

## Approximation of Sturm-Liouville problems by exponentially weighted Legendre-Gauss Tau Method

Mohamed K. El Daou

**Abstract**—We construct an exponentially weighted Legendre-Gauss Tau method for solving differential equations with oscillatory solutions. The proposed method is applied to Sturm-Liouville problems. Numerical examples illustrating the efficiency and the high accuracy of our results are presented.

**Keywords**—Oscillatory functions, Sturm-Liouville problems, Legendre Polynomial, Gauss points.

### I. INTRODUCTION

THE accurate computation of Sturm-Liouville problems eigenvalues continues to be a challenging problem for computational physicists. In the past there has been much interest in standard numerical methods such as Numerov, Runge-Kutta or de Vogelaere (see [5]). But due to the unsatisfactory performance of standard methods in detecting the strong oscillations exhibited by the eigenfunctions, efforts have concentrated on developing modern techniques that have proven to be highly accurate and effective in treating this type of problems. Such techniques are based on piecewise coefficient perturbation and on exponential fitting (see [2] and [4]).

This paper is mainly devoted to construct an exponentially weighted approach for a spectral method called *Legendre-Gauss Tau method*, (see [6], [8] and [1]). The main idea of the classical Legendre-Gauss Tau method (LGT) is to find an approximation  $\tilde{y}$  for  $y$  expressed in terms of Legendre polynomial  $\{L_i(x)\}$  as  $\tilde{y} = \sum_{i=0}^{n+1} a_i L_i(x)$ , where  $\{a_i; i = 0, 1, 2, \dots, n\}$  are fixed, by imposing some prescribed initial/boundary conditions on  $\tilde{y}$  and by forcing the residual produced by  $\tilde{y}$  to vanish at  $n$  Gauss points. The proposed method, that will be called Exponentially weighted Legendre-Gauss Tau method (ELGT), is an extension of LGT; it seeks approximations in terms of an exponentially weighted Legendre polynomials basis  $\{L_i(x)e^{\omega x}\}$ , where the frequencies  $\omega$ 's are determined in terms of the local behaviour of the solution. These  $\omega$ 's are accurately estimated using the Piecewise Constant Perturbation Method (see [9] and [2]).

### II. LEGENDRE-GAUSS TAU METHOD LGT

LGT was invented by Lanczos in [6] and later developed by Ortiz [8] and by Gottlieb and Orszag [1] to treat problems with different degrees of complexities. It has two equivalent approaches: recursive and spectral.

Mohamed K. El Daou is with the College of Technological Studies, Kuwait, email: mk.eldaou@paaet.edu.kw. This work is supported by the Public Authority for Applied Education and Training, Kuwait, (Project number TS-6-07)

#### A. Recursive formulation of LGT

Given an initial value problem (i.v.p.) of order  $\nu \in \mathbf{N}$ , with variable coefficients  $\{P_i(x), i = 0, 1, \dots, \nu\}$ ,

$$(Dy)(x) := \sum_{i=0}^{\nu} P_i(x) \frac{d^i y}{dx^i} = f(x); \quad x \in [a, b], \quad (1)$$

$$y^{(k)}(a) = \alpha_k \in \mathbf{R}; \quad k = 0, 1, \dots, \nu - 1, \quad (2)$$

Let us assume that  $P_\nu(x)$  does not vanish in the domain of integration  $I := [a, b]$ .

The recursive formulation of LGT ([6], [8]) consists in replacing  $f(x)$  by an approximation  $\tilde{f}(x)$  in a way that the solution  $\tilde{y}$  of,

$$(D\tilde{y})(x) := \sum_{i=0}^{\nu} P_i(x) \frac{d^i \tilde{y}}{dx^i} = \tilde{f}(x); \quad x \in I,$$

$$\tilde{y}^{(k)}(a) = \alpha_k \in \mathbf{R}; \quad k = 0, 1, \dots, \nu - 1,$$

is an exact polynomial. In practice  $\tilde{f}(x)$  takes the form,

$$\tilde{f}(x) = f(x) + H_N(x)$$

where,

- $H_N(x) := (\sum_{i=0}^r \tau_i x^i) L_N(x)$ ;  $L_k(x)$  stands for the  $k$ th Legendre polynomial shifted to interval I.
- $\{\tau_i\}$  are free parameters adjusted so that  $\tilde{y}$  is an exact polynomial satisfying the initial conditions (2).

