SLEIGN2: THE HELP FILE

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This copy of the HELP data has been written in AMS-LaTeX in view of the considerable amount of mathematical formulae involved in the text. The user should note that when HELP is accessed in MAKEPQW and/or DRIVE the corresponding data is given in Fortran notation. The best use of this HELP data can be made by printing out a copy of this AMS-LaTeX file to have available when the code files are in use.

HELP may be called at any point where the program halts and displays (h?), by pressing "h <ENTER>". To RETURN from HELP, press "r <ENTER>". To QUIT at any program halt, press "q <ENTER>".

This AMS-LaTeX file is supplied as a separate text file within the SLEIGN2 package; it can be accessed on-line in both the MAKEPQW (if used) and DRIVE files.

HELP contains information to aid the user in entering data: on the coefficient functions p, q, w; on the self-adjoint, separated and coupled, regular and singular, boundary conditions; on the limit-circle boundary condition functions u, v at the endpoint a and U, V at the endpoint b of the interval (a, b); on the endpoint classifications of the differential equation; on DEFAULT entry; on eigenvalue indexes; on IFLAG information; and on the general use of the program SLEIGN2.

The 17 sections of HELP are:

H1: Overview of HELP. H2: File name entry. H3: The differential equation. H4: endpoint classification. H5: DEFAULT entry. H6: Self-adjoint limit-circle boundary conditions. H7: General self-adjoint boundary conditions. H8: Recording the results. H9: Type and choice of interval. H10: Entry of endpoints. H11: endpoint values of p, q, w. H12: Initial value problems. H13: Indexing of eigenvalues. H14: Entry of eigenvalue index, initial guess, and tolerance. H15: IFLAG information. H16: Plotting. H17: Indexing of eigenvalues.

HELP can be accessed at each point in MAKEPQW and DRIVE where the user is asked for input, by pressing "h <ENTER>"; this places the user at the appropriate HELP section. Once in HELP, the user can scroll the further HELP sections by repeatedly pressing "h <ENTER>", or jump to a specific HELP section Hn (n =1,2,...17) by typing "hn <ENTER>"; to return to the place in the program from which HELP is called, press "r <ENTER>".

H2: File name entry.

MAKEPQW is used to create a Fortran file containing the coefficients p, q, w defining the differential equation, and the boundary condition functions u, v and U, V if required. The file must be given a NEW filename which is acceptable to your Fortran compiler. For example, it might be called bessel.f or bessel.for depending upon your compiler.

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The same naming considerations apply if the Fortran file is prepared other than with the use of MAKEPQW.

H3: The differential equation.

The prompt "Input p (or q or w) =" requests you to type in a Fortran expression defining the function p, which is one of the three coefficient functions defining the Sturm-Liouville differential equation

$$(*) \qquad -(py')' + qy = \lambda wy$$

to be considered on some interval (a, b) of the real line. The actual interval used in a particular problem can be chosen later, and may be either the whole interval (a, b) where the coefficient functions p, q, w are defined, or on any sub-interval (a', b') of (a, b); $a = \infty$ and/or $b = +\infty$ are allowable choices for the endpoints.

The coefficient functions p, q, w of the differential equation may be chosen arbitrarily but must satisfy the following conditions:

(1) p, q, w are real-valued throughout (a, b).

(2) p, q, w are piece-wise continuous and defined throughout the interior of the interval (a, b).

(3) p and w are strictly positive in (a, b).

For better error analysis in the numerical procedures, condition (2) above is often replaced with

(2′) p, q, w are four times continuously differentiable on (a, b).

The behaviour of p, q, w near the endpoints a and b is critical to the classification of the differential equation (see H4 and H11).

H4: endpoint classification.

The correct classification of the endpoints a and b is essential to the working of the SLEIGN2 program. To classify the endpoints, it is convenient to choose a point c in (a, b); *i.e.* $a < c < b$. Subject to the general conditions on the coefficient functions p, q, w (see H3):

(1) a is REGULAR (say R) if $-\infty < a$, p, q, w are piece-wise continuous on $[a, c]$, and $p(a) > 0, w(a) > 0$.

