# On a computer assisted proof of eigenvalues below the essential spectrum of the Sturm-Liouville problem

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## 1 Introduction

This paper is a follow up of [3]. In [3] the authors presented a new method for proving the existence of an eigenvalue below the essential spectrum of Sturm-Liouville operators defined by

$$-y^{''} + qy = \lambda y, \text{ on J} = [0, \infty), \text{ y}(0) = 0, \tag{1}$$

where $q$ is a real $L^1(0, \infty)$ perturbation of a real-valued periodic function on $J$. This method combines operator theory and "standard" numerical analysis with interval analysis and interval arithmetic, and is illustrated by showing that there is at least one eigenvalue for

$$q(x) = \sin(x + \frac{1}{1 + x^2}) \tag{2}$$

which lies below the essential spectrum.

In this paper we extend and develop further the notions in [3] to cover additional classes of problems. In Section 2 we introduce the relevant notation and review the approach taken in [3]. In Section 3 we show how some of the restrictions required by the approach in [3] may be removed enabling us to prove the existence of several eigenvalues below the essential spectrum of (1). For completeness we include in Section 3 a short review of the interval analytic background that is relevant to our work. Section 4 contains examples, some of which are of physical interest, which illustrate our method.

## 2 Mathematical formulation of the method

Of particular interest are the two cases (i) $q \in L^1(0, \infty)$ or (ii) $q$ is an $L^1(0, \infty)$ perturbation of a periodic function $p$ with fundamental periodic interval $[a, b]$. It is well known that in both cases $q$ is in the limit-point case at infinity and that therefore (1) determines a unique self-adjoint operator $S$ in $L^2[0, \infty)$ with domain

$$\{y \in L^2(0,\infty) : y, y' \in \mathrm{AC_{loc}}[0,\infty),\ -y'' + qy \in L^2(0,\infty),\ y(0) = 0\}.$$

For both cases (i) and (ii) the potential $q$ ensures that $S$ has an essential spectrum $\sigma_e(q)$, bounded below and extending to infinity. Indeed in case (i), $\sigma_e(q)$ occupies the nonnegative real axis, while for case (ii) it is known that $\sigma_e(q) = \sigma_e(p)$ and $\sigma_e(q)$ lies in bands, bounded below and extending to infinity. We denote by $\sigma(q)$ the spectrum of $S$ and write

$$\sigma_0(q) = \inf \sigma_e(q).$$

In order to describe our approach to proving the existence of eigenvalues $\lambda_n$ below the essential spectrum of the operator $S$ we introduce the following notation. Denote by $\lambda_j^N([a,b],q)$, $\lambda_j^D([a,b],q)$, $\lambda_j^P([a,b],q)$, $(0 \le j \le k-1)$ the first $k$ Neumann, Dirichlet and periodic eigenvalues respectively, of the regular Sturm-Liouville problems (SLP) consisting of the left-hand side of (1) together with either Neumann $y'(a) = 0 = y'(b)$, Dirichlet $y(a) = 0 = y(b)$ or periodic $y(a) = y(b)$, $y'(a) = y'(b)$ boundary conditions.

The well-known inequality

$$\lambda_0^N([a,b],q) \le \lambda_0^P([a,b],q) < \lambda_0^D([a,b],q) < \lambda_1^P([a,b],q) \tag{3}$$

may be found in [11, Theorem 13.10, pages 209-212].

Our proof of the existence of eigenvalues below the essential spectrum depends on the following

**Theorem 2.1** *(Bailey, Everitt, Weidmann, Zettl) If*

$$\lambda_j^D([0,b],q) < \sigma_0(q) \tag{4}$$

*for some* $b$, $0 < b < \infty$, *and some* $j = 0, 1, 2, \ldots$, *then* $S$ *has at least* $j+1$ *eigenvalues* $< \sigma_0(q)$.

**Proof** See [2].

Our approach to proving the existence of $j$ eigenvalues below $\sigma_0(q)$ is first to compute a verified lower bound $l$ for $\sigma_0(q)$ and a verified upper bound $u$ for $\lambda_j^D([0,b],q)$ such that

$$u < l$$

for some $b$ and some $j$. Note that $\lambda_j^D([0,b],q)$ is a decreasing function of $b$ and, by [2], $\lambda_j^D([0,b],q) \to \lambda_j < \sigma_0$ implies that $\lambda_j \in \sigma(S)$.

