

The MATSLISE test set

1 Introduction

A collection of more than 50 examples of Sturm-Liouville problems of the form

$$-(p(x)y'(x))' + q(x)y(x) = Ew(x)y(x) \quad x \in (a, b)$$

has been predefined in the MATSLISE package. This MATSLISE test set collects problems which are commonly used to test Sturm-Liouville software, some examples from physical applications and some classical mathematical problems. Many examples have been taken from earlier test sets:

- the list of test problems provided by John D. Pryce in the book *Numerical Solution of Sturm-Liouville Problems*, Oxford University Press, 1993, and the SLTSTPAK package: *A test package for Sturm-Liouville solvers*, ACM Trans. Math. Software 25 (1999).
- the catalogue of Sturm-Liouville problems composed by W.N. Everitt: *A Catalogue of Sturm-Liouville differential equations*, in: *Sturm-Liouville Theory. Past and Present*, W.O. Amrein, A.M. Hinz, D.B. Pearson (eds), Birkhuser-Verlag 2005.

For some of the examples explicit information on the spectrum of associated boundary value problems is provided against which the program calculated results can be compared.

2 List of Test Problems

1. **Airy equation.** (`Airy.mat`). (SLTSTPAK #27).

$$\begin{aligned} p(x) &= 1 & q(x) &= x & w(x) &= 1 \\ a &= 0 & \text{Regular} & & y(a) &= 0 \\ b &= +\infty & \text{LPN} & & & \end{aligned}$$

Number of eigenvalues: ∞ continuous spectrum: none

Eigenvalues are the zeros of Airy function $Ai(E) = (J_{1/3} + J_{-1/3})(\frac{2}{3}E^{1/3})$.

$$E_0 = 2.3381074104 \quad E_9 = 12.828776753$$

Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p.91.

2. **Anharmonic oscillator potential.** (`anharm_oscillator.mat`).

$$\begin{aligned} p(x) &= 1 & q(x) &= x^2 + \lambda x^2 / (1 + g x^2) & w(x) &= 1 \\ \lambda, g & \text{parameters} \\ a &= -\infty & \text{LPN} \\ b &= +\infty & \text{LPN} \end{aligned}$$

Number of eigenvalues: ∞ continuous spectrum: none

$$\lambda = 0.1, g = 0.1 : \quad E_0 = 1.043173713$$

$$\lambda = 10.0, g = 10.0 : \quad E_0 = 1.580022327$$

Reference: V. Fack and G. Vanden Berghe. (Extended) Numerov method for computing eigenvalues of specific Schrödinger equations. *J. Phys. A: Math. Gen.*, 20 (1987), 4153-4160.

3. Associated Legendre equation in Liouville normal form.

(associated_Legendre_normalform.mat). (SLTSTPAK #16).

$$p(x) = 1 \quad q(x) = -1/4 + (c - 1/4) \sec(x)^2 \quad w(x) = 1$$

Let $c = \nu^2 \geq 0$

$$a = -\pi/2, b = +\pi/2$$

$\nu = 0$: LCN

$\nu = 1/2$: Regular

$0 < \nu < 1, \nu \neq 1/2$: LCN

$\nu \geq 1$: LPN

Number of eigenvalues: ∞ continuous spectrum: none

$$E_k = (k + \nu + 1)(k + \nu), \quad k = 0, 1, \dots$$

Reference: Dunford and Schwartz 1963, Linear Operators: Part II: Spectral Theory, Self Adjoint Operators in Hilbert Space. Pure and Applied Mathematics. Wiley-Interscience, New York, NY p. 1510.

4. BaileyEtAl.mat. (SLTSTPAK #33).

$$p(x) = 1 \quad q(x) = -7x^2 + 0.5x^3 + x^4 \quad w(x) = 0.5$$

$a = -\infty$ LPN

$b = \infty$ LPN

Number of eigenvalues: ∞ continuous spectrum: none

$$E_0 = -24.5175977072 \quad E_5 = 8.10470769427.$$

Reference: P.B. Bailey, M.K. Gordon and L.F. Shampine. Solving Sturm-Liouville eigenproblems. *Sandia Tech. Rep. SAND76-0560*, (1976).

also: Coll and Melius. Theoretical calculation of Raman scattering cross-sections for use in flame analysis. *Rep. SAND79-8204*, (1976).

5. Bender_Orszag.mat. (SLTSTPAK #14).

$$p(x) = 1 \quad q(x) = -m(m+1)/\cosh^2 x \quad w(x) = 1$$

m parameter

$a = -\infty$ LPN/O

$b = +\infty$ LPN/O

Number of eigenvalues: Number of integers in range $0 \leq k < m$

Continuous spectrum: $(0, \infty)$

$$E_k = -(m - k)^2, \quad 0 \leq k < m.$$

Reference: Bender and Orszag. *Adv. Math. Methods for Scientists and Engineers*. McGraw-Hill, N.Y., 1978, p. 28.