(2) a is WEAKLY REGULAR (say WR) if $-\infty < a$, a is not R and

$$\int_a^c \left\{p^{-1} + |q| + w\right\} < +\infty.$$

If endpoint a is neither R nor WR, then a is SINGULAR; that is, either $-\infty = a$, or $-\infty < a$ and

$$\int_a^c \left\{p^{-1} + |q| + w\right\} = +\infty.$$

(3) The SINGULAR endpoint a is LIMIT-CIRCLE NON-OSCILLATORY (say LCNO) if for some real value of the spectral parameter λ ALL real-valued solutions y of the differential equation

$$-(py')' + qy = \lambda wy \text{ on } (a, c]$$

satisfy the conditions:

$$\int_a^c w\,|y|^2 < +\infty$$

and y has at most a finite number of zeros in $(a, c]$.

(4) The SINGULAR endpoint a is LIMIT-CIRCLE OSCILLATORY (say LCO) if for some real λ ALL real-valued solutions of the differential equation (*) satisfy the conditions:

$$\int_a^c w\,|y|^2 < +\infty$$

and y has an infinite number of zeros in $(a, c]$.

(5) The SINGULAR endpoint a is LIMIT POINT (say LP) if for some real λ at least one solution of the differential equation $(*)$ satisfies the condition:

$$\int_a^c w\,|y|^2 = +\infty.$$

There is a similar classification of the endpoint b into one of the five distinct cases R, WR, LCNO, LCO, LP.

Although the classification of singular endpoints invokes a real value of the parameter λ, this classification is invariant in λ; all real choices of λ lead to the same classification.

In determining the classification of singular endpoints for the differential equation $(*)$, it is often convenient to start with the choice $\lambda = 0$ in attempting to find solutions (particularly when $q = 0$ on (a, b)); however, see example 7 below.

See H6 on the use of maximal domain functions to determine the classification at singular endpoints.

EXAMPLES:

1. $-y'' = \lambda y$ is R at both endpoints of (a, b) when a and b are finite.

2. $-y'' = \lambda y$ on $(-\infty, +\infty)$ is LP at both endpoints.

3. $-\left(x^{1/2}y'(x)\right)' = \lambda x^{-1/2}y(x)$ for all $x \in (0, +\infty)$ is WR at 0 and LP at $+\infty$ (take $\lambda = 0$ in $(*)$). See the file xamples.f, #10 (Weakly Regular).

4. $-((1 - x^2)y'(x))' = \lambda y(x)$ for all $x \in (-1, +1)$ is LCNO at both ends (take $\lambda = 0$ in $(*)$). See xamples.f, #1 (Legendre).

5. $-y''(x) + Cx^{-2}y(x) = \lambda y(x)$ for all $x \in (0, +\infty)$ is LP at $+\infty$; however at 0 the equation illustrates a number of different classifications(take $\lambda = 0$ in $(*)$) as follows:

LP $C \geq 3/4$; LCNO for $-1/4 \leq C < 3/4$ (but $C \neq 0$); LCO for $C < -1/4$.

6. $-(xy'(x))' - x^{-1}y(x) = \lambda y(x)$ for all $x \in (0, \infty)$ is LCO at 0 and LP $+\infty$ (take $\lambda = 0$ in $(*)$ with solutions $\cos(\ln(x))$ and $\sin(\ln(x))$. See xamples.f, #7 (BEZ).

7. $-(xy'(x))' - xy(x) = \lambda x^{-1}y(x)$ for all $x \in (0, +\infty)$ is LP at 0 and LCO at $+\infty$ (take $\lambda = -1/4$ in $(*)$ with solutions $x^{-1/2}\cos(x)$ and $x^{-1/2}\sin(x)$). See xamples.f, #6 (Sears-Titchmarsh).

8. $-y''(x) + x\sin(x)y(x) = \lambda y(x)$ on $(0, +\infty)$ is R at 0 and LP at $+\infty$. See xamples.f #30 (Littlewood-McLeod).

H5: DEFAULT entry.

The complete range of problems for which SLEIGN2 is applicable can only be reached by appropriate entries under endpoint classification and boundary conditions. However, there

is a DEFAULT application which requires no detailed entry of endpoint classification or boundary conditions, subject to:

1) The DEFAULT application CANNOT be used at a LCO endpoint.

2) If an endpoint a is R, then the Dirichlet boundary condition $y(a) = 0$ is automatically used.

3) If an endpoint a is WR, then the following boundary condition is automatically applied:

(i) if $p(a) = 0$, and both q and w are bounded near a, then the Dirichlet boundary condition $y(a) = 0$ is used

(ii) if $p(a) > 0$, and q and/or w are not bounded near a, then the Neumann boundary condition $y'(a) = 0$ is used.

