

## A LOWER BOUND AND ESTIMATE OF THE LOWEST EIGENVALUE OF A SECOND ORDER FLOQUET EQUATION

BY

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**Abstract.** A bound on the lowest eigenvalue of a second order Floquet problem is derived by applying the Cauchy Integral Theorem. Specifically, we chose a special function which depends on an arbitrary positive parameter  $S \geq 1$ . We use the residue theorem and show that its residue at the origin determines an infinite sum composed of reciprocals of the eigenvalues raised to the  $2S$  power. A simple bound gives us our result. We show that the residue depends explicitly on the power series expansions, in the eigen-parameter, of the original equation's fundamental solutions. The coefficients of these power series are computed recursively.

Three typical examples are presented, and it is shown for these cases that the lower bound, derived in this paper, actually affords a good approximation to the first eigenvalue. We show this for the case only of  $S = 1$ .

**1. Preliminaries.** We are interested in achieving a lower bound or estimate of the lowest eigenvalue  $\lambda_1$  of the Floquet problem

$$\frac{d^2}{dx^2}\psi + \lambda p(x)\psi = 0, \quad 0 < x < 1 \quad (1a)$$

$$\psi(1) = e^{i\alpha}\psi(0), \quad \frac{d}{dx}\psi(1) = e^{i\alpha}\frac{d}{dx}\psi(0), \quad (1b)$$

where  $\alpha$  is a fixed real number in the interval  $[-\pi, \pi]$ . Here  $\lambda_1(\alpha)$ , and  $p(x) > 0$  is a smooth function that is defined on  $[0, 1)$ . It is known that the  $\{\lambda_j\}$  are real and non-decreasing for  $j \geq 0$ ; that is, the differential operator and boundary conditions in (1) form a Hermitian operator [1]. Finally, we note here that the boundary conditions (1b) become periodic when  $\alpha = 0$ . For this case  $\lambda_1 = 0$  and  $\psi = 1$ , as can be directly shown by computation. The bound and approximation we obtain in this paper directly bear out the former result for this case.

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Floquet problems, such as (1), are not only of natural mathematical interest [1] but arise naturally in the stability studies of periodic mechanical motion [2], as well as the study of waves in a periodic media. Indeed, in the last context one-dimensional models such as (1) are prototypes for more complicated photonic structures [3]. In this application  $\lambda_1(\alpha)$  corresponds to the first pass-band of the periodic structure.

To begin the description of our method we let  $U$  and  $V$  be fundamental solutions of (1a). That is, they satisfy (1a) and the initial conditions

$$U(0) = 0, \quad \frac{dU}{dx}(0) = 1, \quad V(0) = 1, \quad \frac{dV}{dx}(0) = 0, \quad (2a)$$

for all  $\lambda$ . Moreover, the Wronskian for these fundamental solutions  $W = V \frac{dU}{dx} - U \frac{dV}{dx}$  is

$$W(x) = W(0) = 1. \quad (2b)$$

In addition both  $U$  and  $V$  are entire functions [1] of  $\lambda$ , as can be deduced from (1a). Accordingly they are given by the convergent series

$$U = \sum_{n=0}^{\infty} U_n(x) \lambda^n, \quad V = \sum_{n=0}^{\infty} V_n(x) \lambda^n, \quad (2c)$$

respectively, for all  $x \in [0,1]$ . The series both converge for all  $\lambda$ .

The coefficients  $U_n$  and  $V_n$  sequentially satisfy the initial value problems

$$\frac{d^2}{dx^2} U_0 = 0, \quad (3a)$$

$$\frac{d^2}{dx^2} U_n = -p(x) U_{n-1}, \quad n \geq 1, \quad (3b)$$

$$U_n = 0, \quad \text{and} \quad \frac{d}{dx} U_n = \delta_{n0}, \quad x = 0, \quad n \geq 0, \quad (3c)$$

and

$$\frac{d^2}{dx^2} V_0 = 0, \quad (4a)$$

$$\frac{d^2}{dx^2} V_n = -p(x) V_{n-1}, \quad n \geq 1, \quad (4b)$$

$$V_n(0) = \delta_{n0}, \quad \frac{d}{dx} V_n(0) = 0, \quad n \geq 1, \quad (4c)$$

respectively. The solutions of these equations are

$$U_0 = x, \quad U_n(x) = - \int_0^x (x-t) p(t) U_{n-1}(t) dt, \quad n \geq 1, \quad (5a)$$

$$V_0(x) = 1, \quad V_n(x) = - \int_0^x (x-t) p(t) V_{n-1}(t) dt, \quad n \geq 1. \quad (5b)$$

