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Solution & visualization in The Sturm - Liouville problem

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Outline

1. Introduction. The regular Sturm - Liouville problem.
2. The Two - Center Problem in quantum mechanics.
3. SLEIGN2
 - 3.1 Manual for program package SLEIGN2
 - 3.2 SLEIGN2 with BARSIC

1. Introduction. The regular Sturm - Liouville problem.

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

(a, b) - open interval

$\{p, q, w\}$ - coefficients defined on the open interval (a, b)

λ - spectral parameter

Boundary conditions:

- Regular (R)
- Singular (S)
- Separated
- Coupled

Regular boundary conditions:

- separated boundary conditions

$$A_1 y'(a) + A_2 y(a) = 0$$

$$B_1 y'(b) + B_2 y(b) = 0$$

- coupled boundary conditions

$$y(a) = y(b)$$

$$(py')(a) = (py')(b)$$

Eigen solution of the regular Sturm - Liouville problem -

$$\{ \lambda , y \}$$

λ — eigenvalue, for which differential equation has nontrivial solution ψ

y — eigenfunction, corresponds to eigenvalue, satisfies boundary conditions

The regular Sturm - Liouville problem & Schrödinger problem

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

(a, b) - is the integration interval and the boundary conditions

$$-y''(x) + q(x)y(x) = \lambda y(x), x \in (a, b)$$

(a, b) - is the integration interval and the boundary conditions

2. The Two - Center Problem in quantum mechanics.

$$\Delta \psi (r ; R) + 2 \left(E - \frac{Z_1}{r_1} - \frac{Z_2}{r_2} \right) \psi (r ; R) = 0$$

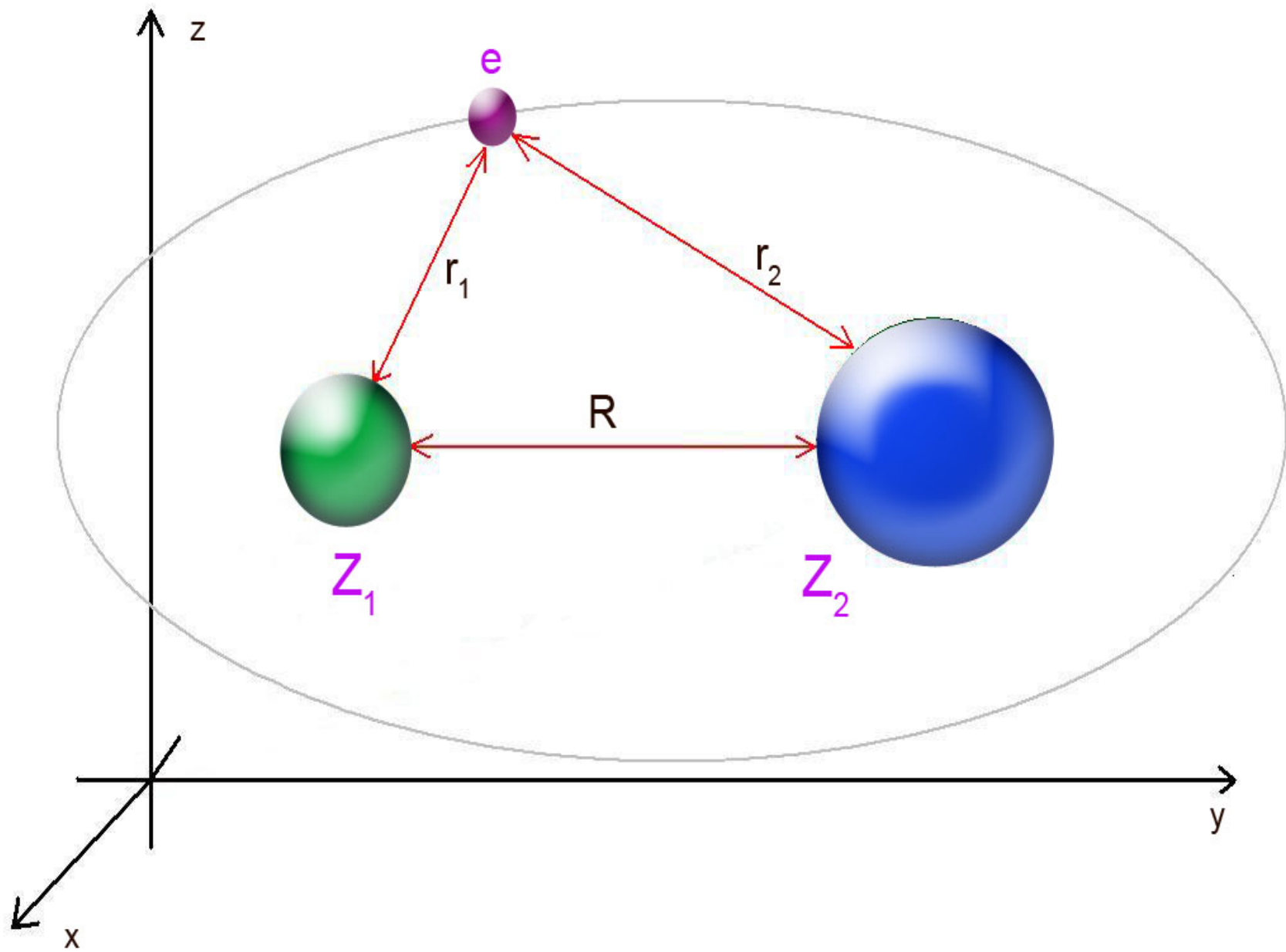
$$\hbar = m_e = e$$

Z_1 and Z_2 - nuclear charges

r_1 and r_2 - distance between electron and Z_1, Z_2

R - internuclear distance

$E = E(R)$ - energy term



Prolate spheroidal coordinate system

$$\zeta = \frac{r_1 + r_2}{R}, \quad \eta = \frac{r_1 - r_2}{R}, \quad \varphi = \arctan(y/x)$$

$\zeta = 1, \eta = +1$ - coordinates of charge Z_1

$\zeta = 1, \eta = -1$ - coordinates of charge Z_2

$$\psi_j = \psi_{kqm}(\zeta, \eta, \varphi; R) = N_{kqm}(R) X_{mk}(\zeta; R) Y_{mq}(\eta; R) e^{im\varphi}$$

$j = \{k, q, m\}$ - set of quantum numbers

k - principal quantum number

q - orbital quantum number

m - magnetic quantum number

$$\int_V \psi_{kqm}^*(\xi, \eta, \varphi; R) \psi_{k'q'm'}(\xi, \eta, \varphi; R) dV = \delta_{kk'} \delta_{qq'} \delta_{mm'}$$

$$\frac{d}{d\zeta}(\zeta^2 - 1) \frac{d}{d\zeta} X_{mk}(\zeta; R) + \left[-\lambda - p^2(\zeta^2 - 1) + a\zeta - \frac{m^2}{\zeta^2 - 1} \right] X_{mk}(\zeta; R) = 0$$

$$\frac{d}{d\eta}(1 - \eta^2) \frac{d}{d\eta} Y_{mq}(\eta, R) + \left[-\tilde{\lambda} - p^2(1 - \eta^2) + b\eta - \frac{m^2}{1 - \eta^2} \right] Y_{mq}(\eta, R) = 0$$

$$p_j^2 = -\frac{E_j R^2}{2} \quad (p > 0) \quad - \text{energy parameter}$$

$$a = (Z_1 + Z_2) R, \quad b = (Z_2 - Z_1) R \quad - \text{charge parameter}$$

$$\lambda = \lambda_{mk}^{(\zeta)}(p, a), \quad \tilde{\lambda} = \lambda_{mq}^{(\eta)}(p, b) \quad - \text{separation constants}$$

$$\lambda_{mk}^{(\zeta)}(p, a) = \lambda_{mq}^{(\eta)}(p, b)$$

Quasiradial equation

$$\frac{d}{d\zeta}(\zeta^2 - 1) \frac{d}{d\zeta} X_{mk}(\zeta; R) + \left[-\lambda - p^2(\zeta^2 - 1) + a\zeta - \frac{m^2}{\zeta^2 - 1} \right] X_{mk}(\zeta; R) = 0$$

$$|X_{mk}(1; R)| < \infty, \quad |X_{mk}(\zeta; R)| \xrightarrow{\zeta \rightarrow \infty} 0, \quad \zeta \in [1, \infty)$$