#### B. Spectral approach of LGT

The spectral approach of LGT, which this paper is concerned with, seeks an approximation  $y_N$  of the form

$$y_N = \sum_{i=0}^{N+\nu-1} a_i L_i(x).$$

The unknown coefficients  $\{a_i; i = 0, 1, \dots, n + \nu - 1\}$  are determined by

- imposing the initial conditions (2) on  $y_N$ ,
- $$y_N^{(k)}(a) = \alpha_k; \quad k = 0, 1, \dots, \nu - 1,$$
- and, either, by projecting orthogonally the residual  $R_N(x) := Dy_N(x) - f(x)$  against the subspace  $\text{span}\{L_0(x), L_1(x), \dots, L_{N-1}(x)\}$ ,

$$\int_a^b R_N(t) L_k(t) dt = 0, \quad l = 0, 1, 2, \dots, N - 1,$$

- or, by forcing  $R_N(x)$  to vanish at the  $N$  Gauss points  $\{z_i; i = 1, 2, \dots, N\} \subset I$ , (which are the zeros of  $L_N(x)$ ),

$$R_N(z_i) = 0, \quad i = 1, 2, 3, \dots, N.$$



A. Structure of CP-Method residual

In this section we will suppress the  $i$  indices and let  $X$  designate one of the  $x_i$ . Adding up the reference equation and the first  $m$  correction equations, we find that

$$Y_m'' + b(x)Y_m = -\delta b y_m, \quad x \in [X, X + h] \quad (7)$$

$$Y_m(X) = \eta_0, \quad Y_m'(X) = \eta_1$$

where  $\{\eta_0, \eta_1\}$  are generic values available from the approximation computed on the previous subinterval  $[x_{i-2}, x_{i-1}]$ .

Comparing (7) with the original i.v.p, (4), we observe that when the PPM approximant  $Y_m$  is substituted in the original differential equation, it produces a residual made up of  $\delta b(x)$ , the perturbation in  $b(x)$ , and the  $m$ th correction  $y_m(x)$ ,

$$R(x) = -\delta b y_m.$$

In other words,  $Y_m$  is the exact solution of a perturbed version of the original one where the perturbation occurs in the right hand side.

In particular, if  $\tilde{b}(x) \equiv \bar{b}$  is constant, (CP-Method), and  $\omega = \sqrt{-\bar{b}}$ , then

- the CP-reference  $y_0$  is given as

$$y_0(x) = p_{10}e^{\omega x} + p_{20}e^{-\omega x}$$

where  $\{p_{10}, p_{20}\}$  are constants fixed in terms of the initial conditions associated with (5),

- the  $k$ th CP-correction has the form

$$y_k(x) = p_{1k}(x)e^{\omega x} + p_{2k}(x)e^{-\omega x},$$

for some polynomials  $\{p_{1k}, p_{2k}\}$  that involve two constants fixed in terms of the initial conditions  $y_k(X) = y_k'(X) = 0$ .

- the CP-approximant  $Y_m := y_0 + y_1 + \dots + y_m$  can be written as,

$$Y_m = P_{m1}(x)e^{\omega x} + P_{m2}(x)e^{-\omega x}.$$

Further from (7) follows that, for  $x \in [X, X + h]$ ,  $Y_m$  satisfies

$$Y_m'' + b(x)Y_m = -(\delta b p_{1m})e^{\omega x} - (\delta b p_{2m})e^{-\omega x},$$

$$Y_m(X) = \eta_0, \quad Y_m'(X) = \eta_1$$

If we compare the latter with the original i.v.p, (4), we find that the CP approximant  $Y_m$  produces the residual

$$R(x) = -(\delta b p_{1,m})e^{\omega x} - (\delta b p_{2,m})e^{-\omega x}. \quad (8)$$

This structure of CP-residual will be very constructive in assuring the close dependence between the error function and the quality of perturbation measured by  $\delta b(x)$ . Subsequently this will allow to propose a technique that reduces the error substantially.

B. Error analysis

Let  $e_m(x) := y(x) - Y_m(x)$  denote the  $m$ th error function. The difference between (4) and (7) gives the error equation,

$$e_m'' + b(x)e_m = (\delta b p_{1m})e^{\omega x} + (\delta b p_{2m})e^{-\omega x},$$

$$e_m(X) = \epsilon_m, \quad e_m'(X) = \epsilon_m$$

where  $x \in [X, X + h]$ .  $e_m(x)$  is formally represented as

$$e_m(x) = \int_X^x G^*(x, t)\delta b(t)dt + G(x, X)\epsilon' + G_x(x, X)\epsilon. \quad (9)$$

$G(x, t)$  is the Green function associated with  $D$  and

$$G^*(x, t) := G(x, t) [p_{1,m}(t)e^{\omega t} + p_{2,m}(t)e^{-\omega t}]$$

For the local truncation error (l.t.e.), let  $\epsilon = \epsilon' = 0$  and take norms in (9)

$$\|e_m\| \leq \kappa \|\delta b\|, \quad \text{where } \|G^*\| \leq \kappa$$

for some constant  $\kappa = \kappa(\omega)$ .