If $p(a) = 0$, and q and/or w are not bounded near a, then no reliable information, in general, can be given on the DEFAULT boundary condition.

4) If an endpoint is LCNO, then in most cases the principal or Friedrichs boundary condition is applied (see H6).

5) If an endpoint is LP, then the normal LP procedure is applied (see H7(1.)).

If you choose the DEFAULT condition, then no entry is required for the u, v and U, V boundary condition functions.

H6: Limit-circle (LC) boundary conditions.

At an endpoint a, the LC type separated boundary condition is of the form (similar remarks throughout apply to the endpoint b with U, V being boundary condition functions at b)

$$A1[y, u](a) + A2[y, v](a) = 0 \tag{**}$$

where y is a solution of the differential equation

$$-(py')' + qy = \lambda wy \text{ on } (a, b) \tag{*}$$

Here $A1, A2$ are real numbers, not both zero; u and v are boundary condition functions at a; and for real-valued y and u the form $[y, u](\cdot)$ is defined by

$$[y, u](x) = y(x)(pu')(x) - (py')(x)u(x) \text{ for all } x \in (a, b).$$

If neither endpoint is LP then there are also self-adjoint coupled boundary conditions. These have a canonical form given by

$$Y(b) = \exp(i\alpha)\mathbf{K}Y(a)$$

where

(i) $\mathbf{K}$ is a real 2×2 matrix with $\det(\mathbf{K}) = 1$

(ii) the parameter α is restricted to $\alpha \in (-\pi, \pi]$

(iii) Y is the solution column vector $Y(a) = [y(a), (py')(a)]^T$ at a regular R endpoint a, and Y is the "singular solution vector" $Y(a) = [[y, u](a), [y, v](a)]^T$ at a singular LC endpoint a. Similarly at the right endpoint b with U, V.

The object of this section is to provide help in choosing appropriate functions u and v in $(**)$ (or in choosing U, V) given the differential equation $(*)$. Full details of the boundary conditions for $(*)$ are discussed in H7; here it is sufficient to say that the limit-circle type boundary condition $(**)$ must be applied at any endpoint in the LCNO, LCO classification,

but can also be used in the R, WR classification subject to the appropriate choice of u and v, and U and V.

Let $(*)$ be R, WR, LCNO, or LCO at endpoint a and choose c in (a,b).. Then *either* u and v are a pair of linearly independent real solutions of $(*)$ on $(a,c]$ for any chosen real value of λ, *or* u and v are a pair of real-valued maximal domain functions defined on $(a,c]$ satisfying $[u,v](a) \neq 0$.

The maximal domain $D(a,b)$ is defined by

$$D(a,b) = \{f : (a,b) \to \mathbb{C} : \begin{array}{l}(i)\ f \text{ and } pf' \in AC_{\mathrm{loc}}(a,b) \\ (ii)\ f \text{ and } w^{-1}(-(pf')' + qf) \in L^2((a,b);w)\}.\end{array}$$

The domains $D(a,c]$ and $D[c,b)$ are the restrictions of the functions $D(a,b)$ to the sub-intervals. It is known that for all $f, g \in D(a,c]$ the limit

$$[f,g](a) = \lim_{x \to a} [f,g](x)$$

exists and is finite. If $(*)$ is LCNO or LCO at a, then all solutions of (*) belong to $D(a,c]$ for all values of λ. The boundary condition $(**)$ is essential in the LCNO and LCO cases but can also be used with advantage in some R and WR cases.

In the R, WR, and LCNO cases, but not in the LCO case, the boundary condition functions can always be chosen so that

$$\lim_{x \to a} \frac{u(x)}{v(x)} = 0$$

and it is recommended that this normalisation be effected, but this is not essential; this normalization has been entered in the examples given below. In this case, the boundary condition $[y,u](a) = 0$ (*i.e.* $A1 = 1, A2 = 0$ in $(**)$) is called the principal or Friedrichs boundary condition at a.

In the case when endpoints a and b are, independently, in the R, WR, LCNO, or LCO classification, it may be that symmetry or other reasons permit one set of boundary condition functions to be used at both end-points (see xamples.f, #1 (Legendre)). In other cases, different pairs must be chosen for each endpoint (see xamples.f: #16 (Jacobi), #18 (Dunsch), and #19 (Donsch)).