Jaffé expansion

$$t = (\zeta - 1)/(\zeta + 1) \quad - \text{transformation of variable}$$

$$\zeta \rightarrow t, \quad -1 \rightarrow +\infty, \quad +1 \rightarrow 0, \quad \infty \rightarrow +1 \quad - \text{transformation of equilibrium points}$$

$$\zeta \in [1; \infty) \rightarrow t \in [0; 1) \quad - \text{transformation of interval}$$

$$X_{mk}(\zeta; R) = e^{-p\zeta} (\zeta^2 - 1)^{m/2} (\zeta + 1)^\sigma \sum_{s=1}^{\infty} g_s \left(\frac{\zeta - 1}{\zeta + 1} \right)^s$$

$$\delta = a/2p - (m+1)$$

$$\alpha_s g_{s+1} - \beta_s g_s + \gamma_s g_{s-1} = 0 \quad - \text{three-term relation between coefficients } g_s$$

$$\alpha_s = (s+1)(s+m+1)$$

$$\beta_s = 2s(s+2p-\delta) - (m+\delta)(m+1) - 2p\delta + \lambda$$

$$\gamma_s = (s-1-\delta)(s-m-1-\delta)$$

Eigenvalues of the problem are found from the condition of nullifying of the continued fraction.

$$F(p, a, \lambda) = \beta_0 - \frac{\alpha_0 \gamma_1}{\beta_1 - \frac{\alpha_1 \gamma_2}{\beta_2 - \dots}} = 0$$

$$\left| \frac{\alpha_{s-1} \gamma_s}{\beta_{s-1} \beta_s} \right| \xrightarrow{s \rightarrow \infty} \frac{1}{4} \left(1 - \frac{4p}{s} \right) + O\left(\frac{p^2}{s^2}\right)$$

Coefficients of three - termed relation converge for all $p > 0$
It follows from the equation above.

The ratio of the series coefficients

$$\frac{g_{s+1}}{g_s} \xrightarrow{s \rightarrow \infty} 1 - 2 \sqrt{\frac{p}{s}} + O\left(\frac{p}{s}\right)$$

provides the convergence of Jaffé expansion on the complete interval $t \in [0;1)$ or $\zeta \in [1;\infty)$

Quasiangular equation

$$\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}Y_{mq}(\eta; R)+\left[-\tilde{\lambda}-p^2(1-\eta^2)+b\eta-\frac{m^2}{1-\eta^2}\right]Y_{mq}(\eta; R)=0$$

$$\left|Y_{mq}(\pm 1; R)\right|<\infty; -1\leq\eta\leq+1$$

Baber - Hasse expansion

$$Y_{mq}(\eta; R) = e^{-p\eta} \sum_{s=0}^{\infty} c_s P_{s+m}^m(\eta)$$

$$\rho_s c_{s+1} - \chi_s c_s + \delta_s c_{s-1} = 0 \quad \text{- relation between three - terms coefficients } c_s$$

$$\rho_s = \frac{(s + 2m + 1)(b - 2p(s + m + 1))}{2(s + m) + 3}$$

$$\chi_s = (s + m)(s + m + 1) - \lambda$$

$$\delta_s = \frac{s[b + 2p(s + m)]}{2(s + m) - 1}$$

The ratio of succeeding series coefficients at large indexes:

$$\frac{c_{s+1}}{c_s} \sim \frac{p}{s} \xrightarrow{s \rightarrow \infty} 0$$

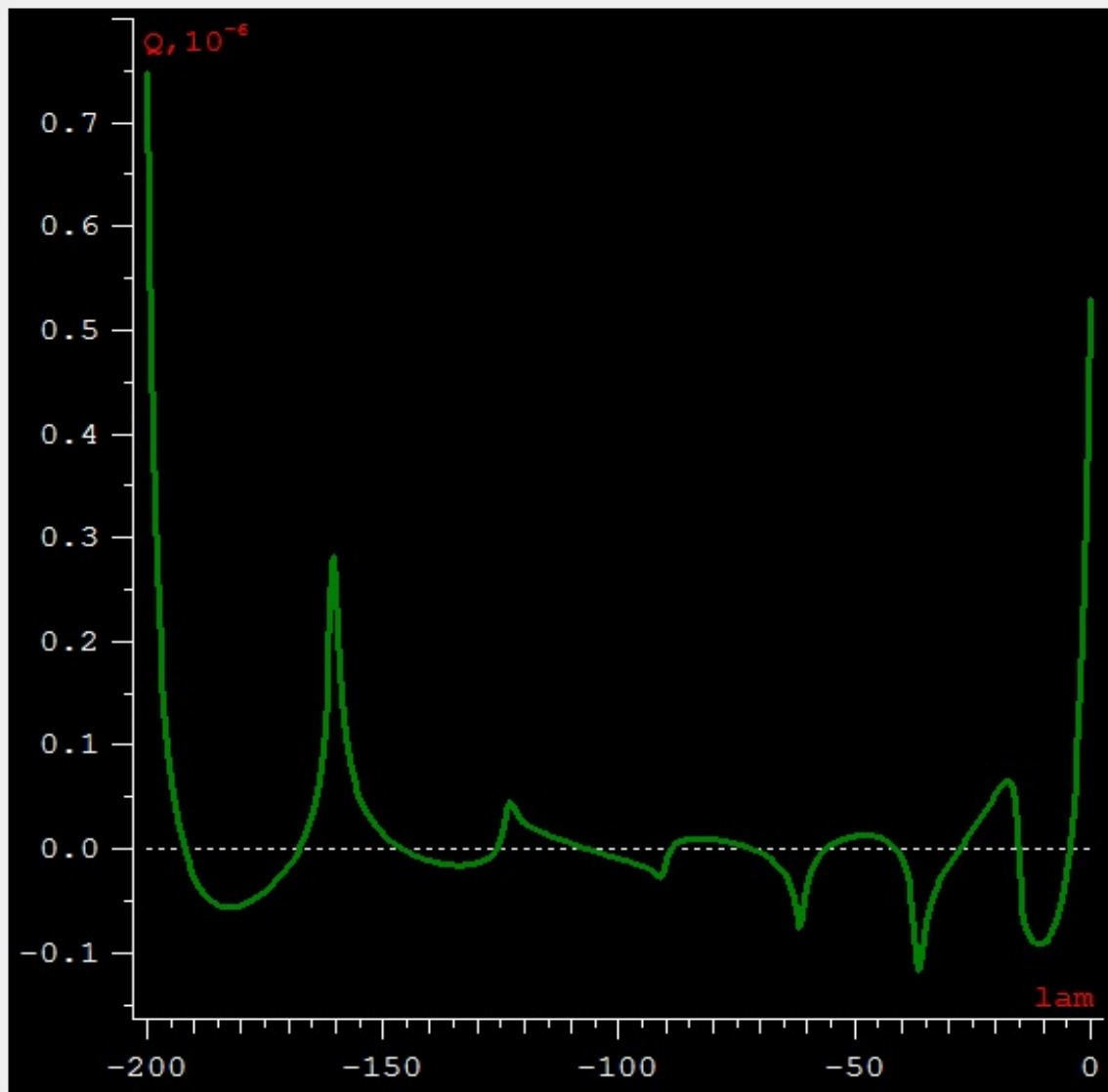
Solutions of $\lambda_{mk}^{(\zeta)}(p, a) = \lambda_{mq}^{(\eta)}(p, b)$ can be found from the equation

$$F^{(\eta)}(p, b, \lambda) = k_0 - \frac{\rho_0 \delta_1}{k_1 - \frac{\rho_1 \delta_2}{k_2 - \dots}} = 0$$