With the coefficients  $U_n$  and  $V_n$  now determined, (2c) gives  $U(x)$  and  $V(x)$ , which are particularly valuable as  $\lambda \rightarrow 0$ .

On the other hand, when  $\lambda \rightarrow \infty$  the leading order WKB approximations of  $U$  and  $V$  are [4]

$$U \sim \frac{1}{\sqrt{\lambda} p(0)^{1/4} p(x)^{1/4}} \{ \sin \sqrt{\lambda} \int_0^x \sqrt{p(t)} dt \}, \quad V \sim \frac{p(0)^{1/4}}{p(x)^{1/4}} \{ \cos \sqrt{\lambda} \int_0^x \sqrt{p(t)} dt \}. \quad (6)$$

This result is true for  $0 < \text{arg}(\lambda) \leq 2\pi$ ; that is, (6) is uniform in  $\lambda$  as  $\lambda \rightarrow \infty$ .

Now any solution of (1a) can be written as a linear combination of  $U$  and  $V$ . Specifically we have

$$\psi = c_1U(x) + c_2V(x), \tag{7a}$$

where  $c_1$  and  $c_2$  are constants to be determined. By applying the quasi-periodic boundary conditions (1b),  $c_1$  and  $c_2$  satisfy a linear homogeneous pair of equations whose determinant  $\Delta$  must be equal to zero. This last condition demands that

$$\Delta \equiv V(1, \lambda) + \frac{d}{dx}U(1, \lambda) - 2 \cos \alpha = 0, \tag{7b}$$

and note that it is an entire analytic function of  $\lambda$ . It is important to observe here that the zeroes of  $\Delta$  are the eigenvalue of (1) and vice versa. The power series for  $\Delta$  is explicitly given by

$$\Delta(\lambda) = \sum_{n=0}^{\infty} \Delta_n \lambda^n, \tag{8a}$$

where

$$\Delta_0 \equiv V_0(1) + \frac{d}{dx}U_0(1) - 2 \cos \alpha, \tag{8b}$$

$$\Delta_n \equiv V_n(1) + \frac{d}{dx}U_n(1), \quad n \geq 1, \tag{8c}$$

which is a good representation of  $\Delta$  as  $\lambda \rightarrow 0$ .

On the other hand, as  $\lambda \rightarrow \infty$ , it follows from (6) and (7) that

$$\Delta \sim \left\{ \left[ \frac{p(0)}{p(1)} \right]^{1/4} + \left[ \frac{p(1)}{p(0)} \right]^{1/4} \right\} \cos(\lambda I) - 2 \cos \alpha, \tag{9a}$$

where

$$I = \int_0^1 p(x)^{1/2} dx. \tag{9b}$$

Again, this asymptotic result is uniform in the complex plane as  $\lambda \rightarrow \infty$ .

When one sets  $\Delta = 0$  and  $p(0) = p(1)$  as in the above estimate, one obtains the asymptotic result  $\lambda_n \sim \alpha^2 + \frac{n^2\pi^2}{I^2} \sim \frac{n^2\pi^2}{I^2}$  as  $n \rightarrow \infty$ .

**2. The lower bound and estimate.** With all the necessary ingredients from the previous section we begin now by considering

$$f(\lambda) = \frac{\Delta_\lambda}{\lambda^{2S} \Delta} \tag{10}$$

as a function of  $\lambda$  for a fixed positive integer  $2S$ . It has simple poles at  $\lambda_n$  with residues of  $\frac{1}{\lambda_n^{2S}}$ .