Note that a solution pair u, v is always a maximal domain pair, but not necessarily vice versa. EXAMPLES:

1. $-y'' = \lambda y$ on $[0,\pi]$ is R at 0 and R at π. At 0, with $\lambda = 0$, a solution pair is

$$u(x) = x, v(x) = 1 \text{ for all } x \in [0,\pi].$$

At π,with $\lambda = 1$, a solution pair is

$$U(x) = \sin(x), V(x) = \cos(x) \text{ for all } x \in [0,\pi].$$

2. $-(x^{1/2}y'(x))' = \lambda x^{-1/2} y(x)$ on $(0,1]$ is WR at 0 and R at 1. (The general solutions of this equation are $u(x) = \cos(2x^{1/2}\sqrt{\lambda})$ and $v(x) = \sin(2x^{1/2}\sqrt{\lambda})$.)

At 0, $\lambda = 0$, a solution pair is

$$u(x) = 2x^{1/2}, v(x) = 1.$$

At 1, with $\lambda = \pi^2/4$, a solution pair is

$$U(x) = \sin(\pi x^{1/2}), V(x) = \cos(\pi x^{1/2}).$$

Also at 1, with $\lambda = 0$, a solution pair is

$$U(x) = 2(1 - x^{1/2}), V(x) = 1.$$

See also xamples.f, #10 (Weakly Regular).

3. $-((1 - x^2)y'(x))' = \lambda y(x)$ on $(-1, +1)$ is LCNO at both endpoints.

At both ± 1, $\lambda = 0$, a solution pair is

$$u(x) = 1, v(x) = \ln((1 + x)/(1 - x))/2$$

At $+1$, a maximal domain pair is $U(x) = 1, V(x) = \ln(1 - x)$. At -1, a maximal domain pair is $u(x) = 1, v(x) = \ln(1 + x)$.

See also xamples.f, #1 (Legendre).

4. $-y''(x) - (4x^2)^{-1}y(x) = \lambda y(x)$ on $(0, +\infty)$ is LCNO at 0 and LP at $+\infty$.

At 0, a maximal domain pair is

$$u(x) = x^{1/2}, v(x) = x^{1/2}\ln(x).$$

See also xamples.f, #2 (Bessel).

5. $-y''(x) - 5(4x^2)^{-1}y(x) = \lambda y(x)$ on $(0, +\infty)$ LCO at 0 and LP at $+\infty$.

At 0, $\lambda = 0$, a solution pair is

$$u(x) = x^{1/2}\cos(\ln(x)), v(x) = \sin(\ln(x)).$$

See also xamples.f, #20 (Krall).

6. $-y''(x) = \lambda y(x)$ on $(0, +\infty)$ is LCNO at 0 and LP at +infinity.

At 0, a maximal domain pair is

$$u(x) = x, v(x) = 1 - x\ln(x).$$

See also xamples.f, #4(Boyd).

7. $-(x^{-1}y'(x))' + (kx^{-2} + k^2x^{-1})y(x) = \lambda y(x)$ on $(0, 1]$ with k real and $k \neq 0$, is LCNO at 0 and R at 1.

At 0, a maximal domain pair is

$$u(x) = x^2, v(x) = x - k^{-1}$$

See also xamples.f, #8 (Laplace Tidal Wave).

H7: General self-adjoint boundary conditions.

Boundary conditions for Sturm-Liouville boundary value problems

$$(*) \qquad -(py')' + qy = \lambda wy \text{ on } (a, b)$$

are *either* SEPARATED, with at most one condition at endpoint a and at most one condition at endpoint b,

or COUPLED, when both a and b are, independently, in one of the end-point classifications R, WR, LCNO, LCO, in which case two independent boundary conditions are required which link the solution values near a to those near b. The SLEIGN2 program allows for all self-adjoint boundary conditions; separated self-adjoint conditions and all cases of coupled self-adjoint conditions.

Separated Conditions: the boundary conditions to be selected depend upon the classification of the differential equation at the endpoint, say, a:

1. If the endpoint a is LP, then no boundary condition is required or allowed.

2. If the endpoint a is R or WR, then a separated self-adjoint boundary condition is of the form

$$A1y(a) + A2(py')(a) = 0$$

where $A1, A2$ are real constants the user must choose, not both zero.

3. If the endpoint a is LCNO or LCO, then a separated boundary condition is of the form

$$A1[y, u](a) + A2[y, v](a) = 0$$

where $A1, A2$ are real constants the user must choose, not both zero; here u, v are the pair of boundary condition functions the user has previously selected when the input Fortran file was being prepared with makepqw.f.

