mathrm{i}$	6×10^{-10}
	$11.1403893^{12}_{08} + 18.3574034^{12}_{07}\mathrm{i}$	5×10^{-9}
	$17.57719^{61}_{54} + 9.60261^{36}_{29}\mathrm{i}$	7×10^{-7}
95	$3.7478593^{12}_{08} + 27.13963285^{69}_{44}\mathrm{i}$	3×10^{-9}
	$11.3957869^{53}_{43} + 19.7243635^{75}_{65}\mathrm{i}$	10^{-8}
	$18.113718^{51}_{24} + 10.847200^{47}_{31}\mathrm{i}$	3×10^{-7}
100	$3.81954995^{22}_{15} + 28.63848557^{24}_{11}\mathrm{i}$	2×10^{-9}
	$11.639859^{41}_{39} + 21.0931999^{78}_{68}\mathrm{i}$	10^{-8}
	$18.62757^{82}_{78} + 12.10064^{73}_{69}\mathrm{i}$	4×10^{-7}

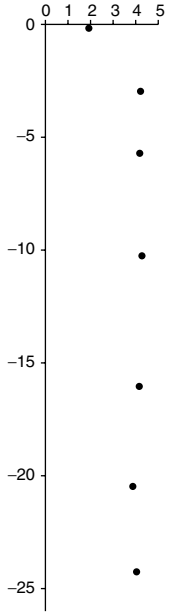

Figure 2. Resonances for the potential $q(x) = x^2\,\mathrm{e}^{-0.2x^2}$.

Table 2. Resonances for $q(x) = x^2\,\mathrm{e}^{-0.2x^2}$.

Box $\mathcal{R} + \mathcal{C}$ enclosing the resonance	Bound for the error
$2.028256180{74}^{22}_{15} - 0.2499499460{6}^{32}_{25}\mathrm{i}$	7×10^{-13}
$3.27512973359^{97}_{71} - 2.47261836482^{73}_{47}\mathrm{i}$	3×10^{-12}
$3.9740981036^{35}_{14} - 6.1009927234^{37}_{20}\mathrm{i}$	2×10^{-11}
$4.0714200408^{63}_{57} - 10.6443394965{1}^{67}_{14}\mathrm{i}$	6×10^{-12}
$3.9527029180^{17}_{08} - 16.4309490422^{27}_{13}\mathrm{i}$	2×10^{-11}
$3.6673855{1}^{54}_{45} - 20.8630054731^{74}_{03}\mathrm{i}$	9×10^{-11}
$3.8343858{1}^{11}_{08} - 24.64757551{4}^{31}_{11}\mathrm{i}$	2×10^{-10}

Acknowledgments

This work was supported by The British Council and Deutscher Akademischer Austauschdienst, DAAD, under the British–German Academic Research Collaboration, ARC. The second author acknowledges the support of the British Engineering and Physical Sciences Research Council, EPSRC, grant no GR/R40753.

Appendix. Introduction to interval arithmetic and initial value problem enclosure algorithms

In this appendix we give a brief overview of the concepts of interval arithmetic that are needed in this work together with a short account of interval based initial value problem solvers.

All computer realizations of algorithms consist of finitely many instances of the four basic operations of arithmetic. When these are applied to real numbers, modelled in a finite number

of bits, rounding errors can occur. Interval arithmetic seeks to provide safe upper and lower bounds on a calculation which take these into account. A simple minded implementation of this concept would lead to an explosion in the interval width and many sophisticated techniques are available to control this problem [3].

An interval based initial value problem (IVP) solver is a computer program that, given an ODE with symbolically defined coefficients and intervals in which numerical parameter values lie, together with a value x of the independent variable at which the solution is required, returns a u-interval which is an enclosure of the solution value $u(x)$. It uses the arithmetic operations described above to perform the calculations and also uses algorithms that take account of the other approximation errors which must also contribute to the width of the final enclosure.

More specifically, suppose that the ODE is the IVP

$$u' = f(x, u) \qquad u(0) = u_0 \tag{A.1}$$

where $f\colon [0, \infty) \times \mathbb{R}^n \to \mathbb{R}^n$ is sufficiently smooth. An approach to enclose the solution of the IVP uses a polynomial to model the solution in the x-interval $[x_0, x_0 + h]$ together with some truncation error $\varepsilon(x_0, h)$. The error term is usually not known exactly but often fixed-point arguments implemented in interval arithmetic are used to obtain interval valued upper and lower bounds for this error term. It is often the case that in order to implement this approach and get tight enclosures, a high degree polynomial needs to be used. This means that the coefficient function in the IVP must be differentiable a suitable number of times. The coefficients are specified in a symbolic form to the program and an automatic differentiation package is used to calculate the required derivatives, without the need of a symbolic algebra system. In any given implementation much effort is expended to ensure that the interval enclosures are as tight as possible. We refer the reader to [16, 19] for details of actual implementations. Lohner [16] reports on a work where a Taylor polynomial is used to approximate the solution while the method chosen in [19] is an Obrechkoff method and is therefore based on Padé approximants.