6. Bessel equation, order 1/2. (Bessel.mat). (SLTSTPAK #19).

$$p(x) = x \quad q(x) = \alpha/x \quad w(x) = x$$

$$\alpha = \nu^2, \nu = \frac{1}{2}$$

$a = 0$ LCN

$b = 1$ Regular $y(b) = 0$

$$E_k = ((k+1)\pi)^2, \text{ this is } -v'' = Ev \text{ transformed by } v = x^{1/2}u.$$

Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p.81.

7. **Bessel equation in normal form, order 1/4.** (Bessel_normalform.mat). (SLTSTPAK #13).
 $p(x) = 1 \quad q(x) = (\alpha - 1/4)/x^2 \quad w(x) = 1$
 $\alpha = 1/2$
 $a = 0$ LCN
 $b = 1$ Regular $y(b) = 0$
Number of eigenvalues: ∞ continuous spectrum: none.
 $E_0 = 11.7768123, E_9 = 1007.256998$
8. **Bessel equation in normal form, order 0.** (Bessel_normalform0.mat). (SLTSTPAK #18).
 $p(x) = 1 \quad q(x) = (\alpha - 1/4)/x^2 \quad w(x) = 1$
 $\alpha = 0$
 $a = 0$ LCN
 $b = 1$ Regular $y(b) = 0$
 $E_0 = 5.78318596295 \quad E_{19} = 3850.01252885$.
Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p.81.
9. **Bessel equation in normal form, order 0.01.** (Bessel_normalform0.01.mat). (SLTSTPAK #43).
Bessel equation in normal form with $\alpha = 0.01$.
LCN for small $\alpha \geq 0$
Number of eigenvalues: ∞ continuous spectrum: none
 $E_0 = 6.540555712 \quad E_{24} = 6070.441468$.
10. **Biswas potential.** (Biswas.mat).
 $p(x) = 1 \quad q(x) = \mu x^2 + \nu x^4 \quad w(x) = 1$
 μ, ν parameters
 $a = -\infty$ LPN
 $b = +\infty$ LPN
Number of eigenvalues: ∞ continuous spectrum: none
 $\mu = 0.0, \nu = 1.0 : E_0 = 1.06036209$
 $\mu = 1.0, \nu = 1.0 : E_0 = 1.39235164$.
Reference: S.N. Biswas, K. Datta, R.P. Saxena, P.K. Srivastava and V.S. Varma. Eigenvalues of λx^{2m} anharmonic oscillators . *J. Math. Phys.*, 14 (1973), 1190.
also: V. Fack and G. Vanden Berghe. A finite difference approach for the calculation of perturbed oscillator energies. *J. Phys. A: Math. Gen.*, 18 (1985), 3355-3363.
11. **Border of LPN and LCN.** (border_LPN_LCN.mat). (SLTSTPAK #44).
 $p(x) = 1 \quad q(x) = x^{\alpha-2} \quad w(x) = 1$
 $a = 0$ LCN ($\alpha > 0$), LPN ($\alpha \leq 0$)
 $b = 1$ Regular $y(b) = 0$
Number of eigenvalues: ∞ continuous spectrum: none
 $\alpha = +0.01 : E_0 = 15.87305674, E_{24} = 6316.899940$
 $\alpha = -0.01 : E_0 = 15.96808975, E_{24} = 6325.038047$.

12. **Boyd equation.** (Boyd1.mat).

$$p(x) = 1 \quad q(x) = -1/x \quad w(x) = 1$$

$$a = 0 \quad \text{LCN}$$

$$b = 1 \quad \text{Regular} \quad y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_0 = 7.373985, E_4 = 242.705559$$

Reference: J.P. Boyd. Sturm-Liouville eigenvalue problems with an interior pole. *J. Math. Phys.*, 22 (1981), 1575.

also: P.B. Bailey, W.N. Everitt and A. Zettl. Computing eigenvalues of singular Sturm-Liouville problems. *Results in Mathematics*, 20 (1991) 391.

13. **Boyd equation.** (Boyd2.mat).

$$p(x) = r(x)^2 \quad q(x) = -r(x)^2 \ln(x)^2 \quad w(x) = r(x)^2, \quad r(x) = \exp(-(x \ln(x) - x))$$

$$a = 0 \quad \text{LCN}$$

$$b = 1 \quad \text{Regular} \quad y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

Reference: J.P. Boyd. Sturm-Liouville eigenvalue problems with an interior pole. *J. Math. Phys.*, 22 (1981), 1575.

also: P.B. Bailey, W.N. Everitt and A. Zettl. Computing eigenvalues of singular Sturm-Liouville problems. *Results in Mathematics*, 20 (1991) 391.