Continuous fraction converges due to following limit:

$$\left| \frac{\rho_{s-1} \delta_s}{\chi_{s-1} \chi_s} \right| \xrightarrow{s \rightarrow \infty} \left(\frac{2p}{s} \right)^2$$

Plot $Q_r(\text{lam})$



Parameters

$q1 = -2$

$q2 = 3$

$R = 15$

$m = 0$

$p = 1$

$\text{lam1} = -200$

$\text{lam2} = 0$

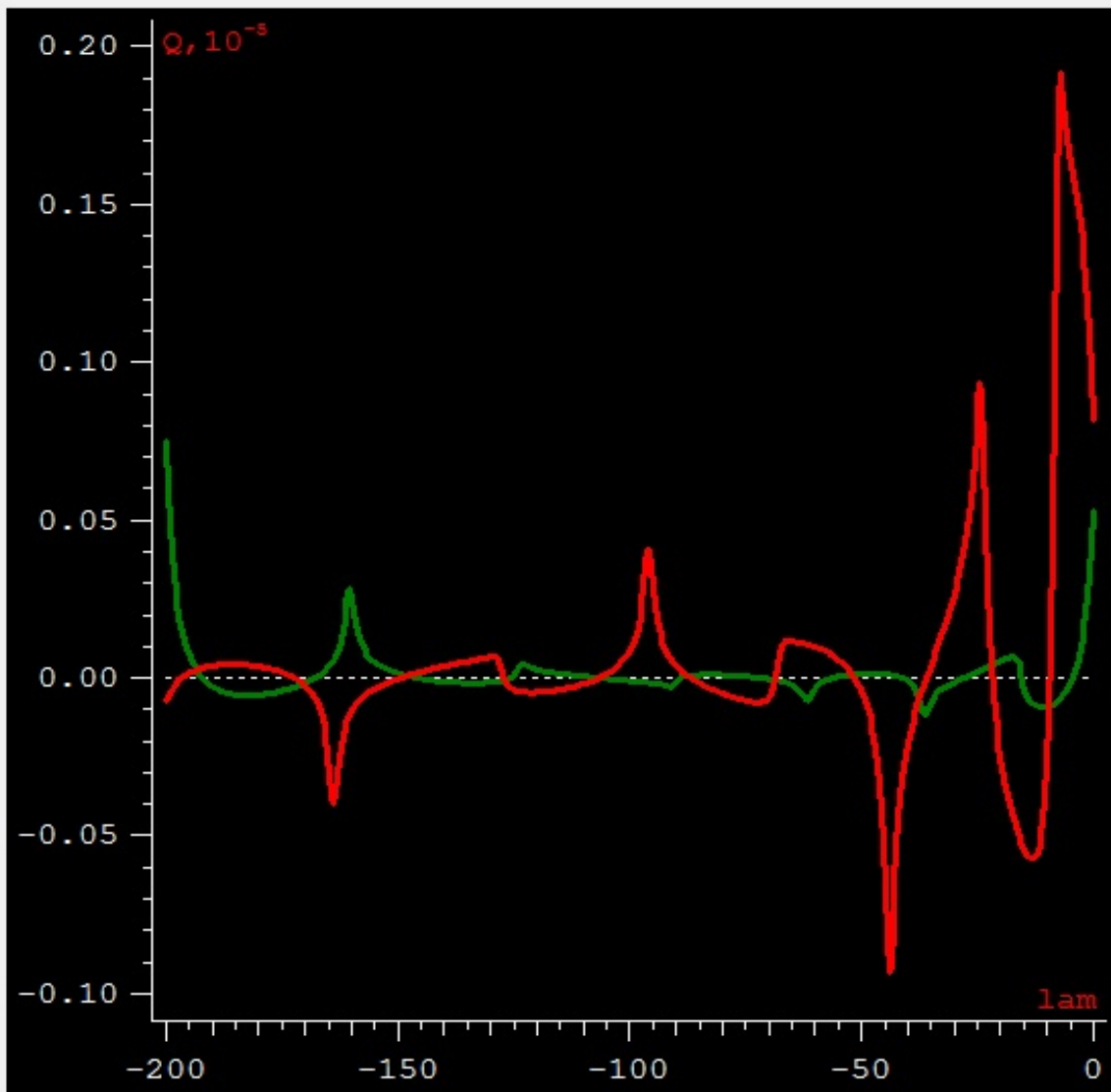
$N_{\text{max}} = 50$

Plot

Clear

Quit

Plot $Q_r(\text{lam})$



Parameters

q1 = -2

q2 = 3

R = 15

m = 0

p = 1.5

lam1 = -200

lam2 = 0

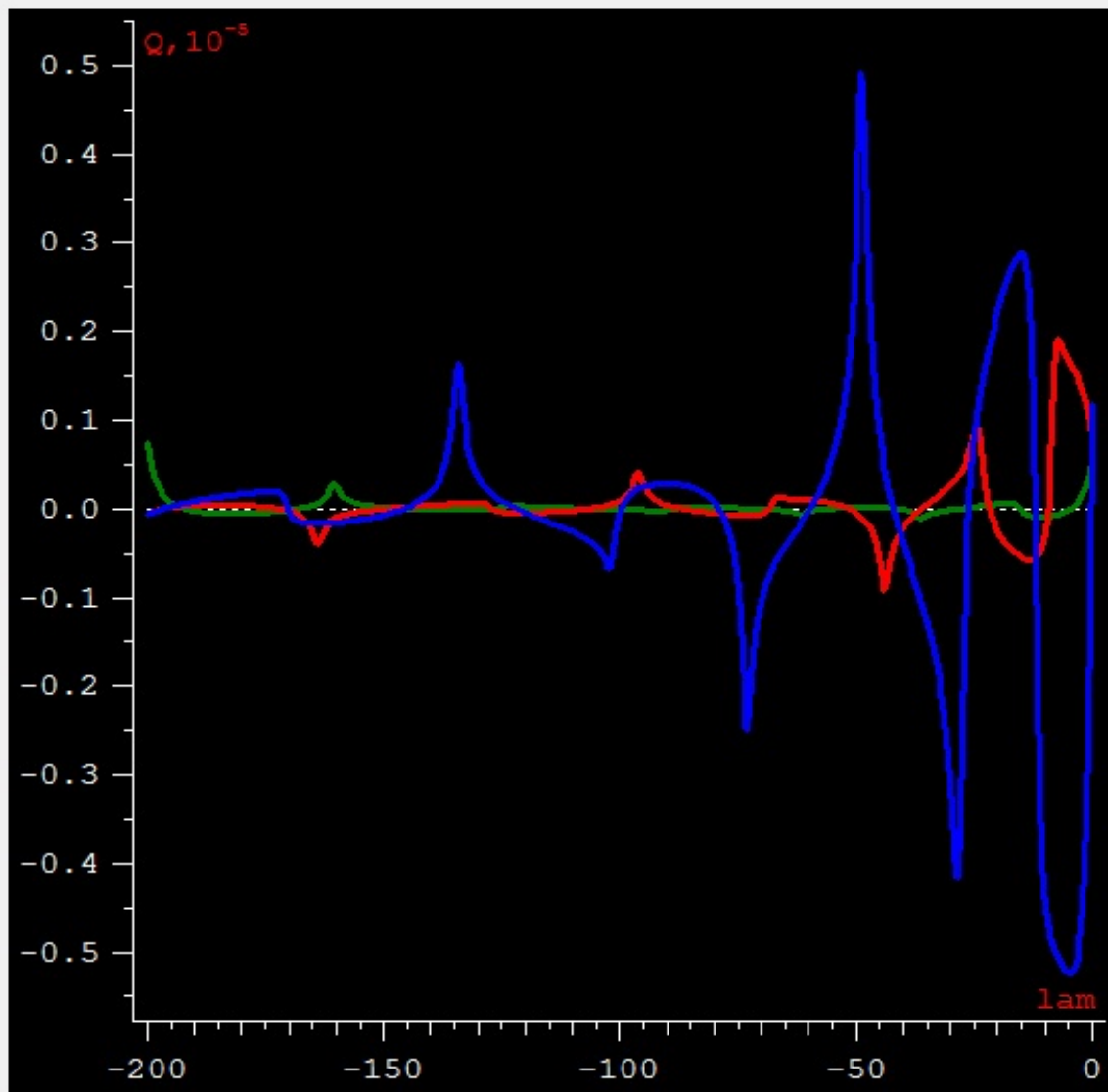
Nmax = 50

Plot

Clear

Quit

Plot $Q_r(\lambda)$



Parameters

q1 =

q2 =

R =

m =

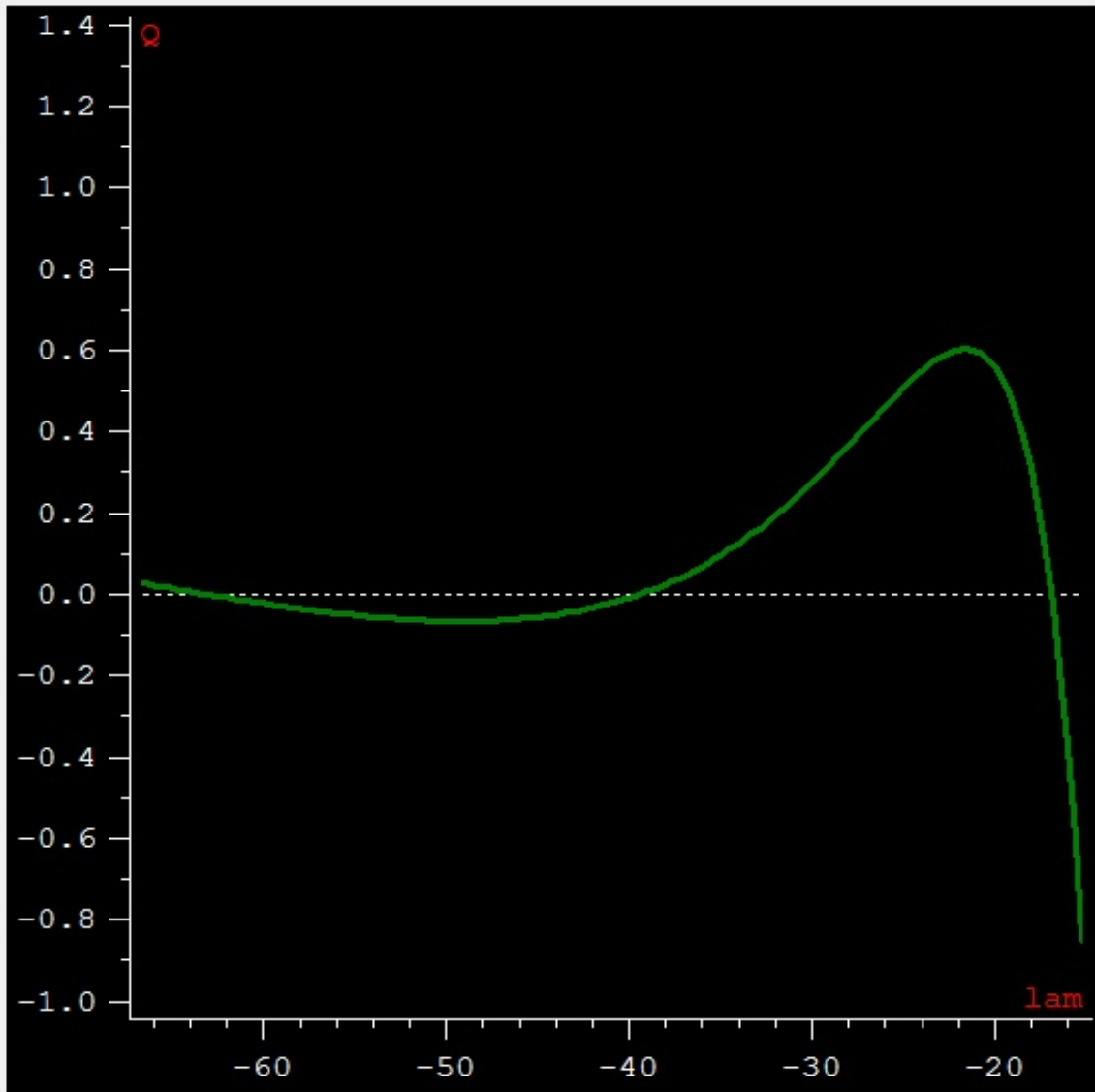