We find by direct multiplication that the power series of  $f(\lambda)$  is

$$f(\lambda) = \sum_{n=0}^{\infty} f_n \lambda^{n-2S}, \tag{11a}$$

where

$$f_0 = \frac{\Delta_1}{\Delta_0}, \tag{11b}$$

$$f_n = \frac{(n+1)\Delta_{n+1} - \sum_{r=1}^n \Delta_r f_{n-r}}{\Delta_0}, \quad n \geq 1, \tag{11c}$$

and the  $f_n$  are computed sequentially. For example,  $f_1 = \frac{2\Delta_2 - \Delta_1 f_0}{\Delta_0}$ ,  $f_2 = \frac{3\Delta_3 - \Delta_1 f_1 - \Delta_2 f_0}{\Delta_0}$ , etc.

From (10) it is clear that  $f$  has a pole of order  $2S$  at the origin. But its residue there,  $r_{-1}$  [5], is the coefficient of  $\lambda^{-1}$ , namely  $f_{2S-1}$ , which is obtained from (11a) and (11c). That is,

$$r_{-1} = f_{2S-1}, \tag{12}$$

where  $f_{2S-1}$  is given by (11). When  $S = 1/2$ , the residue at the origin,  $r_{-1} = f_0 = \frac{\Delta_1}{\Delta_0} = -\frac{\langle p \rangle}{4 \sin^2(\alpha/2)}$  by applying (11b), (8), (3), and (4), respectively. Similarly, when  $S = 1$ ,  $r_{-1} = f_1 = \frac{2\Delta_2 - \Delta_1 f_0}{\Delta_0}$ . After some algebraic manipulations this becomes

$$r_{-1} = \frac{[\langle p \rangle - \langle P \rangle]^2 + \langle p \rangle[\langle P \rangle - \langle x^2 p \rangle] - \langle P^2 \rangle}{2 \sin^2(\frac{\alpha}{2})} - \frac{\langle p \rangle^2}{16 \sin^4(\frac{\alpha}{2})}, \tag{13}$$

where  $P = \int_0^t p(\eta) d\eta$  and  $\langle * \rangle = \int_0^1 * dx$ .

To find and simplify  $r_{-1}$  for an  $S > 1$  requires more effort, although the calculations are elementary. Although the results of the following section are valid for  $S \geq 1/2$ , we shall pursue explicitly neither the cases of  $1 > S > 1/2$ , for reasons of accuracy, nor the cases of  $S > 1$ , for simplicity.

Now let  $S_n$  denote the square in the complex plane which encloses the origin and whose sides are parallel to the real and imaginary axes. The sides cut the axes at the points  $\pm \frac{1}{2}(\lambda_{n+1} + \lambda_n)$  and  $\pm i \frac{1}{2}(\lambda_{n+1} + \lambda_n)$ , where the  $\lambda_n \rightarrow \infty$ .

We now apply Cauchy's residue theorem [5] to  $f(\lambda)$ , defined by (10), in the region inside of  $S_n$  and obtain

$$\oint_{S_n} f(\lambda) d\lambda = \sum_{j=1}^n \frac{1}{\lambda_j^{2S}} + r_{-1}, \tag{14}$$

where the sum terms come from the residues at the eigenvalues and the single term from the residue at the origin.

Now we deduce from (9)-(10) that the integrand in (14) is the product of the two factors

$$\frac{-I}{\lambda^{2S}} \cdot \frac{\eta \sin \sqrt{\lambda} I}{\sqrt{\lambda}(\eta \cos \sqrt{\lambda} I - 2 \cos \alpha)}$$

where

$$\eta = \frac{p(1)}{p(0)} + \frac{p(0)}{p(1)}.$$

The second is clearly bounded on the sides of  $S_n$ , and the first gives the proper decay, as long as  $S > 1/2$ . Hence the integral in (14) is  $o(1)$  as  $\lambda \rightarrow \infty$ . Letting  $S > 1/2$  be fixed and  $n \rightarrow \infty$  we find from (14) that

$$\sum_{j=1}^{\infty} \frac{1}{\lambda_j^{2S}} = -r_{-1}. \tag{15}$$

Since all the  $\lambda_j^{2S}$  are positive, we find that (15) implies  $\lambda_1^{2S} \geq -1/r_1$  or, equivalently,

$$\lambda_1 \geq \left[ \frac{-1}{r_1} \right]^{\frac{1}{2S}}. \tag{16}$$

This is our lower bound. If the  $\lambda_j \rightarrow \infty$  at a sufficiently rapid rate, then the inequality sign in (16) may be replaced by an approximate equal sign. That is, the lower bound (16) may be a good approximation of our first eigenvalue.