14. **Close-eigenvalues problem.** (Close_eigenvalues.mat). (SLTSTPAK #38).

$$p(x) = 1 \quad q(x) = x^4 - 25x^2 \quad w(x) = 1$$

Double well version of quartic anharmonic oscillator

$$a = -\infty \quad \text{LPN} \quad \text{Trunc. BC.: } y(a) = 0$$

$$b = +\infty \quad \text{LPN} \quad \text{Trunc. BC.: } y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_0 = -149.2194561 \quad E_1 = -149.2194561 \quad E_{40} = 75.69072485$$

15. **Coffey-Evans equation.** (Coffey_Evans.mat). (SLTSTPAK #7).

$$p(x) = 1 \quad q(x) = -2\beta \cos 2x + \beta^2 \sin^2 2x \quad w(x) = 1$$

$$a = -\pi/2 \quad \text{Regular} \quad y(a) = 0$$

$$b = \pi/2 \quad \text{Regular} \quad y(b) = 0$$

As β increases there are very close eigenvalue triplets $\{E_2, E_3, E_4\}, \{E_6, E_7, E_8\}, \dots$ with the other eigenvalues well separated. E_0 is very close to zero.

$$\beta = 20 : E_0 = 0.000000000000 \quad E_3 = 151.46322365766$$

$$\beta = 30 : E_0 = 0.000000000000 \quad E_3 = 231.66492931296$$

$$\beta = 50 : E_0 = 0.000000000000 \quad E_3 = 391.808191489.$$

16. **Collatz.mat.**

$$p(x) = 1 \quad q(x) = 0 \quad w(x) = 3 + \cos(x)$$

$$a = -\pi \quad \text{Regular} \quad y(a) = 0$$

$$b = +\pi \quad \text{Regular} \quad y(b) = 0$$

$$E_1 = 0.071250472.$$

Reference: L. Collatz. *Differential equations, An Introduction with Applications*. Wiley, Chichester, 1986.

17. **Coulomb potential.** (Coulomb.mat). (SLTSTPAK #30).

With $b = 1$, $u(b) = 0$ also called Boyd equation.

$$p(x) = 1 \quad q(x) = -1/x \quad w(x) = 1$$

$$a = 0 \quad \text{LCN}$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$

$$E_k = -1/[4(k+1)^2], \quad k = 0, 1, \dots$$

Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p.98.

Also: P.B. Bailey, W.N. Everitt and A. Zettl. Computing eigenvalues of singular Sturm-Liouville problems. *Results in Mathematics*, 20 (1991), 391–423.

18. **Mysterious exact $E_0 = 7$. (exact7.mat).** (SLTSTPAK #26).

$$p(x) = x^3 \quad q(x) = x^3 \quad w(x) = x^2$$

$$a = 0 \quad \text{LPN}$$

$$b = 1 \quad \text{regular} \quad y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_0 = 7.0000000000, \quad E_9 = 284.53608972.$$

Reference: S. Pruess, C. Fulton and Y. Xie, Performance of the Sturm-Liouville software package SLEDGE, 1991.

19. **Partially screening exponential-cosine potential. (Expon_cosine_part_screening.mat).**

$$p(x) = 1 \quad q(x) = l(l+1)/x^2 - 2Z_0V_{ec}(x, \lambda, \mu) - 2Z_{as}(1/x - V_{ec}(x, \lambda, \mu)) \quad w(x) = 1$$

$$V_{ec}(x, E, \mu) = e^{-\lambda x} \cos(\mu x)/x.$$

$$a = 0 \quad \text{LCN } (l = 0), \text{ LPN } (l = 5, 10)$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$

$$l = 0, Z_0 = 50, Z_{as} = 1, \lambda = \mu = 0.025: E_0 = -2497.550000612$$

$$l = 5, Z_0 = 50, Z_{as} = 1, \lambda = \mu = 0.025: E_0 = -66.9947751270$$

$$l = 10, Z_0 = 50, Z_{as} = 1, \lambda = \mu = 0.025: E_0 = -18.2144512404$$

Reference: L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe. Highly accurate eigenvalues for the distorted Coulomb potential. *Phys. Rev. E*, 61 (2000).

20. **Screening exponential-cosine potential. (Expon_cosine_screening.mat).**

$$p(x) = 1 \quad q(x) = l(l+1)/x^2 - 2ZV_{ec}(x, \lambda, \mu) \quad w(x) = 1$$

$$V_{ec}(x, \lambda, \mu) = e^{-\lambda x} \cos(\mu x)/x.$$

$$a = 0 \quad \text{LCN } (l = 0), \text{ LPN } (l = 5, 10)$$

$$b = +\infty \quad \text{LPN/O}$$

$l = 0$: Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$

$l = 5$: Number of eigenvalues: 30 continuous spectrum: $(0, \infty)$

$l = 10$: Number of eigenvalues: 25 continuous spectrum: $(0, \infty)$

Reference: L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe. Highly accurate eigenvalues for the distorted Coulomb potential. *Phys. Rev. E*, 61 (2000).