In [3] we dealt with the case when $q$ is an $L^1(0,\infty)$ perturbation of a periodic potential $p$. Here it follows that $\sigma_e(p) = \sigma_e(q)$ and further from the Flochet theory [8], [11] that $\inf \sigma_e(p) = \lambda_0^P([a,b],p)$. Thus it follows from (3) that we can take $l = \lambda_0^N([a,b],p)$. We remark that when $q \in L^1(0,\infty)$, $\sigma_0(q) = 0$ we can take $l = 0$.

In [3] we illustrated the above method by taking $q(x) = \sin(x + \frac{1}{1+x^2})$. This is an $L^1(0,\infty)$ perturbation of $\sin(x)$ and since the essential spectrum is invariant under a unitary map $\sigma_e(\sin) = \sigma_e(\cos)$. It follows then that we can take $l = \lambda_0^N([0,2\pi],\cos)$. We remark that for this problem, since cos is an even function that $\lambda_0^N([0,2\pi],\cos) = \lambda_0^P([0,2\pi],\cos)$ giving in this example the optimal value for $l$. However we can not hope for this to occur in more general examples.

In this paper we turn to wider considerations and address the problem of computing several eigenvalues below $\sigma_e(q)$ both when $q \in L^1(0,\infty)$ and when $q$ is an $L^1(0,\infty)$ perturbation of a periodic potential $p$. It is clear that in both of these classes of example the method that we have outlined above has two principal components to proving the existence of $\lambda_j < \sigma_e(q)$, $j \geq 0$ viz:

1. finding a lower bound $l$ for $\sigma_e(q)$;
2. finding an upper bound $u$ for $\lambda_j$ satisfying $u < l$.

We discuss a new method to achieve this in the next subsection.

## 2.1 A new algorithm to prove the existence of eigenvalues below $\sigma_0$.

Upper bounds for eigenvalues of $S$ may be obtained from the BEWZ approximation [2]. This shows that for operators $S$ with $k$ eigenvalues below $\sigma_0(q)$ and any $X < \infty$ that

$$\lambda_j^D([0,X],q) \to \lambda_j([0,\infty],q), \quad (0 \leq j \leq k-1)$$
$$\lambda_j^D([0,X],q) \to \sigma_e(q) \quad (k \leq j)$$

the convergence being from above.

As we remarked above when $q \in L^1(0,\infty)$ we have $\sigma_0(q) = 0$ and so in this case the problem of determining a lower bound for the number of eigenvalues below the essential spectrum is to find an integer $j$ such that

$$\lambda_j^D([0,X],q) < 0.$$

When $q$ is an $L^1(0,\infty)$ perturbation of $p$ our previous method used $\lambda_0^N([a,b],p)$ as a lower bound for $\sigma_0(q)$. This has the disadvantage that eigenvalues $\lambda_j([0,\infty],q)$ with

$$\lambda_0^N([a,b],p) \leq \lambda_j([0,\infty),q) < \sigma_0(q)$$

fail to be detected. In this paper we use a lower bound for $\sigma_0(q)$ which is better than $\lambda_0^N([a,b],p)$ and thus are able to find eigenvalues of $S$ satisfying (2.1).

We first introduce some notation. Assume $q$ is an $L^1(a,\infty)$ perturbation of a periodic function $p$ with fundamental periodic interval $[a,b]$. Let $\phi_1(x,\lambda)$ be the solution of

$$-y'' + qy = \lambda y$$

on $[a,b]$ determined by the initial conditions $y(a) = 0,\ y'(a) = 1$ and let $\phi_2(x,\lambda)$ be the solution determined by $y(a) = 1,\ y'(a) = 0$. Let

$$\begin{aligned} \Phi_1(\lambda) &= \phi_1(b,\lambda), \\ \Phi_2(\lambda) &= \phi_2(b,\lambda), \end{aligned}$$

with a similar notation for the derivatives. Then defining

$$D(\lambda) = \Phi_1(\lambda) + \Phi_2'(\lambda) \tag{5}$$

it follows from Flochet theory that the periodic eigenvalues $\lambda_n^P([a,b],p)$ are the roots of the equation

$$D(\lambda) = 2. \tag{6}$$

Our method of obtaining, in some sense an optimal interval enclosure for $\sigma_0(q)$, is to obtain an enclosure $[\mu]$ for the solution $\mu$ of (6) such that