p =

lam1 =

lam2 =

Nmax =

Plot $Q_u(\lambda)$



Parameters

$q1 = -2$

$q2 = 3$

$R = 15$

$m = 0$

$p = 1$

$\lambda_{1} = -200$

$\lambda_{2} = 0$

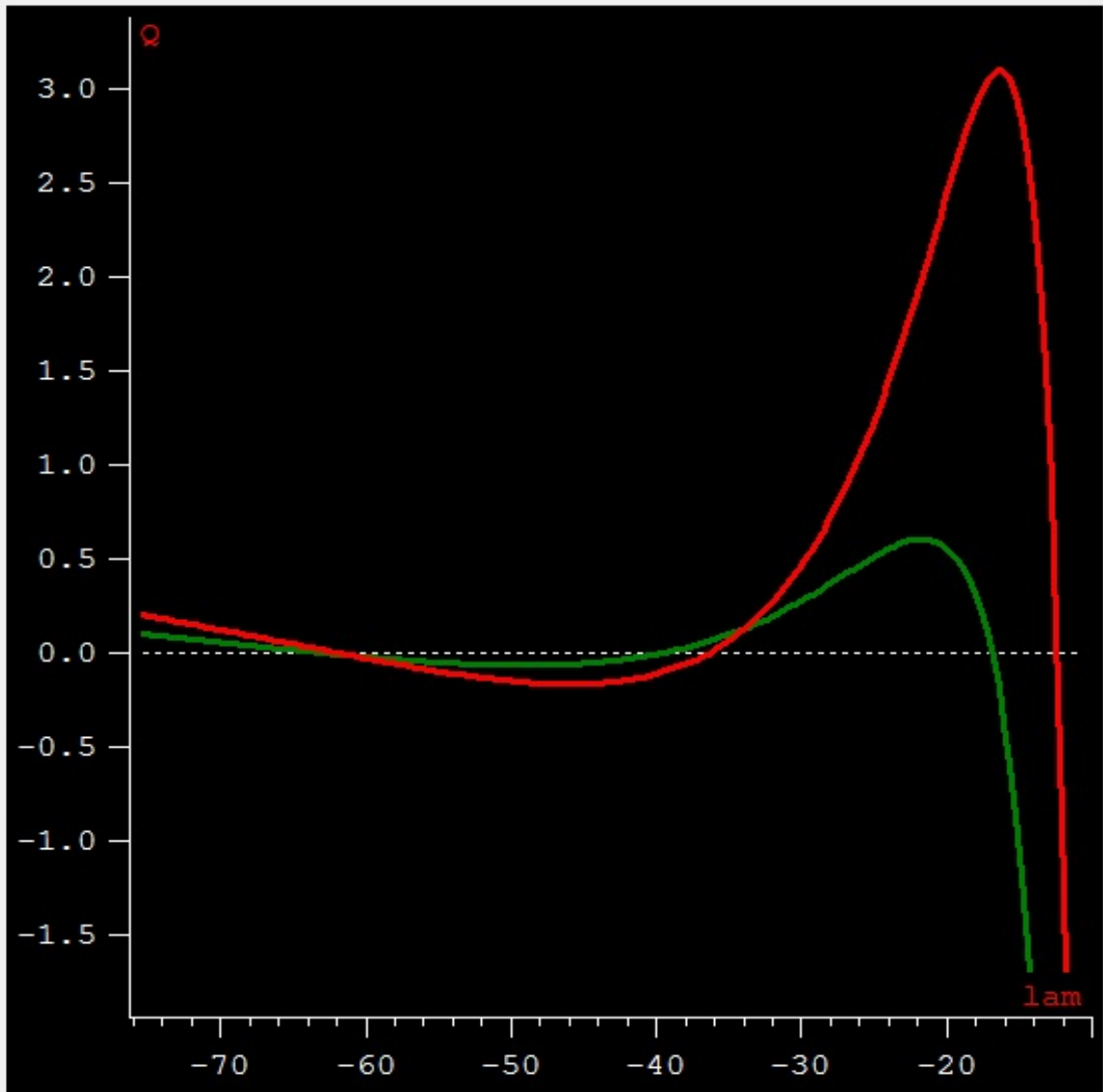
$N_{\max} = 50$

Plot

Clear

Quit

Plot $Q_u(\lambda)$



Parameters

q1 =

q2 =

R =

m =

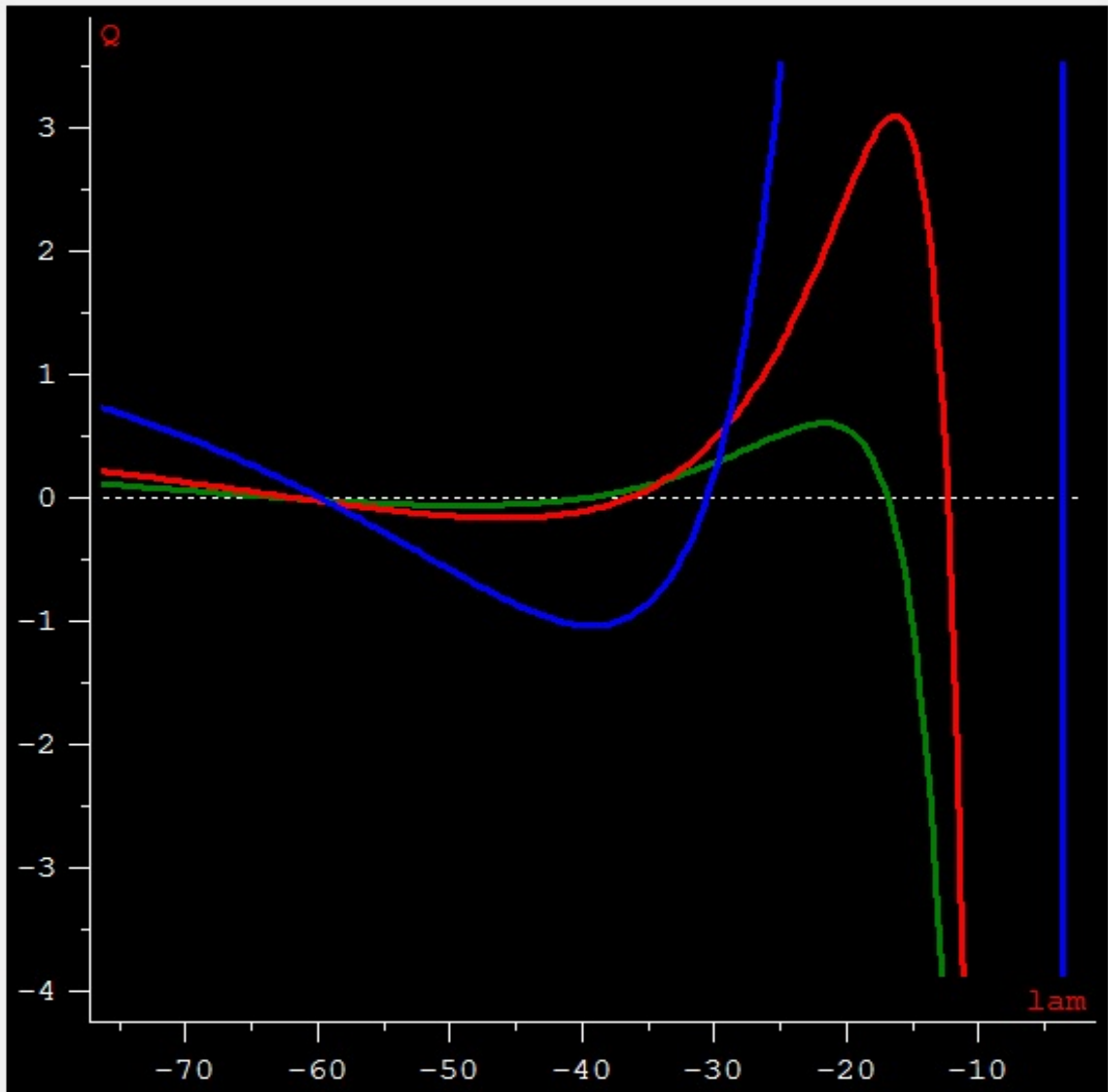
p =

lam1 =

lam2 =

Nmax =

Plot $Q_u(\lambda)$



Parameters

$q_1 =$

$q_2 =$

$R =$

$m =$

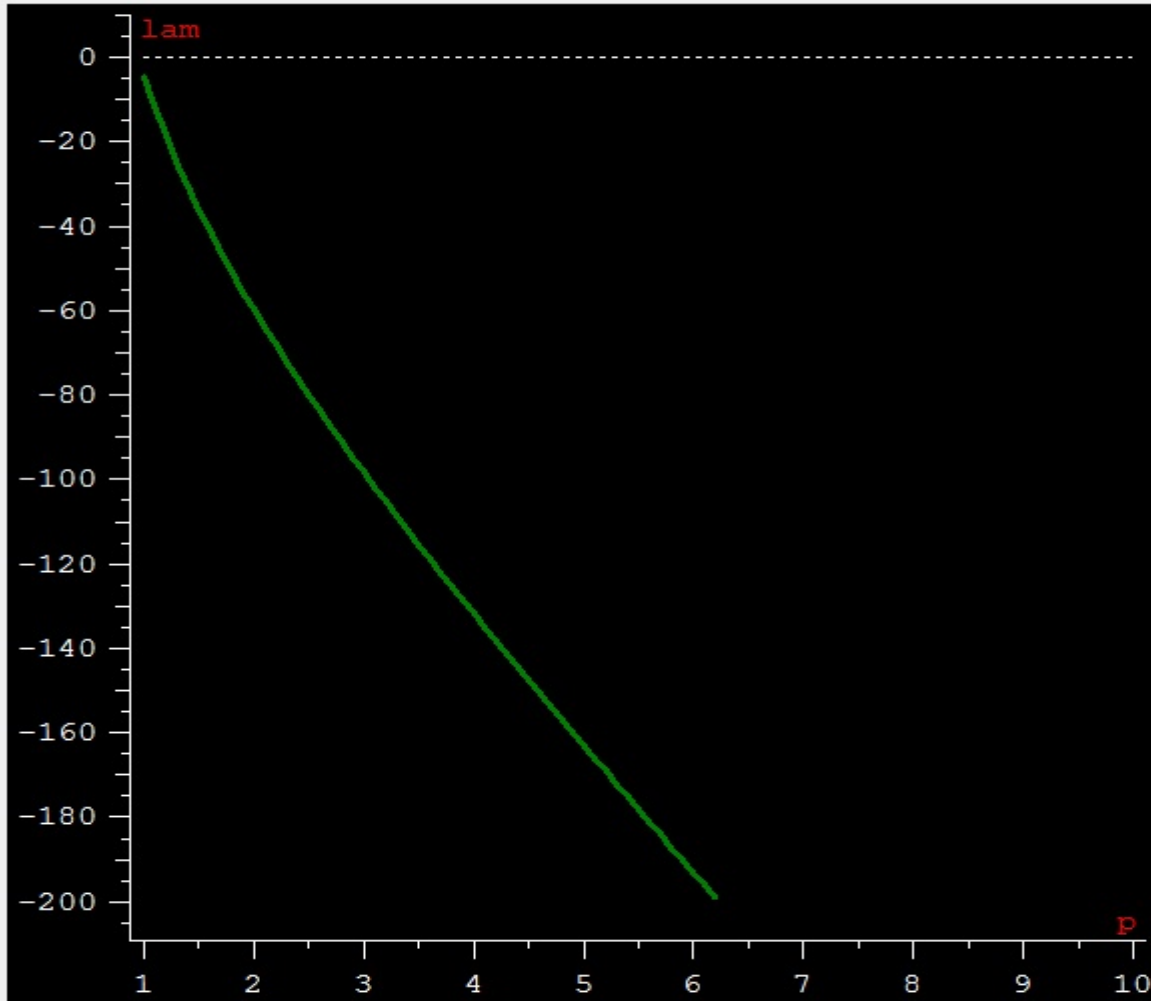
$p =$

$\lambda_{1} =$

$\lambda_{2} =$

$N_{max} =$

Plot lam r(p)



Parameters

q1 = q2 = R = m = p1 = p2 = dp = lam1 = lam2 = k =

View parameters

p min = lam min = p max = lam max =

Apply