4. If the endpoint a is LCNO and the boundary condition pair u, v has been chosen so that

$$\lim_{x \to a} \frac{u(x)}{v(x)} = 0$$

(which is always possible), then $A1 = 1, A2 = 0$ (*i.e.* $[y, u](a) = 0$) gives the principal (Friedrichs) boundary condition at a.

5. If a is R or WR and boundary condition functions u, v have been entered in the Fortran input file, then 3 and 4 above apply to entering separated boundary conditions at such an endpoint; the boundary conditions in this form are equivalent to the point-wise conditions in 2 (subject to care in choosing $A1, A2$). This singular form of a regular boundary condition may be particularly effective in the WR case if the boundary condition form in 2 leads to numerical difficulties. Conditions 2,3,4,5 apply similarly at endpoint b (with U, V as the boundary condition functions at b).

6. If a is R, WR, LCNO, or LCO and b is LP, then only a separated condition at a is required and allowed (or instead at b if a and b are interchanged).

7. If both endpoints a and b are LP, then no boundary conditions are required or allowed.

The indexing of eigenvalues for boundary value problems with separated conditions is discussed in H13.

Coupled Conditions:

8. Coupled regular self-adjoint boundary conditions on (a, b) apply only when both endpoints a and b are R or WR.

H8: Recording the results.

If you choose to have a record kept of the results, then the following information is stored in a file with the name you select:

1. The file name.
2. The header line prompted for (up to 32 characters of your choice).
3. The interval (a, b) selected by the user.

For SEPARATED boundary conditions:

4. The endpoint classification.
5. A summary of coefficient information at WR, LCNO, LCO endpoints.

6. The boundary condition constants $(A1, A2), (B1, B2)$ if entered.
7. (NUMEIG,EIG,TOL) or (NUMEIG1,NUMEIG2,TOL), as entered.
For COUPLED boundary conditions:
8. The boundary condition parameter α and the coupling matrix $\mathbf{K}$, see H6.
For ALL self-adjoint boundary conditions:
9. The computed eigenvalue, EIG, and its estimated accuracy, TOL.
10. IFLAG reported (see H15).

H9: Type and choice of interval.
You may enter any interval (a, b) for which the coefficients p, q, w are well defined by your Fortran statements in the input file, provided that (a, b) contains no interior singularities.

H10: Entry of endpoints.
Endpoints a and b should generally be entered as real numbers to an appropriate number of decimal places.

H11: endpoint values of p, q, w.
The program SLEIGN2 needs to know whether the coefficient functions p, q, w as defined by the Fortran expressions entered in the input file, can be evaluated numerically without running into difficulty. If, for example, either q or w is unbounded at a, or $p(a) = 0$, then SLEIGN2 needs to know this information so that a is not chosen for functional evaluation.

H12: Initial value problems.
The initial value problem facility for Sturm-Liouville problems

$$(*) \qquad -(py')' + qy = \lambda wy \text{ on } (a, b)$$

allows for the computation of a solution of $(*)$ with a user-chosen value λ and any one of the following initial conditions:
1. From endpoint a of any classification except LP towards endpoint b of any classification
2. From endpoint b of any classification except LP back towards endpoint a of any classification
3. From endpoints a and b of any classifications except LP towards an interior point of (a, b) selected by the program.

Initial values at a are of the form $y(a) = \alpha 1, (py')(a) = \alpha 2$ when a is R or WR; and $[y, u](a) = \alpha 1, [y, v](a) = \alpha 2$ when a is LCNO or LCO.
Initial values at b are of the form $y(b) = \beta 1, (py')(b) = \beta 2$ when b is R or WR; and $[y, u](b) = \beta 1, [y, v](b) = \beta 2$ when b is LCNO or LCO.
In $(*)$, λ is a user-chosen real number; while in the above initial values, $(\alpha 1, \alpha 2)$ and $(\beta 1, \beta 2)$ are user-chosen pairs of real numbers not both zero.
In the initial value case 3 above when the interval (a, b) is finite, the interior point selected by the program is generally near the midpoint of (a, b); when (a, b) is infinite, no general rule can be given. Also if, given $(\alpha 1, \alpha 2)$ and $(\beta 1, \beta 2)$, the λ chosen is an eigenvalue of the associated boundary value problem, the computed solution may not be the corresponding eigenfunction – the signs of the computed solutions on either side of the interior point may be opposite.