21. **Fourier equation. (Fourier.mat).**

$$p(x) = 1 \quad q(x) = 0 \quad w(x) = 1$$

$$a = 0 \quad \text{Regular} \quad y(a) + y'(a) = 0$$

$$b = \infty \quad \text{Regular} \quad y(b) = 0$$

There is an isolated eigenvalue $E_0 = -1$, with eigenfunction $\exp(-x)$ and a continuous spectrum on $[0, \infty)$

22. **Truncated Gelfand-Levitan.** (`Gelfand_Levitan_truncated.mat`). (SLTSTPAK #6).
 $p(x) = 1$ $q(x) = 2(T \sin 2x + \cos^4 x)/T^2$, $T = 1 + x/2 + \sin(2x)/4$ $w(x) = 1$
 $a = 0$ Regular $y(a) - y(a) = 0$
 $b = 100$ Regular $y(b) = 0$
Non-uniform oscillations of decreasing size in $q(x)$.
Reference: I. Gelfand and B. Levitan. On the determination of a differential equation from its spectral function. *AMS Translations*, 1 (1955), 253-304.
23. **Harmonic oscillator.** (`Harmonic_oscillator.mat`). (SLTSTPAK #28).
 $p(x) = 1$ $q(x) = x^2$ $w(x) = 1$
 $a = -\infty$ LPN
 $b = +\infty$ LPN
Number of eigenvalues: ∞ continuous spectrum: none
 $E_k = 2k + 1$, $k = 0, 1, \dots$
Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p. 1536.
24. **Half-range anharmonic oscillator.** (`HR_anharm_oscillator.mat`). (SLTSTPAK #17).
 $p(x) = 1$ $q(x) = x^\alpha$ $w(x) = 1$, $\alpha > 0$
 $a = 0$ Regular $y(a) = 0$
 $b = +\infty$ LPN
Number of eigenvalues: ∞ continuous spectrum: none
 $\alpha = 2$: $E_k = 4k + 3$, $k = 0, 1, 2, \dots$ (alternate eigenvalues of harmonic oscillator)
 $\alpha = 3$: $E_0 = 3.4505626899$ $E_{24} = 228.52088139$
 $\alpha = 4$: $E_0 = 3.7996730298$ $E_{24} = 397.14132678$
 $\alpha = 5$: $E_0 = 4.0891593149$ $E_{24} = 588.17824969$.
Reference: M. Marletta. Theory and implementation of algorithms for Sturm-Liouville computations. *PhD thesis*. Royal Military College of Science, Cranfield, 1991.
25. **Hulthén partially screening potential.** (`Hulthen_part_screening.mat`).
 $p(x) = 1$ $q(x) = l(l+1)/x^2 - 2Z_0 V_H(x, \lambda) - 2Z_{as}(1/x - V_H(x, \lambda))$ $w(x) = 1$
 $V_H(x, \lambda) = \frac{\lambda e^{-\lambda x}}{1 - e^{-\lambda x}} = \frac{e^{-\lambda x/2}}{x \eta_0((\lambda x/2)^2)}$.
 $a = 0$
 $b = +\infty$ LPN/O
Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$
 $l = 0$, $Z_0 = 50$, $Z_{as} = 1$, $\lambda = 0.025$: $E_0 = -2498.775153125$
 $l = 5$, $Z_0 = 50$, $Z_{as} = 1$, $\lambda = 0.025$: $E_0 = -68.2234257245$
 $l = 10$, $Z_0 = 50$, $Z_{as} = 1$, $\lambda = 0.025$: $E_0 = -19.4490716959$.
Reference: L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe. Highly accurate eigenvalues for the distorted Coulomb potential. *Phys. Rev. E*, 61 (2000).
26. **Hulthén screening potential.** (`Hulthen.mat`).
 $p(x) = 1$ $q(x) = l(l+1)/x^2 - 2Z V_H(x, \lambda)$ $w(x) = 1$
 $V_H(x, \lambda) = \frac{\lambda e^{-\lambda x}}{1 - e^{-\lambda x}}$.
 $a = 0$
 $b = +\infty$ LPN/O
Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$
Exact eigenvalues only known for $l = 0$: $E_k = -[2Z - (k+1)^2 \lambda]^2 / 4(k+1)^2$, $k = 0, 1, \dots, k_{max} =$

$$\left| \sqrt{2Z/\lambda} \right| - 1.$$

$$Z = 50, \lambda = 0.025, l = 0: E_0 = -2498.7501562500, E_9 = -23.76562500$$

$$Z = 50, \lambda = 0.025, l = 5: E_0 = -68.1985069764, E_9 = -9.8947071396$$

$$Z = 50, \lambda = 0.025, l = 10: E_0 = -19.42433530452, E_9 = -5.05679485664$$

Reference: L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe. Highly accurate eigenvalues for the distorted Coulomb potential. *Phys. Rev. E*, 61 (2000).