Restore

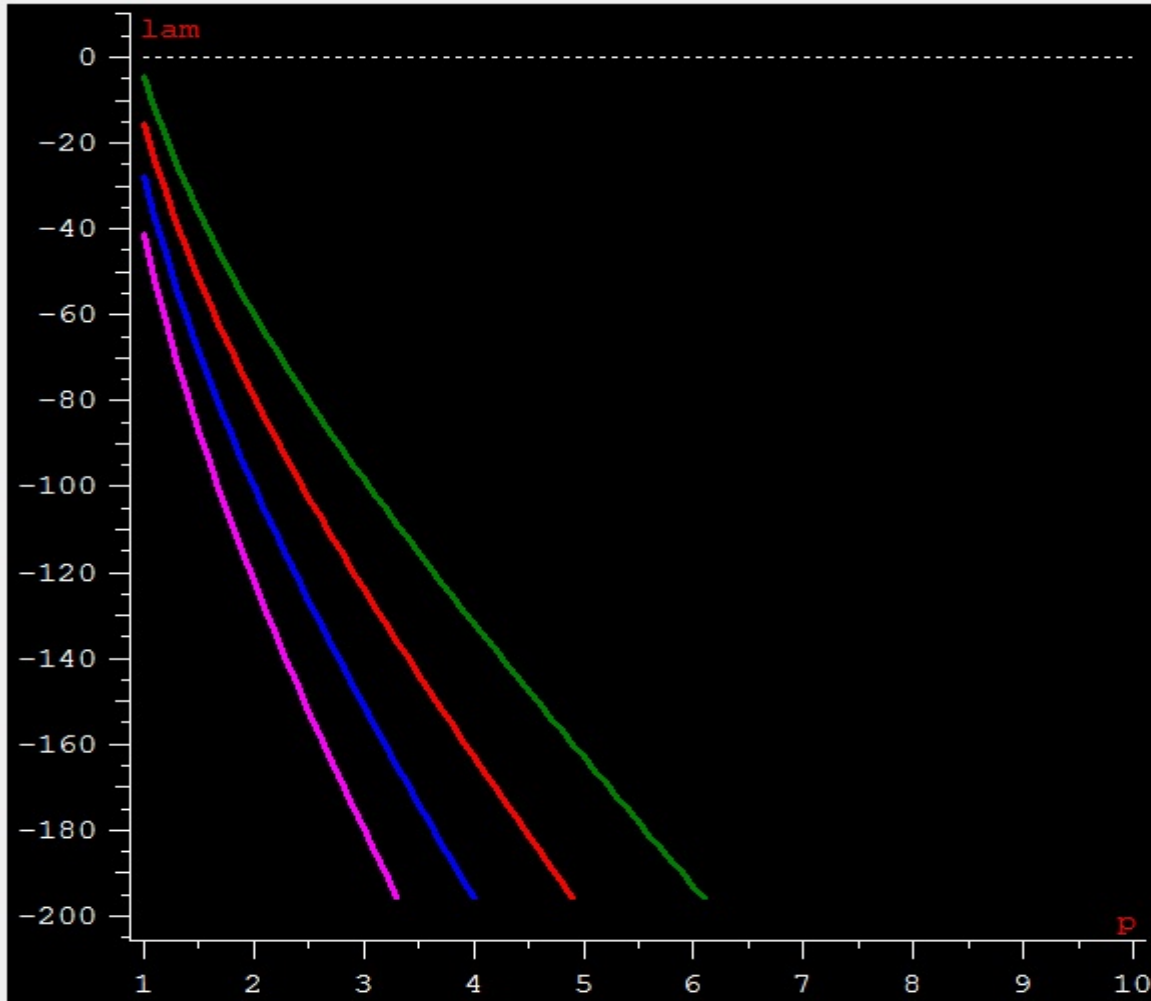
Plot

Clean

Stop

Quit

Plot lam r(p)



Parameters

q1 = q2 = R = m = p1 = p2 = dp = lam1 = lam2 = k =

View parameters

p min = lam min = p max = lam max =

Apply

Restore

Plot

Clean

Stop

Quit

3. SLEIGN2

General-purpose programs for computing the eigenvalues and eigenfunctions of Sturm - Liouville problem

- Program SLEIGN has been developed by Bailey, Gordon and Shampine , programming language FORTRAN
- Code in the NAG Library has been developed by Pryce and Marletta , programming language FORTRAN
- Program SLEDGE has been developed by Fulton and Pruess , programming language FORTRAN
- Program SLEIGN2 has been developed by Bailey Everitt and Zettl , programming language FORTRAN

To meet the needs of numerical computing techniques was made the following assumptions:

1. The interval (a, b) of \mathbb{R} may be bounded or unbounded
2. p, q and w are real-valued functions on (a, b)
3. p, q and w piecewise continuous on (a, b)
4. p and w strictly positive on (a, b)

Conditions on the coefficients:

Minimal conditions:

$$p^{-1}, q, w \in L^1(a, b)$$

$$p(x), w(x) > 0$$

Smoothness conditions:

$$p, p', q, w \in C(a, b)$$

$$p(x), w(x) > 0$$

Endpoint classification

To classify endpoints a and b , it is convenient to choose a point $c \in (a, b)$