To make the above theory concrete we take  $S = 1$  so that (16) becomes, with the aid of (13),

$$\lambda_1 \geq \frac{4 \sin^2(\alpha/2)}{\sqrt{\langle p \rangle^2 - 8Q \sin^2(\alpha/2)}}, \tag{17a}$$

$$Q = [\langle p \rangle - \langle P \rangle]^2 + \langle p \rangle [\langle P \rangle - \langle x^2 p \rangle] - \langle P^2 \rangle. \tag{17b}$$

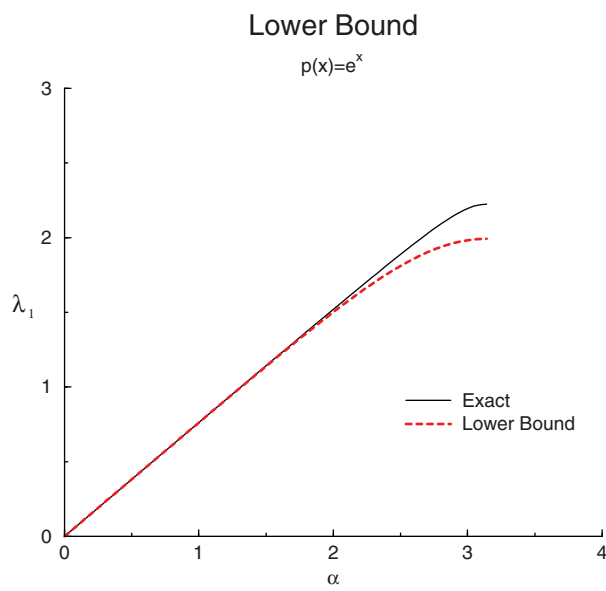
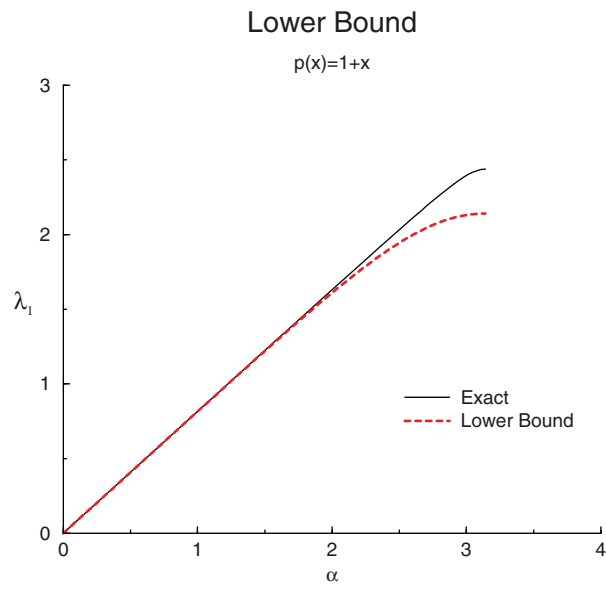
**3. Examples.** In this section we shall present several examples by functionally varying  $p(x)$ . In all of these cases we take  $S = 1$  and find that our lower bound on  $\lambda_1$  actually provides a good approximation over a range of  $\alpha$ . Our results are shown in the following figures. The lower bounds are given as dashed curves, whereas the solid curves are the results of a shooting technique [6] applied to the original problem (1). The latter may be taken as exact.