27. Hydrogen atom. (hydrogen.mat). (SLTSTPAK #29).

$$p(x) = 1 \quad q(x) = -1/x + 2/x^2 \quad w(x) = 1$$

$$a = 0 \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$

$$E_k = -1/(2k+4)^2, k = 0, 1, \dots$$

Reference: E.C. Titchmarsh. *Eigenfunction expansions associated with second-order differential equations*. Oxford University Press, 1946, p.98.

28. Truncated hydrogen equation. (hydrogen_truncated.mat). (SLTSTPAK #4).

$$p(x) = 1 \quad q(x) = -1/x + 2/x^2 \quad w(x) = 1$$

$$a = 0 \quad \text{LPN}$$

$$b = 1000 \quad \text{Regular} \quad y(b) = 0$$

$$E_0 = -6.2500000000 \cdot 10^{-2} \quad E_9 = -2.066115702478 \cdot 10^{-3}$$

$$E_{17} = -2.5757359232 \cdot 10^{-4} \quad E_{18} = 2.873901310 \cdot 10^{-5}$$

The lower eigenvalues approximate those of the infinite problem.

29. Jörgens equation. (Jorgens.mat).

$$p(x) = 1 \quad q(x) = \exp(2x)/4 - k \exp(x) \quad w(x) = 1$$

k parameter

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN}$$

continuous spectrum: $(0, \infty)$

$k \leq 1/2$: no eigenvalues

$$h < k - 1/2 \leq h + 1 \text{ for } h = 0, 1, 2, 3, \dots: E_n = -(k - 1/2 - n)^2, n = 0, 1, 2, \dots, h.$$

Reference: P.B. Bailey, W.N. Everitt and A. Zettl. The SLEIGN2 Sturm-Liouville code.

30. Klotter.mat. (SLTSTPAK #3).

$$p(x) = 1 \quad q(x) = 3/(4x^2) \quad w(x) = 64\pi^2/(9x^6)$$

$$a = 8/7 \quad \text{Regular} \quad y(a) = 0$$

$$b = 8 \quad \text{Regular} \quad y(b) = 0$$

$$E_k = (k+1)^2, k = 0, 1, \dots$$

Transformation of $-d^2v/dt^2 = Ev$, $v(\pi/48) = 0 = v(49\pi/48)$ by $t = \frac{4\pi}{3x^2}$, $u = x^{3/2}v$. (The original reference had $a = 1$, $b = 2$ corresponding to $v(\pi/3) = 0 = v(4\pi/3)$ which is much tamer.

Reference: Klotter. *Technische Schwingungslehre*, I. Heidelberg, 1978, p.12.

31. Laguerre's equation. (Laguerre.mat). (SLTSTPAK #32).

$$p(x) = 1 \quad q(x) = x^2 + 3/(4x^2) \quad w(x) = 1$$

$$a = 0 \quad \text{LPN} \quad \text{Trunc. BC: } y(a) = 0$$

$$b = +\infty \quad \text{LPN} \quad \text{Trunc. BC: } y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_k = 4(k+1), k = 0, 1, \dots$$

32. **Latzko equation.** (`Latzko.mat`). (SLTSTPAK #24).

$p(x) = 1 - x^7$ $q(x) = 0$ $w(x) = x^7$
 $a = 0$ Regular $y(a) = 0$
 $b = 1$ LCN
Number of eigenvalues: ∞ continuous spectrum: none
 $E_0 = 8.7274703526$, $E_2 = 435.06333218$.

33. **Legendre equation.** (`Legendre.mat`).

$p(x) = (1 - x^2)$ $q(x) = 1/4$ $w(x) = 1$
 $a = -1$ LCN
 $b = 1$ LCN
Number of eigenvalues: ∞ continuous spectrum: none
 $E_k = k(k+1) + 1/4$, $k = 0, 1, \dots$

34. **Legendre equation.** (`Legendre2.mat`). (SLTSTPAK #20).

$p(x) = (1 - x^2)$ $q(x) = 0$ $w(x) = 1$
 $a = -1$ LCN
 $b = 1$ LCN
Number of eigenvalues: ∞ continuous spectrum: none
 $E_k = k(k+1)$, $k = 0, 1, \dots$

35. **Truncated Lennard-Jones LJ(12,6).** (`LennardJones.mat`). (SLTSTPAK #8).

$p(x) = 1$ $q(x) = \frac{1.92}{16.858056} D_e ((R_e/x)^{12} - 2(R_e/x)^6) + \frac{l(l+1)}{x^2}$ $w(x) = 1$
 $D_e = 62$, $R_e = 3.56$, $l = 7$
 $a = 0$ LPN
 $b = 38.85$ Regular $y(b) = 0$
This shows that close eigenvalues can happen with highly asymmetric potentials
 $E_0 = 0.0899594272$, $E_1 = 0.0899769187$
As b varies from the value 38.85 the splitting $E_1 - E_0$ increases.
 $q(x)$ gets very large at 0.

36. **log.mat.** (SLTSTPAK #11).