As far as CP-method is concerned, in the uniform norm  $\|\cdot\|_\infty$  the smallest  $\|\delta b\|_\infty$  is realized when  $\bar{b}$  is the best zeroth approximation of  $b(x)$ ,

$$\bar{b} = b(X + \frac{h}{2}), \quad \omega = \sqrt{-b(X + \frac{h}{2})}$$

Alternatively, for the  $L^2$ -norm,  $\|\cdot\|_2$ , the smallest  $\|\delta b\|_2$  is achieved if  $\bar{b}$  is the best zeroth approximation of  $b(x)$  in  $L^2[X, X + h]$ ,

$$\bar{b} = \int_0^1 b(X + ht)dt$$

Hence, whether  $\|\cdot\|_\infty$  or  $\|\cdot\|_2$  is adopted,  $\delta b(x)$  is of the form

$$\delta b(x) = L_{1,h}(x) \times \text{function of } x$$

We conclude that the residual (8) can be written as

$$R(x) = L_{1,h}(x)\tau_1(x)e^{\omega x} + L_{1,h}(x)\tau_2(x)e^{-\omega x} \quad (10)$$

This result suggests that there could be PPM other than CPM that would lead to a residual whose the same structure as (10), except that the coefficients of the exponentials  $e^{\pm\omega x}$  must be multiples of higher order Legendre polynomial,  $L_{N,h}(x)$  say. In other words, we wish to find a method whose the residual is of the form

$$R_N(x) = L_{N,h}(x)\tau_1(x)e^{\omega x} + L_{N,h}(x)\tau_2(x)e^{-\omega x} \quad (11)$$

Next section demonstrates that LGT can be extended to achieve this goal.

IV. EXPONENTIALLY WEIGHTED LGT METHOD, ELGT

The investigation in this section will be carried out for homogenous and nonhomogenous o.d.e.

A. Case 1:  $y'' + b(x)y = 0$

For each  $\omega \in \mathbb{C}$  let us associate to  $Du := u'' + b(x)u(x)$  the auxilliary operator  $D_\omega$  defined as

$$D_\omega u := u'' + 2\omega u' + [\omega^2 + b(x)]u.$$

THEOREM 1. The exact solution of

$$Dy := y'' + b(x)y(x) = 0 \quad (12)$$

is expressible as a linear combination of two exponentials  $e^{\pm\omega x}$ ,

$$\omega = \sqrt{-b(\bar{X})}$$

whose the coefficients  $\{\phi_1, \phi_2\}$  are the exact solutions of the auxiliary equations

$$D_{\pm\omega}\phi = \phi'' \pm 2\omega\phi' + \delta b(x)\phi = 0. \quad (13)$$

In other words, solving  $Dy = 0$  is equivalent to solving  $D_{\omega}\phi_1 = 0$  and  $D_{-\omega}\phi_2 = 0$ .

The proof of this theorem is based on the following two lemmas:

LEMMA 1. The following assertions hold true:

- 1) For any  $\omega$ ,  $D_{\omega}\phi = 0 \Rightarrow D[\phi(x)e^{\omega x}] = 0$ .
- 2) For any constants  $\{\omega_i, c_i; i = 1, 2\}$

$$\{D_{\omega_1}\phi_1 = D_{\omega_2}\phi_2 = 0\} \Rightarrow D[c_1\phi_1e^{\omega_1x} + c_2\phi_2e^{\omega_2x}] = 0$$

LEMMA 2. Let  $\omega_{1,2} = \pm\omega = \pm\sqrt{-b(\bar{X})}$ . Then

- 1)  $D_{\pm\omega}\phi = \phi'' \pm 2\omega\phi' + \delta b(x)\phi$ ,
- 2) For any constants  $\{c_i; i = 1, 2\}$

$$\{D_{\omega}\phi_1 = D_{-\omega}\phi_2 = 0\} \Rightarrow D[c_1\phi_1e^{\omega x} + c_2\phi_2e^{-\omega x}] = 0 \quad (14)$$

Theoretically,  $y(x)$  can be found, once  $\{\phi_1, \phi_2\}$  are available, and the constants  $c_1$  and  $c_2$  in  $y = c_1\phi_1(x)e^{\omega x} + c_2\phi_2(x)e^{-\omega x}$  are fixed according to the given initial conditions. Analytically, solving (13) is not easier, however, than solving the original problem (12). Computationally, numerical methods that approximates the smooth solutions of (13) could be more successful than approximating (12) directly, specially when  $y(x)$  exhibits sharp variations. Next I will propose an algorithm for LGT that can effectively generate approximations  $\{\tilde{\phi}_1, \tilde{\phi}_2\}$  for  $\{\phi_1, \phi_2\}$  defined by (13) and subsequently construct approximation  $\tilde{y}$  for  $y$  as  $\tilde{y} = c_1\tilde{\phi}_1e^{\omega x} + c_2\tilde{\phi}_2e^{-\omega x}$ .

I will refer to this procedure by ELGT(M,N) where  $M$  indicates the number of steps and  $N$  is the number of Gauss points in each subinterval  $[x_{i-1}, x_i]$ .