The output for a solution of an initial value problem is in the form of stored numerical data which can be plotted on the screen (see H16), or printed out in graphical form if graphics software is available.

H13: Indexing of eigenvalues.

The indexing of eigenvalues is an automatic facility in SLEIGN2. The following general results hold for the separated boundary condition problem (see H7):

1. If neither endpoint a or b is LP or LCO, then the spectrum of the eigenvalue problem is discrete (eigenvalues only), simple (eigenvalues all of multiplicity 1), and bounded below with a single cluster point at $+\infty$. The eigenvalues are indexed as $\{\lambda_n : n = 0, 1, 2, ...\}$, where $\lambda_n < \lambda_{n+1}$ $(n = 0, 1, 2, ..)$, $\lim_{n\to+\infty} \lambda_n = +\infty$; and if $\{\psi_n : n = 0, 1, 2, ...\}$ are the corresponding eigenfunctions, then ψ_n has exactly n zeros in the open interval (a, b).

2. If neither endpoint a or b is LP but at least one endpoint is LCO, then the spectrum is discrete and simple as for 1, but with cluster points at both $\pm\infty$. The eigenvalues are indexed as $\{\lambda_n : n = 0, \pm1, \pm2, ...\}$, where $\lambda_n < \lambda_{n+1}$ (for $n < n + 1$ and $n = 0, \pm1, \pm2, ..$), with λ_0 the smallest non-negative eigenvalue; $\lim_{n\to-\infty} \lambda_n = -\infty$ and $\lim_{n\to+\infty} \lambda_n = +\infty$; and if $\{\psi_n : n = 0, \pm1, \pm2, ...\}$ are the corresponding eigenfunctions, then every ψ_n has infinitely many zeros in (a, b).

3. If one or both endpoints is LP, then there can be one or more intervals of continuous spectrum for the boundary value problem in addition to some (necessarily simple) eigenvalues. For these essentially more difficult problems, SLEIGN2 can be used as an investigative tool to give qualitative and possibly quantitative information on the spectrum.

For example, if a problem has continuous spectrum starting at a real number L, then there may be no eigenvalues below L, any finite number of eigenvalues below L, or an infinite (but countable) number of eigenvalues below L. SLEIGN2 can be used to compute L (see the paper BEWZ on the SLEIGN2 home page for an algorithm to compute L), and to determine the number of these eigenvalues and compute them. In this respect, see xamples.f: #13 (Hydrogen Atom), #17 (Morse Oscillator), #21 (Fourier), and #27 (Jörgens) as examples of success; and #2 (Mathieu), #14 (Marletta), and #28 (Behnke-Goerisch) as examples of failure.

The problem need not have a continuous spectrum, in which case if its discrete spectrum is bounded below, then the eigenvalues are indexed and the eigenfunctions have zero counts as in 1. If, on the other hand, the discrete spectrum is unbounded below, then all the eigenfunctions have infinitely many zeros in the open interval (a, b). SLEIGN2 can, in principle, compute these eigenvalues if neither endpoint is LP although this is a computationally difficult problem. Note however, that SLEIGN2 has no algorithm when the spectrum is discrete, unbounded above and below and one endpoint is LP, as in xamples.f #30.

In respect to the five classes of endpoints, the following identified examples from xamples.f illustrate the spectral property of these boundary value problems:

1. Neither endpoint is LP or LCO:
#1 (Legendre), #2 (Bessel) with $-1/4 < C < 3/4$, #4 (Boyd), #5 (Latzko).
2. Neither endpoint is LP, but at least one is LCO:
#6 (Sears-Titchmarsh), #7 (BEZ), #19 (Donsch)
3. At least one endpoint is LP:

#13 (Hydrogen Atom), #14 (Marletta), #20 (Krall), #21 (Fourier) on [0,infinity).

H14: Entry of eigenvalue index, initial guess, and tolerance.

For all self-adjoint boundary condition problems (see H7), SLEIGN2 calls for input information options to compute *either*

1. a single eigenvalue, *or*
2. a series of eigenvalues.

In each case indexing of eigenvalues is called for (see H13).