$p(x) = 1$ $q(x) = \ln x$ $w(x) = 1$
 $a = 0$ Regular $y(a) = 0$
 $b = 4$ Regular $y(b) = 0$
 $E_0 = 1.1248168097$ $E_{24} = 385.92821596$.

Reference: 11th problem in the Pruess-Fulton test set (S. Pruess, C.T. Fulton and Yuantao Xie. Performance of the Sturm-Liouville software package SLEDGE. *Technical Report MCS-91-19*. Colorado School of Mines, 1991.).

37. **Lohner equation.** (`Lohner.mat`).

$p(x) = 1$ $q(x) = -1000x$ $w(x) = 1$
 $a = 0$ Regular $y(a) = 0$
 $b = 1$ Regular $y(b) = 0$.
 $E_0 = -766.189259$, $E_9 = 508.10800738$, $E_{49} = 24174.8549$.

38. **Marletta equation.** (`Marletta.mat`).

problem with 'pseudo-eigenvalue': some codes report $E = 0$ as a second eigenvalue.
 $p(x) = 1$ $q(x) = \frac{3(x-31)}{4(x+1)(x+4)^2}$ $w(x) = 1$
 $a = 0$ Regular $5y(a) + 8y'(a) = 0$
 $b = +\infty$ LPN

Number of eigenvalues: 1 continuous spectrum: $(0, \infty)$
 $E_0 = -1.18521$

39. **Mathieu equation.** (`Mathieu.mat`). (SLTSTPAK #2).

$$p(x) = 1 \quad q(x) = 2r \cos(2x) \quad w(x) = 1$$

r parameter

$$a = 0 \quad \text{Regular} \quad y(a) = 0$$

$$b = \pi \quad \text{Regular} \quad y(b) = 0.$$

$$r = 1: E_0 = -0.110248816992, E_9 = 100.00505067516$$

Lower eigenvalues cluster in moderately tight pairs as r becomes large negative.

40. **Version of Mathieu equation.** (`Mathieu_version.mat`). (SLTSTPAK #5).

$$p(x) = 1 \quad q(x) = c \cos(x) \quad w(x) = 1$$

c parameter

$$a = 0 \quad \text{Regular} \quad y(a) = 0$$

$$b = 40 \quad \text{Regular} \quad y(b) = 0$$

The lower eigenvalues form clusters of 6; more and tighter clusters as c increases.

$$c = 5: E_0 = -3.4842389, E_5 = -3.4841397, E_6 = -0.599544, E_{11} = -0.595602, E_{12} = 1.9329149, \\ E_{17} = 1.9954588.$$

41. **Morse potential.** (`Morse1.mat`). (SLTSTPAK #35).

$$p(x) = 1 \quad q(x) = 9e^{-2x} - 18e^{-x} \quad w(x) = 1$$

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: 3 continuous spectrum: $(0, \infty)$

$$E_k = -0.25 - (3 - k)(2 - k), k = 0, 1, 2.$$

Reference: Morse, *Phys. Rev.*, 34 (1929), 59-61.

42. **Morse potential.** (`Morse2.mat`). (SLTSTPAK #39).

$$p(x) = 1 \quad q(x) = 8000e^{-3x} - 16000e^{-3x/2} \quad w(x) = 1$$

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: 60 continuous spectrum: $(0, \infty)$

With this deep well, a large truncated interval seems to be needed to give good approximations to higher eigenvalues.

$$E_0 = -7866.398421 \quad E_{57} = -10.193455 \quad E_{58} = -2.865298.$$

Reference: M. Marletta. Theory and implementation of algorithms for Sturm-Liouville computations. *PhD thesis*. Royal Military College of Science, Cranfield, 1991, Ch.8.

43. **Morse potential.** (`Morse3.mat`). (SLTSTPAK #36).

$$p(x) = 1 \quad q(x) = 2/x^2 - 2000(2e^{-1.7(x-1.3)} - e^{-3.4(x-1.3)}) \quad w(x) = 1$$

$$a = 0 \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN/O}$$

Number of eigenvalues: 26 continuous spectrum: none

$$E_0 = -1923.529655 \quad E_1 = -1777.290819 \quad E_{13} = -473.29712549.$$

Reference: Secrest et al., *J. Chem. Phys.*, 37 (1962), 830-835.

44. **Nasty p^{-1} , nice q and w .** (`nastyP.mat`). (SLTSTPAK #10).

$$p(x) = \sqrt{1 - x^2} \quad q(x) = 0 \quad w(x) = 1$$

Regular problem that looks singular

$a = -1$ Regular $py'(a) = 0$
 $b = 1$ Regular $y(b) = 0$
 $E_0 = 0.385681872027$, $E_{24} = 1031.628249437$.

45. **Nasty w , nice q and p^{-1} . (nastyW.mat). (SLTSTPAK #9).**

$p(x) = 1/\sqrt{1-x^2}$ $q(x) = 0$ $w(x) = 1/\sqrt{1-x^2}$
 Regular problem that looks singular
 $a = -1$ Regular $y(a) = 0$
 $b = 1$ Regular $y(b) = 0$
 $E_0 = 3.55927996$, $E_9 = 258.8005854$, $E_{24} = 1572.635284$.