- a is **Regular (R)**, if

$$-\infty < a < +\infty$$

p, q, w - piecewise continuous on $[a, c]$

$$p(a) > 0, w(a) > 0$$

- a is **Singular (S)**, if

$$a = \pm\infty \text{ or}$$

$$a \in \mathbb{R}, \text{ but } \int_a^c \{(p(x))^{-1} + |q(x)| + w(x)\} dx = +\infty$$

- The singular endpoint a is **Limit Point (LP)** if for some real λ at least one solution of differential equation satisfies the condition

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

- The endpoint a is **Weakly Regular (WR)** if $-\infty < a$ &

$$\int_a^c (p^{-1} + |q| + w) dx < +\infty$$

- The singular endpoint is **Limit-Circle Non-Oscillatory(LCNO)** if for some real value of spectral parameter λ ALL real-valued solutions $y(x, \lambda)$ satisfy the conditions

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

and $y(x, \lambda)$ has at most a finite number of zeros in $(a, c]$

- The singular endpoint is **Limit-Circle Oscillatory(LCO)** if for some real value of spectral parameter λ ALL real-valued solutions $y(x, \lambda)$ satisfy the conditions

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

and $y(x, \lambda)$ has an infinite number of zeros in $(a, c]$

SLP problems are classified into various classes based on the classification of the endpoints and on whether the boundary conditions are separated (S) or coupled (C). We have the following categories:

1. R/R, Separated
2. R/R, Coupled
3. R/LCNO LCNO/R, Separated
4. R/LCNO LCNO/R, Coupled
5. R/LCO LCO/R, Separated
6. R/LCO LCO/R, Coupled
7. LCNO /LCO LCO/ LCNO LCO/ LCO, Separated
8. LCNO /LCO LCO/ LCNO LCO/ LCO, Coupled
9. LP/R LP/LCNO LP/LCO R/LP LCNO/LP LCO/LP
10. LP/LP

The algorithm in SLEIGN2

- Initial interval (a, b) is converted to interval $(-1, +1)$ in the SLEIGN2 package
- The computation procedure is implemented by the use of Prüfer Transform.

Prüfer Transform.

$$y(x) = \rho(x) \sin(\theta(x))$$

$$(py)'(x) = \rho(x) \cos(\theta(x))$$

Differential equation for ρ & θ :

$$\theta'(x) = p(x)^{-1} \cos^2(\theta(x)) + (\lambda w(x) - q(x)) \sin^2(\theta(x))$$

$$\rho'(x) / \rho(x) = (p(x)^{-1} - \lambda w(x) + q(x)) \sin(\theta(x)) \cos(\theta(x))$$

Boundary conditions for θ :

$$\theta(a) = -\operatorname{arctg}(A_2 / A_1)$$

$$\theta(b) - \pi n = -\operatorname{arctg}(B_2 / B_1)$$

The following disadvantages were found in the program package SLEIGN2:

- The interface of the program is organized on the base of console dialog. This approach considerably increase the time for defining the problem paramters.
- The program is unstable towards the input : if numbers are taken in the incorrect format (say, with comma instead of dot) or letters are taking instead of number. In this case the program is terminated and it is required to start work from the very beginning.
- Additional program MAKEPQW is required in order to create own examples.

Solution in BARSIC (Business And Research Scientific Interactive Calculator)

- Numerical algorithms from SLEIGN2 remain unchanged. Subroutines of SLEIGN2 package (programming language FORTRAN) are compiled into 'dll' file ('so' files in case of OS Linux) and then they are called from BARSIC programs.
- Additional functions for calculation of first and second derivatives were created (It's necessary to write them in FORTRAN when SLEIGN2 is used directly)

File Parameters View Information about the problem About

Problem:

THE LEGENDRE EQUATION

EQUATION: $-(p(x)y'(x))' + q(x)y(x) = \text{Eigen_Value} * w(x) * y(x)$ $p(x) = 1 - x*x$ $q(x) = 1/4$ $w(x) = 1$

Interval:

x = -1

..

1

Boundary Conditions ...

Number of Eigen Value =

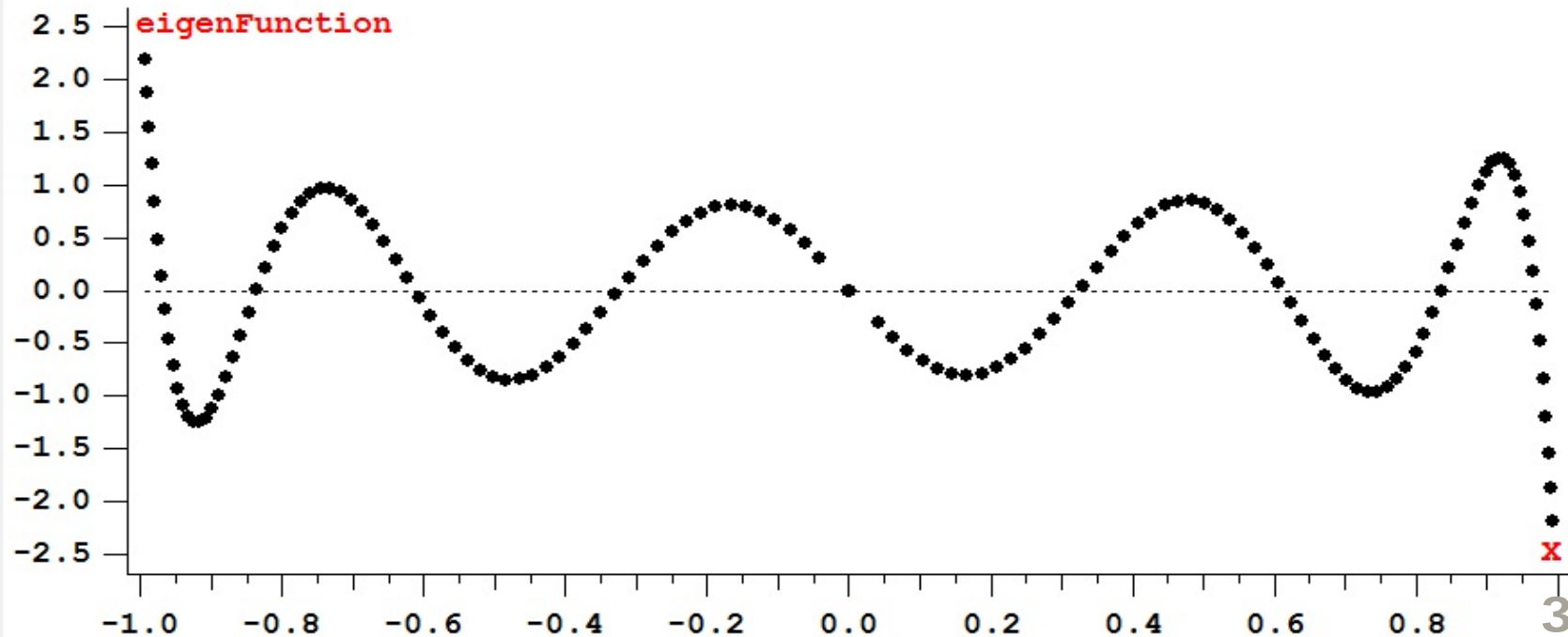
9

+
-

Solve

eigen value =

90.2452011108398



SEPARATED

Left bound X1:

LIMIT_CIRCLE_NON-OSC

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

A1 = 1

A2 = 0

Right bound X2:

LIMIT_CIRCLE_NON-OSC

$$A1*y(\text{leftBound}) + A2*p(\text{leftBound})*y'(\text{leftBound})=0$$

B1 = 1

B2 = 0

u(x) = 1

Set u(x) ...

v(x) = $0.5*\ln((1.0+x)/(1.0-x))$

Set v(x) ...