In our first example we take  $p = 1 + x$ . The calculation of  $\langle x^2 p \rangle$  is trivial for this case, as well as  $\langle p \rangle, \langle P \rangle$ , and  $\langle P^2 \rangle$ . Inserting these numerical values into (17) gives our lower bound (and approximation) to the lowest eigenvalue. The result is shown in Figure 1. Comparing the two graphs it is evident that our lower bound (and approximation) is very accurate for a wide range of  $\alpha$ , but becomes inaccurate as  $\alpha$  approaches the band edge  $\pi$ . As our second example we take  $p = e^x$ . Again, the calculation of  $\langle x^2 p \rangle$  is trivial for this case, as well as  $\langle p \rangle, \langle P \rangle$ , and  $\langle P^2 \rangle$ . Inserting these numerical values into (17) gives our lower bound (and approximation) to the lowest eigenvalue. Our results are shown Figure 2, where the same level of accuracy is again achieved. In the previous two examples  $p(0) \neq p(1)$ . We now consider the case where  $p = 1 + .5 \sin 2\pi x$  and note now that  $p(0) = p(1)$ . Again, the calculation of  $\langle x^2 p \rangle$  is trivial for this case, as well as  $\langle p \rangle, \langle P \rangle$ , and  $\langle P^2 \rangle$ . Inserting these numerical values into (17) gives our lower bound (and approximation) to the lowest eigenvalue. Our results are shown Figure 3, where the same level of accuracy is again achieved.

**4. Conclusion.** In this note we have presented a lower bound for the first eigenvalue of a particular second order Floquet problem. For particular and typical  $p(x)$ 's this bound was shown by examples to yield accurate approximations to  $\lambda_1$ . Although variational techniques [7] are often used to obtain lower bounds, we obtained our result by applying complex variable methods, in particular Cauchy's Residue Theorem [5]. Our result is good for arbitrary powers of  $S$ , although for simplicity the value of  $S = 1$  was chosen.

In closing we make two observations. First, we can easily change the boundary conditions (1b) to the separated case

$$B_1(\psi) \equiv \frac{d\psi}{dx} + \alpha\psi = 0, \quad x = 0, \quad B_2(\psi) \equiv \frac{d\psi}{dx} - \beta\psi = 0, \quad x = 1, \tag{1b'}$$



where  $\alpha \geq 0$  and  $\beta \geq 0$  are arbitrary and fixed. Then, all is the same now except  $\Delta$  is changed to

$$\Delta = B_2(V) - B_2(U). \quad (7b')$$

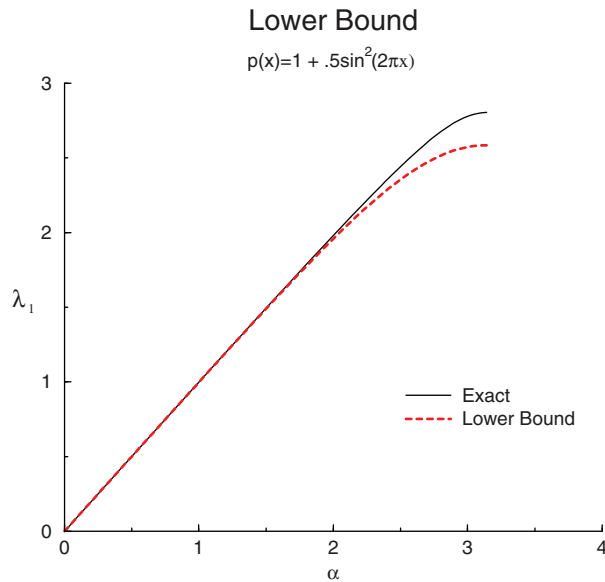


FIG. 3

The fundamental solutions  $U$  and  $V$  remain the same, but the expansion (11) and residue (12) must be recomputed.

Secondly, the differential operator (1a) can be somewhat generalized to

$$\frac{d}{dx}(k(x)\frac{d}{dx}\psi) + \lambda p(x)\psi = 0. \tag{1a'}$$

Then everything remains the same, except the  $U_j$  and the  $V_j$  must be recomputed for a specific  $k$ . The general formulae (3)-(5) are more involved for this scenario.

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