ALGORITHM 1 – Follows is an ELGT(M,N) algorithm that approximates i.v.p. problems of the form:

$$y'' + b(x)y = 0, \quad x \in [a, b]$$

$$y(a) = \alpha_0, \quad y'(a) = \alpha_1$$

- 1) construct a partition  $a = x_0 < x_1 < \dots < x_M = b$  of  $[a, b]$ ; set  $h_i = x_i - x_{i-1}$ .
- 2) provide the  $N$  Gauss points in  $[0,1]$ ;  $\{z_k, k = 1, 2, \dots, N\}$
- 3) for  $i = 1, 2, \dots, M$  repeat (a)-(d)

a) compute the frequency  $\omega_i$  for  $[x_{i-1}, x_i]$ ;  $\omega_i = \sqrt{-b(x_{i-1} + \frac{h_i}{2})}$ ;

b) compute the coefficients  $\{a_{ji}\}$  of  $\phi_{N,i,1} = \sum_{j=0}^N a_{ji}L_{ji}(x)$ ; solve the algebraic linear system,

$$(D_{\omega_i}\phi_{N,i,1})(x_{i-1} + h_iz_k) = 0, \quad k = 1, 2, \dots, N$$

$$\phi_{N,i,1}(x_{i-1}) = 1$$

c) compute the coefficients  $\{b_{ji}\}$  of  $\phi_{N,i,2} = \sum_{j=0}^N b_{ji}L_{ji}(x)$ ; solve the algebraic linear system,

$$(D_{-\omega_i}\phi_{N,i,2})(x_{i-1} + h_iz_k) = 0, \quad k = 1, 2, \dots, N$$

$$\phi_{N,i,2}(x_i) = -1$$

d) construct  $y_{Ni} = c_{1i}\phi_{N,i,1}e^{\omega_ix} + c_{2i}\phi_{N,i,2}e^{-\omega_ix}$ ;  $\{c_{1i}, c_{2i}\}$  are fixed by left-end conditions

$$y_{Ni}(x_{i-1}) = y_{N,i-1}(x_{i-1})$$

$$y'_{Ni}(x_{i-1}) = y'_{N,i-1}(x_{i-1})$$

Next, identify the residual resulting from ELGT(M,N).

THEOREM 2. ELGT(M,N) approximant  $y_{N,i}$  produces a residual of the form (11),

$$R_N(x) = L_{N,h}(x)\tau_1(x)e^{\omega x} + L_{N,h}(x)\tau_2(x)e^{-\omega x}$$

Proof - Parts (b) and (c) imply respectively that

$$(D_{\omega_i}\phi_{N,i,1})(x) = L_{Ni}(x) \times \rho_1(x)$$

$$(D_{-\omega_i}\phi_{N,i,2})(x) = L_{Ni}(x) \times \rho_2(x)$$

Therefore, if  $D$  is operated on  $y_{N,i}$  given in (d) we get

$$Dy_{N,i} = D[c_{1i}\phi_{N,i,1}e^{\omega_ix} + c_{2i}\phi_{N,i,2}e^{-\omega_ix}]$$

$$= c_{1i}D[\phi_{N,i,1}e^{\omega_ix}] + c_{2i}D[\phi_{N,i,2}e^{-\omega_ix}]$$

$$= c_{1i}D_{\omega_i}[\phi_{N,i,1}]e^{\omega_ix} + c_{2i}D_{-\omega_i}[\phi_{N,i,2}]e^{-\omega_ix}$$

$$= c_{1i}L_{Ni}(x)\rho_1(x)e^{\omega_ix} + c_{2i}L_{Ni}(x)\rho_2(x)e^{-\omega_ix}$$

as required.

B. Case 2:  $y'' + a(x)y' + b(x)y = 0$

Extend ELGT to 2nd order o.d.e. involving  $y'$ ,

$$(Dy)(x) := y'' + a(x)y' + b(x)y = 0, \quad x \geq a \quad (15)$$

$$y(a) = \alpha_0, \quad y'(a) = \alpha_1$$

The auxiliary operator  $D_{\omega}$  is defined as

$$D_{\omega}u := u'' + (2\omega + a(x))u' + (\omega^2 + a(x)\omega + b(x))u.$$

Frequencies  $\omega_1$  and  $\omega_2$  are now given by the quadratic equation

$$\omega^2 + a(\bar{X})\omega + b(\bar{X}) = 0, \quad \bar{X} = X + \frac{h}{2},$$

In particular for these  $\omega_j$ 's, the auxiliary operator  $D_{\omega_j}$  becomes

$$D_{\omega_j}u := u'' + (2\omega_j + a(x))u' + (\omega_j\delta a + \delta b)u.$$

Algorithm 1 can be adopted for equation (15) except part (a) which estimates the frequencies. The ELGT would give solution,

$$y_N = c_1\phi_{1,N}(x)e^{\omega_1x} + c_2\phi_{2,N}(x)e^{\omega_2x}$$

where  $c_1$  and  $c_2$  are fixed by the initial conditions.