$$[\lambda_0^N([a,b],p)] < [\mu] < [\lambda_0^D([a,b],p)]. \tag{7}$$

Any verified computation of the above inequality, in view of (3), will exclude all enclosures for the higher periodic eigenvalues. Our algorithm for establishing (7) is to first use SLEIGN2, a "standard numerical analysis" Sturm-Liouville eigenvalue solver to obtain numerical estimates for both $\lambda_0^N([a,b],p)$ and $\lambda_0^D([a,X],q)$. We then use the algorithm and code reported on in [7] to obtain enclosures of these numerical estimates. Next SLEIGN2 is used to find both a numerical approximation of $\lambda_0^P([a,b],p)$ and some $\epsilon$ determined by the error tolerance returned by SLEIGN2. Again the methods of [7] are used to verify that the interval $[\lambda_0^P([a,b],p) - \epsilon, \lambda_0^P([a,b],p) + \epsilon]$ contains $\lambda_0^P([a,b],p)$. This is achieved by computing enclosures for both of

$$D(\lambda_0^P([a,b],p) \pm \epsilon) - 2.$$

Provided these enclosures are of different sign, since $D(\lambda)$ is continuous, this establishes the result. Higher eigenvalues $\lambda_j$ are found similarly.

# 3 Short introduction to interval arithmetic and the AWA algorithm

In this section we give a brief overview of the concepts of interval arithmetic that are need in this work together with both a short account of Lohner's AWA algorithm and an algorithm to enclose eigenvalues. A fuller discussion of these relevant concepts may be found in [3]. An in-depth discussion of interval arithmetic, can be found in [1], Lohner's AWA algorithm is discussed in [9] and [6] and the enclosure algorithm for eigenvalues can be found in [7].

All computer realisations of algorithms consist of finitely many instances of the four basic operations of arithmetic. When these are applied to real numbers, modeled 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 [1].

Most algorithms involve other approximation errors which must also contribute to the final enclosure. An example of this is the numerical solution of an initial value problem (IVP)

$$u^{'} = f(x,u), \quad u(0) = u_0, \tag{8}$$

where $f : [0,\infty) \times R^n \to R^n$ is sufficiently smooth. In addition we shall assume that a solution is known at $x = x_0$. The approach developed by Lohner to enclose the solution of the IVP uses the Taylor method to determine the solution at $x_0 + h$ from its known value at $x_0$ *viz.*

$$u(x_0 + h) = u(x_0) + h\phi(x_0, h) + z_{x_0+h} \tag{9}$$

where $u(x_0) + h\phi(x_0, h)$ is the $(r-1)-th$ degree Taylor polynomial of $u$ expanded about $x_0$ and $z_{x_0+h}$ is the associated local error. The error term is not known exactly since the standard formula give, for some unknown $\tau$,

$$z_{x_0+h} = u^{(r)}(\tau)h^r/r!, \quad \tau \in [x_0, x_0 + h]. \tag{10}$$

Lohner's algorithm uses Banach's fixed-point theorem to compute in interval arithmetic a bound for this error term. We refer the reader to [9] and [6] for a complete discussion of the method.

The enclosures for the eigenvalues that we need are computed using the methods reported on in [7]. Briefly, the equation (1) together with the Prüfer transformation

$$y = \rho \sin\theta, \quad y^{'} = \rho\cos\theta \tag{11}$$

yields

$$\frac{d\theta}{dx} = (\lambda - q(x))\sin^2\theta + \cos^2\theta \tag{12}$$

with initial condition $\theta(0;\lambda) = \theta(0) = \alpha \in [0, \pi)$ where $\tan\alpha = a_2/a_1$, $(a_1 \neq 0)$ and $\alpha = \pi/2$ otherwise. Standard results in the spectral theory of SLP allow us to classify the $n-th$ eigenvalue of the SLP, starting counting at $n = 0$, with the stated separated boundary conditions as that unique $\lambda$ which is such that the equation (12) has a solution $\theta$ with

$$\theta(0, \lambda) = \alpha, \quad \theta(b, \lambda) = \beta + n\pi, \quad \beta \in (0, \pi],$$

where $\tan\beta = b_2/b_1$, $(b_1 \neq 0)$ and $\beta = \pi/2$ otherwise. However it is numerically more convenient to work with a pair of initial value problems for $\theta_L$ and $\theta_R$ defined by (12). The solutions $\theta_L(x,\lambda)$ and $\theta_R(x,\lambda)$ satisfy the initial conditions (13) and (14) respectively:

$$\theta_L(0) = \alpha, \tag{13}$$

$$\theta_R(b) = \beta + n\pi. \tag{14}$$

We next choose a point $c$, with $0 < c < b$ and define the miss-match distance

$$D(\lambda) \equiv \theta_L(c,\lambda) - \theta_R(c,\lambda). \tag{15}$$

The $n-th$ eigenvalue is the unique value $\lambda_n$ with $D(\lambda_n) = 0$. By continuity we have for $\mu_1 < \mu_2$ that if $\text{sign}D(\mu_1) = -\text{sign}D(\mu_2)$ then $\lambda_n \in [\mu_1, \mu_2]$. By sign $D(\mu)$ we mean the sign of any member of the interval $D(\mu)$. This is defined only when all members of $D(\mu)$ have the same sign.

Our algorithm for enclosing the $n^{th}$ eigenvalue $\lambda_n$ proceeds as follows:

**Algorithm 3.1** *1. Obtain an estimate, $\hat{\lambda}_n$, for $\lambda_n$ with a "standard" numerical Sturm-Liouville solver together with an error estimate $\epsilon$, (we use SLEIGN2 for this);*

*2. Form the quantities*

$$\mu_1 = \hat{\lambda}_n - \epsilon, \quad \mu_2 = \hat{\lambda}_n + \epsilon.$$

*3. Use the AWA algorithm to compute*

$$D(\mu_1), \quad D(\mu_2).$$

*4. If (the interval) $signD(\mu_1) = -signD(\mu_2)$ then $\lambda_n \in [\mu_1, \mu_2]$ otherwise increase $\epsilon$ and recompute $D(\mu_j),\ j = 1, 2$.*

# 4 Numerical Examples

In this section we show how the theory and algorithms that we have developed in this paper may be applied to prove results about eigenvalues below the essential spectrum of a number of Sturm-Liouville problems.

## 4.1 $q \in L^1(0, \infty)$

We commence by proving the existence of several eigenvalues below the essential spectrum for a number of problems with $q \in L^1(0, \infty)$.

### 4.1.1 $q(x) = -c \exp(-x/4) \cos(x)$

Here we take $q(x) = -c \exp(-x/4) \cos(x)$ where $c$ is some positive constant. This example has been discussed by Brown et al in [4] in relation to problems of spectral concentration. Since $\sigma_0(q) = 0$ we take $l = 0$ and obtain a lower bound on the number of negative eigenvalues. In table 1 below we give for different values of $c$ the largest eigenvalue together with its index, that we have been able to compute using SLEIGN2. We also give the enclose for it obtained by our method.

| c | eigenvalue index | eigenvalue | enclosure |
|---|---|---|---|
| 26 | 4 | −0.453059 | $[-0.4530^{5}_{6}]$ |
| 19 | 3 | −0.098782 | $[-0.098^{7}_{8}]$ |
| 16 | 2 | −0.181076 | $[-0.18^{1}_{2}]$ |
| 5 | 1 | −0.215400 | $[-0.21^{5}_{6}]$ |
| 4 | 0 | −0.264342 | $[-0.26^{4}_{5}]$ |
| 1.31 | 0 | −0.000451 | $[-0.00045^{1}_{2}]$ |

Table 1: Eigenvalues below the essential spectrum for $q(x) = -c \exp(-x/4) \cos(x)$

### 4.1.2 $q(x) = -c \exp(-x^2)$

For $c = 1$ this example has been discussed in connection with resonances by Siedentop [10] and Brown et al [5]. Again $\sigma_0(q) = 0 = l$ and we find a lower bound for the number of negative eigenvalues. The results are contained in table 2 below.

| c | eigenvalue index | eigenvalue | enclosure |
|---|---|---|---|
| 50 | 2 | $-0.232229$ | $[-0.23_3^2]$ |
| 40 | 1 | $-6.214214$ | $[-6.21_5^3]$ |
| 20 | 1 | $-0.122240$ | $[-0.12_3^2]$ |
| 10 | 0 | $-2.543410$ | $[-2.54_1^3]$ |
| 2.85 | 0 | $-0.000375$ | $[-0.0003_8^7]$ |

Table 2: Eigenvalues below essential spectrum for $q(x) = -c\exp(-x^2)$

## 4.2 Periodic potentials

The examples given here illustrate the power of the methods of this paper to establish the existence of eigenvalues below $\sigma_0(p)$. which we could not reach in [3].