46. **Paine problem 1. (Paine1.mat).**

$p(x) = 1$ $q(x) = e^x$ $w(x) = 1$
 $a = 0$ Regular $y(a) = 0$
 $b = \pi$ Regular $y(b) = 0$
 $E_0 = 4.8966693800$ $E_1 = 10.045189893$.

Reference: Reference: J.W. Paine, F.R. de Hoog, and R.S. Anderssen. On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems. *Computing*, 26 (1981) 123-139.

47. **Paine problem 2. (Paine2.mat). (SLTSTPAK #1).**

$p(x) = 1$ $q(x) = \frac{1}{(x+0.1)^2}$ $w(x) = 1$
 $a = 0$ Regular $y(a) = 0$
 $b = \pi$ Regular $y(b) = 0$
 $E_0 = 1.5198658211$ $E_1 = 4.9433098221$.

Reference: Reference: J.W. Paine, F.R. de Hoog, and R.S. Anderssen. On the correction of finite difference eigenvalue approximations for Sturm-Liouville problems. *Computing*, 26 (1981) 123-139.

48. **PaineSLP.mat.**

$p(x) = (u+x)^3$ $q(x) = 4(u+x)$ $w(x) = (u+x)^5$ $u = \sqrt{0.2}$
 $a = 0$ Regular $y(a) = 0$
 $b = -u + \sqrt{u^2 + 2\pi}$ Regular $y(b) = 0$

Using Liouville's transformation, this problem becomes a Schrodinger equation with $q(x) = 1/(x+0.1)^2$, i.e. Paine problem 2.

Reference: L.Gr. Ixaru, H. De Meyer and G. Vanden Berghe. SLCPM12 - A program for solving regular Sturm-Liouville problems. *Comp. Phys. Comm.*, 118 (1999).

49. **Pruess_Fulton19.mat. (SLTSTPAK #25).**

$p(x) = x^4$ $q(x) = -2x^2$ $w(x) = x^4$
 $a = 0$ LCN
 $b = 1$ Regular $y(b) = 0$
 $E_k = ((k+1)\pi)^2$, $k = 0, 1, \dots$

Reference: 19th problem in the Pruess-Fulton test set.

50. **Pure attractive Coulomb potential. (pure_Coulomb.mat).**

$p(x) = 1$ $q(x) = l(l+1)/x^2 - 2Z/x$ $w(x) = 1$
 $a = 0$ LCN
 $b = +\infty$ LPN/O
 Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$
 $E_k = -Z^2/(n+l+1)^2$, $k = 0, 1, \dots$

51. **Quartic anharmonic oscillator.** (`quartic_anharm_osc.mat`). (SLTSTPAK #37).

$$p(x) = 1 \quad q(x) = x^4 + x^2 \quad w(x) = 1$$

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN}$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_0 = 1.3923516415 \quad E_9 = 46.965069501.$$

Reference: Scott, Shampine and Wing. *Computing*, 4 (1969), 10-23.

52. **The Razavy potential.** (`Razavy.mat`).

$$p(x) = 1 \quad q(x) = (1/8)m^2(\cosh(4x) - 1) - m(n+1)\cosh(2x) \quad w(x) = 1$$

n, m parameters

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN}$$

Number of eigenvalues: ∞ continuous spectrum: none

$$n = 1, m = 1 : E_0 = -2, E_1 = 0$$

$$n = 2, m = 1 : E_0 = -2(1 + \sqrt{2}), E_1 = -4, E_2 = 2(\sqrt{2} - 1)$$

$$n = 1, m = 10 : E_0 = -11, E_1 = 9$$

$$n = 2, m = 10 : E_0 = -2(1 + \sqrt{101}), E_1 = -4, E_2 = 2(\sqrt{101} - 1).$$

Reference: V. Fack, G. Vanden Berghe. (Extended) Numerov method for computing eigenvalues of specific Schrödinger equations. *J. Phys. A: Math. Gen.*, 20 (1987), 4153-4160.

also: M. Razavy. *Am. J. Phys.*, 48 (1980), 285.