1 above asks for data triples NUMEIG, EIG, TOL separated by commas. Here NUMEIG is the integer index of the desired eigenvalue; NUMEIG can be negative only when the problem is LCO at one or both endpoints. EIG allows for the entry of an initial guess for the requested eigenvalue (if an especially good one is available), or can be set to 0 in which case an initial guess is generated by SLEIGN2 itself. TOL is the desired accuracy of the computed eigenvalue. It is an absolute accuracy if the magnitude of the eigenvalue is 1 or less, and is a relative accuracy otherwise. Typical values for TOL might be 0.001 for moderate accuracy and 0.0000001 for high accuracy in single precision. If TOL is set to 0, the maximum achievable accuracy is requested.

If the input data list is truncated with a " / " after NUMEIG or EIG, then the remaining elements default to 0.

2 above asks for data triples NUMEIG1, NUMEIG2, TOL separated by commas. Here NUMEIG1 and NUMEIG2 are the first and last integer indices of the sequence of desired eigenvalues, with NUMEIG1 <NUMEIG2; they can be negative only when the problem is LCO at one or both endpoints. TOL is the desired accuracy of the computed eigenvalues. It is an absolute accuracy if the magnitude of an eigenvalue is 1 or less, and is a relative accuracy otherwise. Typical values for TOL might be 0.001 for moderate accuracy and 0.0000001 for high accuracy in single precision. If TOL is set to 0, the maximum achievable accuracy is requested.

If the input data list is truncated with a " / " after NUMEIG2, then TOL defaults to 0.

For COUPLED self-adjoint boundary condition problems (see H7 and H17), SLEIGN2 also reports which eigenvalues are double. Double eigenvalues can occur only for coupled boundary conditions with the parameter $\alpha = 0$ or π.

H15: IFLAG information.

All results are reported by SLEIGN2 with a flag identification. There are four values of IFLAG:

1. The computed eigenvalue has an estimated accuracy within the
tolerance requested.
2. The computed eigenvalue does not have an estimated accuracy within the tolerance requested, but is the best the program could obtain.
3. There seems to be no eigenvalue of index equal to NUMEIG.
4. The program has been unable to compute the requested eigenvalue.

H16: Plotting.

After computing a single eigenvalue (see H14(1.)), but not a sequence of eigenvalues (see H14(2.)), the eigenfunction can be plotted for separated conditions and for coupled ones

with $\alpha = 0, \pi$. If this data is desired, respond y when asked and SLEIGN2 will then compute eigenfunction data and store them for subsequent use.

The user can ask that the eigenfunction data be in the form of either points (x, y) for $x \in (a, b)$, or points (t, y) for t in the standardized interval $(-1, +1)$ mapped onto from (a, b); the t-choice can be especially helpful when the original interval is infinite. Additionally, the user can ask for a plot of the so-called Prüfer angle, in the x- or t-variables.

In both forms, once the choice has been made of the function to be plotted, a crude plot is displayed on the monitor screen and the user is asked whether or not to save the computed plot points in a file.

H17: Indexing of eigenvalues for coupled self-adjoint problems.

The indexing of eigenvalues is an automatic facility in SLEIGN2. The following general result holds for coupled boundary condition problems (see H7):

The spectrum of the eigenvalue problem is discrete (eigenvalues only). In general the spectrum is not simple, but no eigenvalue exceeds multiplicity 2. The eigenvalues are indexed as $\{\lambda_n : n = 0, 1, 2, ...\}$ where $\lambda_n < \lambda_{n+1}$ for $n = 0, 1, 2, ...$,and $\lim_{n\to+\infty} \lambda_n = +\infty$ if neither endpoint is LCO. If one or both endpoints are LCO the eigenvalues cluster at both $-\infty$ and at $+\infty$, and all eigenfunctions have infinitely many zeros.

If neither endpoint is LCO and $\alpha = 0, \pi$, then the n-th eigenfunction has $n - 1, n, n + 1$ zeros in the half open interval $[a, b)$ (also in $(a, b]$). All three possibilities occur. Recall that in the case of double eigenvalues, although the n-th eigenvalue is well defined there is an ambiguity about which solution is declared as the n-th eigenfunction. If $\alpha \neq 0, \pi$, then the eigenfunction is non-real and has no zero in (a, b), but each of the real and imaginary parts of the n-th eigenfunction have the same zero properties as mentioned above when $\alpha = 0, \pi$.

The following identified examples from xamples.f are of special interest:

#11 (Plum) on $[0, \pi]$, #21 (Fourier) on $[0, \pi]$, #25 (Meissner) on $[-1/2, +1/2]$.

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