ALGORITHM 2 –

- 1) construct a partition  $a = x_0 < x_1 < \dots < x_M = b$  of  $[a, b]$ ; set  $h_i = x_i - x_{i-1}$ .
- 2) provide the  $N$  LG points in  $[0,1]$ ;  $\{z_k, k = 1, 2, \dots, N\}$
- 3) for  $i = 1, 2, \dots, M$  repeat (a)-(d)

a) compute the frequencies  $\{\omega_{1i}, \omega_{2i}\}$  for  $[x_{i-1}, x_i]$  by solving  $\omega^2 + a(\bar{x}_i)\omega + b(\bar{x}_i) = 0$ ,  $\bar{x}_i = x_{i-1} + \frac{h_i}{2}$ ,

b) compute the coefficients  $\{a_{ji}\}$  of  $\phi_{N,i,1} = \sum_{j=0}^N a_{ji}L_{ji}(x)$ ; solve the algebraic linear system,

$$(D_{\omega_{1i}}\phi_{N,i,1})(x_{i-1} + h_iz_k) = 0$$

$$\phi_{N,i,1}(x_{i-1}) = 1, \quad k = 1, 2, \dots, N$$

c) compute the coefficients  $\{b_{ji}\}$  of  $\phi_{N,i,2} = \sum_{j=0}^N b_{ji}L_{ji}(x)$ ; solve the algebraic linear system,

$$(D_{\omega_{2i}}\phi_{N,i,2})(x_{i-1} + h_i z_k) = 0, \\ \phi_{N,i,2}(x_i) = -1, \quad k = 1, 2, \dots, N$$

d) construct  $y_{Ni} = c_{1i}\phi_{N,i,1}e^{\omega_{1i}x} + c_{2i}\phi_{N,i,2}e^{\omega_{2i}x}$ ;  $\{c_{1i}, c_{2i}\}$  are fixed by left-end conditions

$$y_{Ni}(x_{i-1}) = y_{N,i-1}(x_{i-1}) \\ y_{Ni}(x_{i-1}) = y_{N,i-1}(x_{i-1})$$

C. Case 3:  $y'' + a(x)y' + b(x)y = f(x)$

Let us explain how to extend ELGT to solve nonhomogeneous 2nd order o.d.e.

$$(Dy)(x) := y'' + a(x)y' + b(x)y = f(x), \quad x \geq a \quad (16) \\ y(a) = \alpha_0, \quad y'(a) = \alpha_1$$

The general solution of (16) is written as

$$y = \text{const}_1 u_1(x) + \text{const}_2 u_2(x) + Y(x)$$

where  $\{u_1, u_2\}$  are two particular solutions of  $Dy = 0$  and  $Y(x)$  is a particular solution of  $Dy = f$ .

The ELGT solution takes the form,

$$y_N = c_1\phi_{1,N}(x)e^{\omega_{1x}} + c_2\phi_{2,N}(x)e^{\omega_{2x}} + Y_N(x)$$

where  $c_1$  and  $c_2$  are fixed by the initial conditions.

To generate this approximation, replace step (d) by (d)-(e).

ALGORITHM 3 – Algorithm 2 +

(d) compute the coefficients  $\{c_{ji}, j = 0, 1, \dots, N + 1\}$  of

$$Y_{N,i} = \sum_{j=0}^{N/2} c_{ji}L_{ji}(x)e^{\omega_{1i}x} + \sum_{j=0}^{N/2} c_{N/2+1+j,i}L_{ji}(x)e^{\omega_{2i}x}$$

by solving

$$(DY_{N,i})(x_{i-1} + h_i z_k) = f(x_{i-1} + h_i z_k) \\ Y_{N,i}(x_{i-1}) = 0, \quad k = 1, 2, \dots, N \\ Y'_{N,i}(x_{i-1}) = 1$$

(e) compute  $y_{Ni} = c_{1i}\phi_{N,i,1}e^{\omega_{1i}x} + c_{2i}\phi_{N,i,2}e^{\omega_{2i}x} + Y_{N,i}$  where  $\{c_{1i}, c_{2i}\}$  are fixed by left-end conditions

$$y_{Ni}(x_{i-1}) = y_{N,i-1}(x_{i-1}) \\ y_{Ni}(x_{i-1}) = y_{N,i-1}(x_{i-1})$$

Example 1.