References

[1] Abramov A A, Aslanyan A and Davies E B 2001 Bounds on complex eigenvalues and resonances *J. Phys. A: Math. Gen.* **34** 57–72

[2] Aslanyan A and Davies E B 2000 Spectral instability for some Schrödinger operators *Numer. Math.* **85** 525–52

[3] Alefeld G and Herzberger J 1983 *Introduction to Interval Computations* (New York: Academic)

[4] Bailey P B, Garbow B S, Kaper H G and Zettl A 1991 A FORTRAN software package for Sturm–Liouville problems *ACM Trans. Math. Softw.* **17** 500–1

Bailey P B, Garbow B S, Kaper H G and Zettl A 1991 Eigenvalue and eigenfunction computations for Sturm–Liouville problems *ACM Trans. Math. Softw.* **17** 491–9

[5] Brown B M, Eastham M S P, McCormack D K R and Evans W D 1997 Approximate diagonalization in differential systems and an effective algorithm for the computation of the spectral matrix *Math. Proc. Comb. Phil. Soc.* **121** 495–517

[6] Brown B M, Eastham M S P, Evans W D and Kirby V G 1994 Repeated diagonalization and the numerical computation of the Titchmarsh–Weyl $m(\lambda)$-function *Proc. R. Soc.* A **445** 113–26

[7] Brown B M, McCormack D K R and Marletta M 2000 Guaranteed error bounds for eigenvalues of singular Sturm–Liouville problems *Math. Nachr.* **213** 17–33

[8] Brown B M, McCormack D K R, Evans W D and Plum M 1999 On the spectrum of second-order differential operators with complex coefficients *Proc. R. Soc.* A **455** 1235–57

[9] Davies E B 1999 Pseudo-spectra, the harmonic oscillator and complex resonances *Proc. R. Soc.* A **455** 585–99

[10] Eastham M S P 1989 *The Asymptotic Solution of Linear Differential Systems: Applications of the Levinson Theorem (LMS Monographs, New Series 4)* (Oxford: Oxford Science Publications/Clarendon)

[11] Edmunds E E and Evans W D 1987 *Spectral Theory and Differential Operators* (New York: Clarendon/Oxford University Press)

[12] Fulton C T and Pruess S 1993 Mathematical software for Sturm–Liouville problems *ACM Trans. Math. Softw.* **19** 360–76

[13] Greenberg L and Marletta M 2001 Numerical solution of non-selfadjoint Sturm–Liouville problems and related systems *SIAM J. Numer. Anal.* **38** 1800–45

[14] Levinson N 1948 The asymptotic nature of solutions of linear systems of differential equations *Duke Math. J.* **15** 111–26

[15] Lohner R J 1987 Enclosing the solutions of ordinary initial and boundary value problems *Computer Arithmetic: Scientific Computation and Programming Languages (Wiley-Teubner Series in Computer Science)* ed E W Kaucher, U W Kulisch and C Ullrich (Stuttgart: Wiley-Teubner)

[16] Lohner R 1988 Einschließung der Lösung gewöhnlicher Anfangs- und Randwertaufgaben und Anwendungen *PhD Thesis* Universität Karlsruhe

[17] Marletta M and Pryce J D 1992 Automatic solution of Sturm–Liouville problems using the Pruess method *J. Comp. Appl. Math.* **39** 57–78

[18] Nedialkov N S and Jackson K R 2001 The design and implementation of an object-oriented validated ODE solver *Numerical Analysis Technical Reports of the Department of Computer Science at the University of Toronto* webpage http://www.cs.toronto.edu/NA/reports.html#ned.software.01

[19] Nedialkov N S, Jackson K R and Pryce J D 2001 An effective high-order interval method for validating existence and uniqueness of the solution of an IVP for an ODE *Reliab. Comput.* **7** 449–65

[20] Pavlov B S 1975 Conditions for separation of the spectral components of a dissipative operator (Russian) *Math. USSR Izv.* **9** 113–37

[21] Sims A R 1957 Secondary conditions for linear differential operators of the second order *J. Math. Mech.* **6** 247–85

[22] Weyl H 1910 Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen *Math. Ann.* **68** 220–69