### 4.2.1 $q(x) = c\sin(x + \frac{1}{1+x^2})$

The lowest point of the essential spectrum is $\sigma_0 = \lambda_0^P([0, 2\pi], \sin(x))$. In table 3 we give enclosures for $\lambda_0^N([0, 2\pi], \sin)$, $\lambda_0^P([0, 2\pi], \sin)$ and $\lambda_0^D([0, 2\pi], \sin)$ for a selection of differing values of $c$ while in table 4 we give numerical estimates, obtained from SLEIGN2, together with the highest eigenvalue index that we are able to determine and enclosures for the eigenvalues. Thus we see that when $c = 8$ there are at least 3 eigenvalues below $\sigma_0$. We remark that since

$$[\lambda_2^D([0, 20], 8\sin(x + 1/(1 + x^2)))] > [\lambda_0^N([0, 2\pi], 8\sin(x))]$$

(see table 3 and table 4) this result could not have been obtained using the methods of [3].

| c | quantity | eigenvalue | enclosure $\lambda_2([0,20],\sin(x+1/(1+x^2)))$ |
|---|---|---|---|
| 1 | $\lambda_0^N([0,2\pi],\sin)$ | $-0.53370249$ | $[-0.53370_3^2]$ |
| | $\lambda_0^P([0,2\pi],\sin)$ | $-0.378489$ | $[-0.3784_{90}^{89}]$ |
| | $\lambda_0^D([0,2\pi],\sin)$ | $-0.18339010$ | $[-0.1833_{90}^{89}]$ |
| 2 | $\lambda_0^N([0,2\pi],\sin)$ | $-1.23567617$ | $[-1.23567_7^6]$ |
| | $\lambda_0^P([0,2\pi],\sin)$ | $-1.0701309$ | $[-1.0701_3^2]$ |
| | $\lambda_0^D([0,2\pi],\sin)$ | $-0.92090643$ | $[-0.92090_4^3]$ |
| 4 | $\lambda_0^N([0,2\pi],\sin)$ | $-2.77020288$ | $[-2.77020_3^2]$ |
| | $\lambda_0^P([0,2\pi],\sin)$ | $-2.6516838$ | $[-2.651682_5^0]$ |
| | $\lambda_0^D([0,2\pi],\sin)$ | $-2.55827832$ | $[-2.55827_8^6]$ |
| 6 | $\lambda_0^N([0,2\pi],\sin)$ | $-4.41135359$ | $[-4.41135_4^3]$ |
| | $\lambda_0^P([0,2\pi],\sin)$ | $-4.3330181$ | $[-4.333016_6^5]$ |
| | $\lambda_0^D([0,2\pi],\sin)$ | $-4.27201653$ | $[-4.27201_7^6]$ |
| 8 | $\lambda_0^N([0,2\pi],\sin)$ | $-6.11676788$ | $[-6.11676_8^7]$ |
| | $\lambda_0^P([0,2\pi],\sin)$ | $-6.06466963$ | $[-6.0646698_7^6]$ |
| | $\lambda_0^D([0,2\pi],\sin)$ | $-6.02358961$ | $[-6.0235_{90}^{89}]$ |

Table 3: Neumann, periodic and Dirichlet eigenvalues of $q(x)=\sin(x)$

| c | $\sigma_0$ | eigenvalue index | eigenvalue | enclosure $\lambda_2^D([0,20],\sin(x+1/(1+x^2)))$ |
|---|---|---|---|---|
| 1 | $[-0.3784_{90}^{89}]$ | 2 | $-0.34114653$ | $[-0.34114_7^6]$ |
| 2 | $[-1.0701_3^2]$ | 2 | $-1.06208432$ | $[-1.0620_9^8]$ |
| 4 | $[-2.651682_5^0]$ | 2 | $-2.65129447$ | $[-2.651_4^3]$ |
| 6 | $[-4.333016_6^5]$ | 2 | $-4.33348751$ | $[-4.333_{487}^5]$ |
| 8 | $[-6.0646698_7^6]$ | 2 | $-6.06536102$ | $[-6.06536_1^0]$ |

Table 4: Eigenvalues for the perturbed problem $q(x)=c\ \sin(x+\frac{1}{1+x^2})$.

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