Let us resolve problem (3) using ELGT(392,2). The committed errors along those of LGT(392,2) and the frequencies  $\omega_k$  are listed in Table II. One can easily appreciate the significant improvement in the errors over the whole interval and at the right end point of interval of integration.

k	$x_k$	$\omega_k$	$er(x_k)$	$er'(x_k)$	$\sqrt{er^2 + er'^2}$
8	2.0	0.77+3.90i	1.64E-6	1.69E-5	1.70E-5
16	3.0	0.51+5.88i	4.91E-6	1.01E-4	1.01E-4
24	4.0	0.38+7.88i	5.99E-6	1.47E-4	1.47E-4
32	5.0	0.30+9.88i	-8.47E-6	-2.75E-4	2.76E-4
72	10.0	0.15+19.87i	-2.03E-5	-1.19E-3	1.19E-3
112	15.0	0.10+29.87i	-1.69E-4	-2.78E-3	2.78E-3
152	20.0	0.075+39.87i	-9.09E-5	-7.01E-3	7.01E-3
192	25.0	0.060+49.87i	6.42E-4	1.44E-2	1.44E-2
232	30.0	0.050+59.87i	-4.70E-4	9.65E-2	9.65E-2
272	35.0	0.043+69.87i	-1.80E-3	-6.80E-2	6.81E-2
312	40.0	0.037+79.87i	4.472E-4	-1.85E-1	1.85E-1
352	45.0	0.033+89.87i	1.74E-3	1.76E-1	1.76E-1
<b>392</b>	<b>50.0</b>	<b>0.030+99.87i</b>	<b>-3.35E-3</b>	<b>-8.75E-2</b>	<b>8.75E-2</b>

Classical LGT(2,0.05) result:

<b>392</b>	<b>50.0</b>		<b>2.68E+164</b>	<b>1.71E+166</b>	<b>1.71E+166</b>
------------	-------------	--	------------------	------------------	------------------

TABLE II

ELGT(392,2) ERRORS FOR  $y = x \sin x^2 + 2x$  IN  $[1, 50]$ .

V. STURM-LIOUVILLE PROBLEMS

In this section we shall consider equations of this form

$$y'' + (E - V(x))y = 0, \quad x \in [a, b] \\ y(a) = y(b) = 0,$$

where  $V(x)$  is a given function called *potential* and the value of  $E$  is not specified. Finding the values of  $E$  for which there exists a solution  $y \neq 0$  is a part of the so called Sturm-Liouville problem SLP. Many important problems, (e.g quantum physics, quantum chemistry, geophysical applications, vibration and heat flows problems) can be modeled by means of one-dimensional SLP.

We are interested in approximating the eigenvalues  $E$  by means of ELGT(M,N). To this end we adopt the following strategy:

- Take a partition  $a = x_0 < x_1 < \dots < x_M = b$ .
- Solve by ELGT(M,N) a sequence of i.v.p. with  $y(a) = 0$  and  $y'(a)$  arbitrarily chosen.
- Compute the  $\bar{E}$ 's that satisfy  $Y_{MN}(b, \bar{E}) = 0$ .
- These  $\bar{E}$ 's approximate the exact e.v.  $E$ 's.

Example 2.

Let us test ELGT on the following SLP:

$$y'' + (E - V(x))y = 0, \quad [0, x_r]$$

where  $E$  is the energy to be determined and  $V(x)$  is the Woods-Saxon potential,

$$V(x) = v_0 W(x) \left[ 1 - \frac{1 - W(x)}{a_0} \right], \\ W(x) = \left[ 1 + \exp\left(\frac{x - x_0}{a_0}\right) \right]^{-1} \\ v_0 = -50, \quad x_0 = 7, \quad a_0 = 0.6$$

with the conditions (see [7])

$$y(0) = 0 \text{ and } (\sqrt{V(x_r) - E})y(x_r) + y'(x_r) = 0$$

Since  $V(x)$  is negligible for  $x > 15$  we can safely take  $x_r = 15$ .

Exact $E_n$	ELGT(h,N=6)				LPM[4,2]
	M=15	M=30	M=60	M=120	
	h=1	h=1/2	h=1/4	h=1/8	
-49.45778872808258	-2.8E-9	-6.3E-13	< 1.0E-14	< 1.0E-14	
-48.14843042000636	-1.5E-8	-4.28E-12	< 1.0E-14	2.1E-14	
-46.29075395446608	7.4E-9	-1.11E-11	< 1.0E-14	< 1.0E-14	
-43.96831843181423	4.1E-8	-1.5E-11	< 1.0E-14	-2.1E-14	
-41.23260777218022	-1.2E-7	-1.4E-11	< 1.0E-14	-5.0E-14	
-38.12278509672792	1.6E-6	1.32E-10	1.1E-14	-8.0E-14	
-34.67231320569966	4.0E-6	-6.29E-10	5.0E-14	-1.1E-13	
-30.91224748790885	-1.5E-5	8.40E-10	2.6E-14	-1.2E-13	
-26.87344891605987	-1.2E-5	4.81E-10	2.9E-14	-1.1E-13	
-22.58860225769321	2.7E-5	-4.9E-9	2.2E-14	-8.5E-14	
-18.09468828212442	1.3E-5	8.3E-9	-2.4E-13	-6.7E-14	
-13.43686904025008	-7.4E-6	4.0E-9	9.9E-14	-3.4 E-14	
-8.67608167073655	2.8E-5	-3.56E-8	7.4E-14	3.2E-14	
-3.90823248120623	-7.3E-5	3.68E-8	1.6E-13	1.9E-13	

TABLE III

WOODS-SAXON POTENTIAL: THE EXACT EIGNEVALUES AND THE ERRORS FOR ELGT(M,N) FOR SEVERAL UNIFORM STEP SIZES. FOR COMPARAISON, LPM[4,2] ERRORS REPORTED IN [7] ARE ALSO LISTED.