53. **Sears-Titchmarsh.** (`Sears_Titchmarsh.mat`).

$$p(x) = 1 \quad q(x) = -\exp(2x) \quad w(x) = 1$$

$$a = 0 \quad \text{regular}$$

$$b = +\infty \quad \text{LCO}$$

54. **simple_slp1.mat.**

$$p(x) = 1 \quad q(x) = 0 \quad w(x) = 1$$

$$a = 0 \quad \text{Regular} \quad y(a) = 0$$

$$b = 1 \quad \text{Regular} \quad y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_k = ((k+1)\pi)^2.$$

55. **simple_slp2.mat.**

$$p(x) = 1 \quad q(x) = 0 \quad w(x) = 1/x^2$$

$$a = 1 \quad \text{Regular} \quad y(a) = 0$$

$$b = e \quad \text{Regular} \quad y(b) = 0$$

Number of eigenvalues: ∞ continuous spectrum: none

$$E_k = ((k+1)\pi)^2 + 1/4.$$

56. **Symmetric double-well potential.** (`symm_double_well.mat`).

$$p(x) = 1 \quad q(x) = x^6 - Bx^2 \quad w(x) = 1$$

B parameter

$$a = -\infty \quad \text{LPN}$$

$$b = +\infty \quad \text{LPN}$$

Number of eigenvalues: ∞ continuous spectrum: none

$$B = 11: \text{known exact eigenvalues} = \{-8, 0, 8\}$$

$$B = 13: \text{known exact eigenvalues} = \{-11.3137085, 0, 11.3137085\}$$

$B = 15$: known exact eigenvalues = $\{-15.077508510, -3.559316943, 3.559316943, 15.077508510\}$.
Reference: V. Fack, G. Vanden Berghe. (Extended) Numerov method for computing eigenvalues of specific Schrödinger equations. *J. Phys. A: Math. Gen.*, 20 (1987), 4153-4160.

57. **Transformed hydrogen equation.** (`transformedHydrogen.mat`). (SLTSTPAK #31)

$p(x) = x^2$ $q(x) = l(l+1) - x$ $w(x) = x^2$
 $a = 0$ $l = 0$: LCN, $l > 0$: LPN
 $b = +\infty$ LPN/O
Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$
 $E_k = -1/[4(k+l+1)^2]$, $k = 0, 1, \dots$

58. **(Slightly) Tricky $q(x)$.** (`tricky_q.mat`). (SLTSTPAK #21).

$p(x) = 1$ $q(x) = -10/x^{1.5}$, $w(x) = 1$
 $a = 0$ LCN
 $b = 1$ Regular $y(b) = 0$
Number of eigenvalues: ∞ continuous spectrum: none

59. **VandenBerghe.mat.** (SLTSTPAK #42).

$p(x) = 1$ $q(x) = l(l+1)/x^2 + (-1 + 5e^{-2x})/x$ $w(x) = 1$
 $a = 0$ LCN($l = 0$), LPN($l > 0$)
 $b = +\infty$ LPN/O
Number of eigenvalues: ∞ continuous spectrum: $(0, \infty)$
 $l = 0$: $E_0 = -0.156358880971$ $E_2 = -0.023484895664$
 $l = 1$: $E_0 = -0.061681846633$ $E_2 = -0.015501561691$.
Coulomb-type decay at $x = \infty$ similar to hydrogen atom. Need to truncate very far out to obtain higher eigenvalues accurately.
Reference: G. Vanden Berghe, V. Fack and H. de Meyer. *J. Comp. Appl. Math.*, 28(1989), 391-401.

60. **Wicke_Harris.mat.** (SLTSTPAK #40).

$p(x) = 1$ $q(x) = 1250e^{-83.363(x-2.47826)^2} + 3906.25(1 - e^{2.3237-x})^2$ $w(x) = 1$
 $a = 0$ Regular $y(a) = 0$
 $b = +\infty$ LPN/O
Number of eigenvalues: 62 continuous spectrum: $(3906.25, \infty)$
 $E_0 = 163.2238872$ $E_9 = 1277.53684$
This has a spike at the bottom of the well.
Reference: Wicke and Harris, Comparison of three numerical techniques for calculating eigenvalues of an unsymmetrical double minimum oscillator. *J. Chem. Phys.*, 64 (1976), 5236.

61. **Woods-Saxon potential.** (`Woods_Saxon.mat`). (SLTSTPAK #41).

$p(x) = 1$ $q(x) = l(l+1)/x^2 - 50(1 - 5t/(3(1+t)))/(1+t)$ $w(x) = 1$
 $t = e^{(x-7)/0.6}$
 $a = 0$ LPN $y(a) = 0$
 $b = +\infty$ LPN/O
 $l = 0$: Number of eigenvalues: 14 continuous spectrum: $(0, \infty)$
 $E_0 = -49.457788728$ $E_{10} = -18.094688282$
 $l = 2$: Number of eigenvalues: 13 continuous spectrum: $(0, \infty)$
 $E_0 = -48.349481052$ $E_{10} = -13.522303353$.
Reference: G. Vanden Berghe, V. Fack and H. de Meyer, *J. Comp. Appl. Math.*, 28(1989), 391-401.

3 Problems with Discontinuous Coefficients

1. **Approximate Harmonic oscillator.** (`approximateHarmonicOscillator.m`). (SLTST-PAK#53).

$p(x) = 1$ $q(x)$ = piecewise linear function joining the points (x, x^2) for x an integer $w(x) = 1$

$a = -\infty$ LPN

$b = +\infty$ LPN