ELGT(M=15,N)							
n	N=6	N=7	N=8	N=9	N=10	N=11	N=12
0	-2.8E-9	3.8E-12	9.1E-13	1.5E-14	1.8E-16	3.0E-16	3.3E-16
1	-1.5E-8	-7.0E-11	1.9E-12	2.8E-13	-1.8E-15	-1.3E-15	-1.0E-15
2	7.4E-9	-8.4E-10	-1.2E-11	1.9E-12	-1.2E-14	-9.1E-15	-7.6E-15
3	4.1E-8	-2.6E-9	4.3E-11	6.8E-12	-3.9E-14	-7.7E-15	-3.0E-15
4	-1.2E-7	-2.7E-8	2.2E-10	2.2E-11	-8.9E-14	-5.7E-15	1.6E-15
5	1.6E-6	-1.2E-7	-6.6E-10	8.5E-11	4.3E-13	-1.0E-14	2.3E-16
6	4.0E-6	2.4E-7	-6.4E-9	-3.5E-10	2.8E-12	3.1E-13	8.0E-15
7	-1.5E-5	2.8E-7	3.5E-8	-2.6E-10	-3.4 E-11	-2.1E-13	1.8E-14
8	-1.2E-5	-1.2E-6	-8.7E-10	2.07E-9	5.4 E-11	-1.9E-12	-6.1E-14
9	2.7E-5	5.9E-7	-1.2 E-7	-2.6E-9	1.1 E-10	4.9E-12	1.8E-14
10	1.3E-5	3.1E-6	6.6E-8	-2.2E-9	-3.4E-10	-3.1E-12	2.8E-13
11	-7.4E-6	-4.1E-6	9.5E-8	1.3E-8	1.6 E-10	-9.7E-12	-6.5E-13
12	2.8E-5	-1.4E-6	-1.3E-7	-1.4E-8	2.6E-10	2.9E-11	5.0E-13
13	-7.3E-5	2.7E-6	2.0E-7	2.1E-9	-4.2E-10	-4.0E-11	1.6E-13

TABLE IV

WOODS-SAXON POTENTIAL: THE ERROR IN THE COMPUTED EIGENVALUES  $\tilde{E}_n$  OBTAINED BY ELGT(M=15,N) FOR N=6,7,.....,12.

We solved this problem by means of ELGT(M,6) for  $M = 15, 30, 60$  and  $120$ ; (that is  $h = 1, \frac{1}{2}, \frac{1}{4}$  and  $\frac{1}{8}$ ).

Table III displays the errors committed by ELGT(M,N) along the errors obtained by Ledoux et al [7] for the Linear Perturbation Method LPM that employs the Airy functions to construct the eigenfunctions.

In order to observe the behaviour of ELGT(M,N) in terms of  $N$ , we solved Example 2 for fixed step size  $h = 1, (M=15)$ , and for  $N = 6, 7, 8, 9, 10, 11$  and  $12$ . The exact errors are listed in Table IV. Figure 2 shows the variation of  $\ln |E_k - \tilde{E}_{k,N}|$ , for  $k = 5, 9, 13$  along the curve of  $\ln |\frac{1}{N!c_N^N}|$ ,  $N = 6, 7, \dots, 12$  where  $c_N^N$  denotes the leading coefficient of  $L_N^*(x)$ . This is an experimental evidence that the ELGT(M,N) errors has an exponential decay as a function of  $N$ .

Example 3.

We wish to solve SLP with potential function of Coffey-Evans form ([10]):

$$V(x) = -2\beta \cos 2x + \beta^2 \sin^2 2x, \quad \beta = 20$$

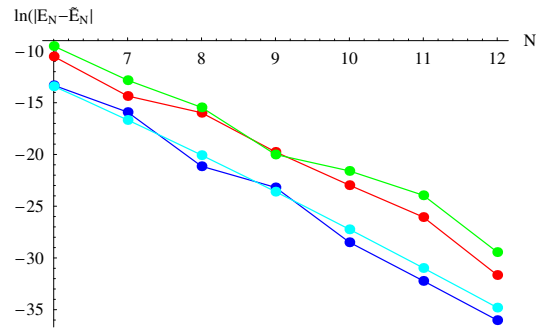


Fig. 2. Experimental evidence for the order of ELGT(M=15,N) in terms of  $N$ . Variation of  $\ln |E_k - \tilde{E}_{k,N}|$ , for  $k = 5, 9, 13$  along the curve of  $\ln |\frac{1}{N!c_N^N}|$ ,  $N = 6, 7, \dots, 12$ .  $C_N^N$ =leading coefficient of  $L_N^*(x)$ .

n	ELGT(M,N=6)			SLCPM12
	$\tilde{E}_N$	M=15 $h = \pi/15$	M=30 $h = \pi/30$	M=28 $h = \pi/38$
0	5.2185E-11	6.8E-7	5.0E-11	-6.9E-10
1	77.91619567704743	1.7E-6	-9.7E-11	-1.3E-9
2	151.46277834649058	-6.1E-6	3.4E-11	2.0E-10
3	151.46322365755634	-5.5E-7	-1.0E-10	-3.6E-10
4	151.46366898838570	-6.0E-6	3.4E-11	2.0E-10
5	220.15422983550180	1.9E-5	2.4E-10	1.2E-9
6	283.09481469529091			
7	283.25074374324649			
8	283.40873540331631			
9	339.37066565320982			

TABLE V

COFFEY-EVANS POTENTIAL: THE ERROR IN THE COMPUTED E.V.S  $\tilde{E}_n$  OBTAINED BY ELGT(M,N=6) FOR  $h = \pi/15$  AND  $h = \pi/30$ . THE LAST COLUMN LISTS RESULTS FROM IXARU [3] OBTAINED BY SLCPM12. NO REFERENCE IS AVAILABLE TO COMPARE THE LAST COMPUTED 4 E.V.S.

in interval  $[a, b]$  where  $a = -\pi/2$  and  $b = \pi/2$  and where  $y(a) = y(b) = 0$ .

The approximate eigenvalues  $\tilde{E}_N$  of this problem were obtained by means of ELGT(M,N) (see Table V). It is obvious that  $\tilde{E}_N$  are close triplets  $\{\tilde{E}_2, \tilde{E}_3, \tilde{E}_4\}$  and  $\{\tilde{E}_6, \tilde{E}_7, \tilde{E}_8\}$ , a characteristic of the (Coffey-Evans) exact eigenvalues.

VI. CONCLUSION

Exponentially Weighted Legendre-Gauss Tau Method ELGT for approximating ODE with strongly oscillatory solution is developed. ELGT procedure produces approximate solution that involves weights  $\{e^{\pm\omega x}\}$  where the frequencies  $\{\omega\}$  are determined by the quadratic equation associated with Constant reference equation. This method is proven to be of high degree of accuracy when used to solve Sturm-Liouville problems and when the interval of integration has a large size.

ACKNOWLEDGMENT

The author acknowledges financial support from the Public Authority for Applied Education and Training in Kuwait (PAAET).

## REFERENCES

- [1] D. Gottlieb and S. A. Orszag, *Numerical Analysis of Spectral Methods: Theory and Applications*, Series in Appl. Math., SIAM, Philadelphia, Pa., 1977
- [2] L. Gr. Ixaru, *Numerical Methods for Differential Equations and Applications*, D.Reidel Publishing Co, Dordrecht, 1984.
- [3] L. Gr. Ixaru, *CP methods for Schrödinger equation*, J. Comput. Appl. Math. 125(2000) 347-357.
- [4] L. Gr. Ixaru and G. Vanden Berghe, *Exponential Fitting*, Kluwer Academic Publishers, Dordrecht, 2004
- [5] J. D. Lambert, *Computational Methods in Ordinary Differential Equations*, Jhon Wiley and Sons, London, 1973.
- [6] C. Lanczos, *Applied Analysis*, Prentice-Hall, Englewood Cliffs, New Jersey, 1956.
- [7] V. Ledoux, M. Rizea, L. Ixaru, G. Vanden Berghe, M. Van Daele, Solution of the Schrödinger equation by a high order perturbation method based on linear reference potential, *Comput. Phys. Commun.* 175:424-439 2006
- [8] E.L. Ortiz, *The Tau Method*, , SIAM J. Numer. Anal. 6(1969) 480-492.
- [9] S. Pruess, Estimating the eigenvalues of Sturm-Liouville problems by approximating the differential equations, *SIAM J. Numer. Anal.* 10:55-68 (1973) .
- [10] J. D. Pryce, *Numerical Solution of Sturm-Liouville Problems*, Clarendon Press, Oxford Science Publications, 1993.
- [11] T.E. Simos, An exponentially-fitted Runge-Kutta method for the numerical integration of initial-value problems with periodic or oscillating solutions, *Comput. Phys. Comm.*, 115:1-8 (1998)



**Mohamed K El Daou.** Born in Lebanon in 1963. I received my M.Sc. in pure mathematics from the University of Leeds, UK in 1988, and in 1992 I completed my Ph.D. in computational mathematics at London Imperial College. Currently I am an associate professor at the Applied Sciences Department in the College of Technological Studies in Kuwait.