Ok

Problem:

THE LEGENDRE EQUATION

EQUATION: $-(p(x) \cdot y'(x))' + q(x) \cdot y(x) = \text{Eigen_Value} \cdot w(x) \cdot y(x)$

$p(x) = 1 - x^2$

$q(x) = 1/4$

$w(x) = 1$

Interval:

$x = -1 \dots 1$

Boundary Conditions ...

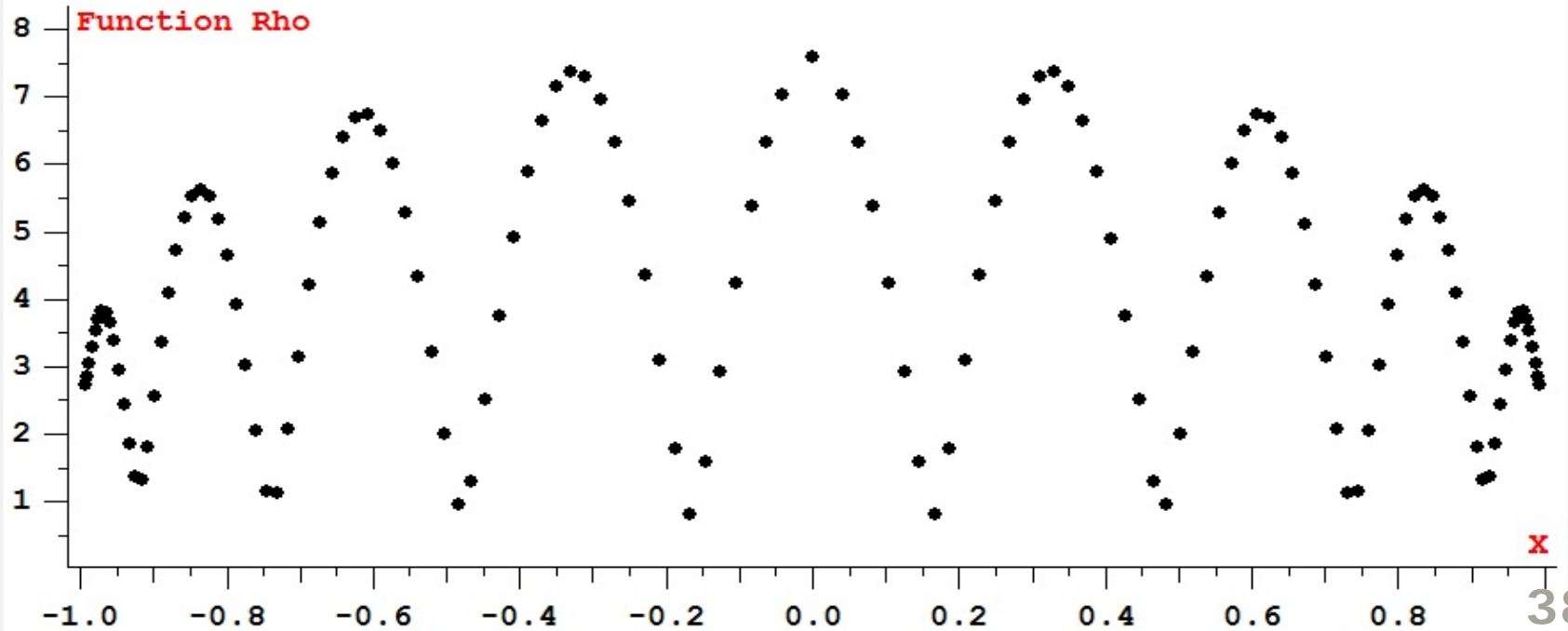
Number of Eigen Value =

9

Solve

eigen value =

90.2452011108398



Problem:

THE LEGENDRE EQUATION

EQUATION: $-(p(x) \cdot y'(x))' + q(x) \cdot y(x) = \text{Eigen_Value} \cdot w(x) \cdot y(x)$

$p(x) = 1 - x^2$

$q(x) = 1/4$

$w(x) = 1$

Interval:

$x = -1$

..

1

Boundary Conditions ...

Number of Eigen Value =

9

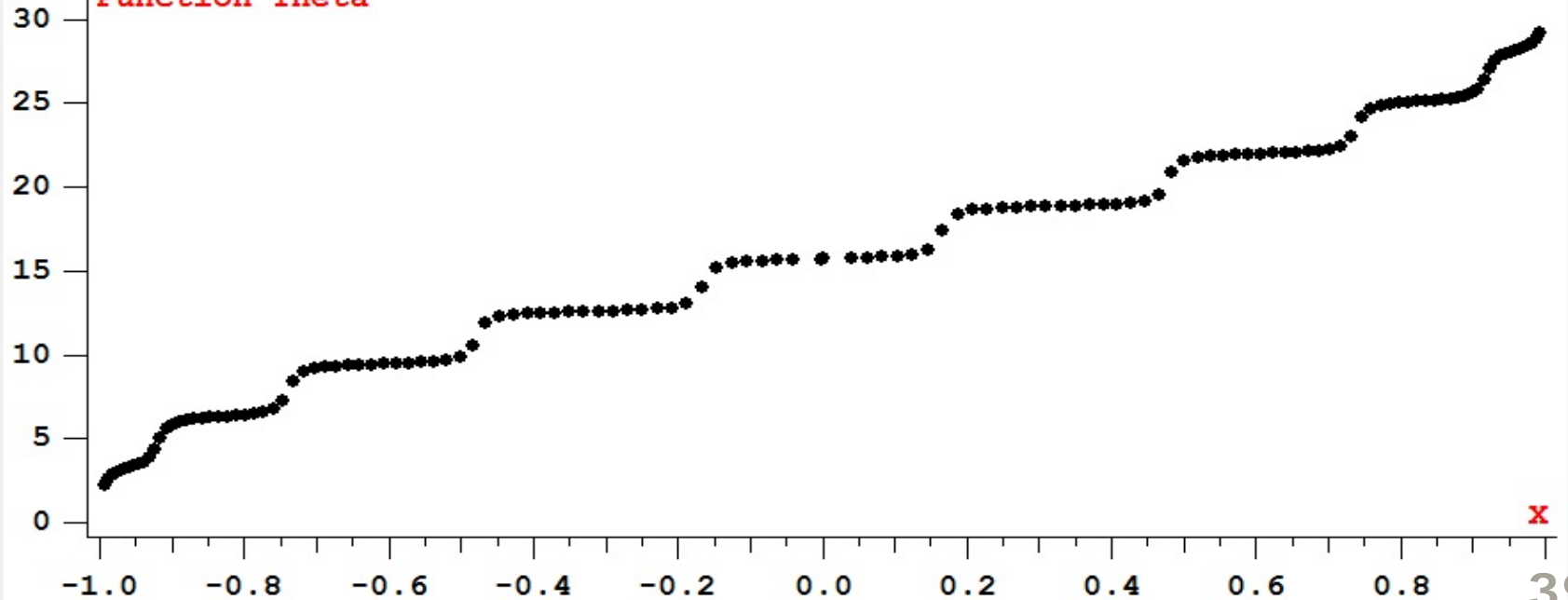


Solve

eigen value =

90.2452011108398

Function Theta



File Parameters View Information about the problem About

Problem: THE BESSEL EQUATION

EQUATION: $-(p(x) \cdot y'(x))' + q(x) \cdot y(x) = \text{Eigen_Value} \cdot w(x) \cdot y(x)$

$p(x) = 1$
 $q(x) = (0.75 \cdot 0.75 - 0.25) / x^2$
 $w(x) = 1$

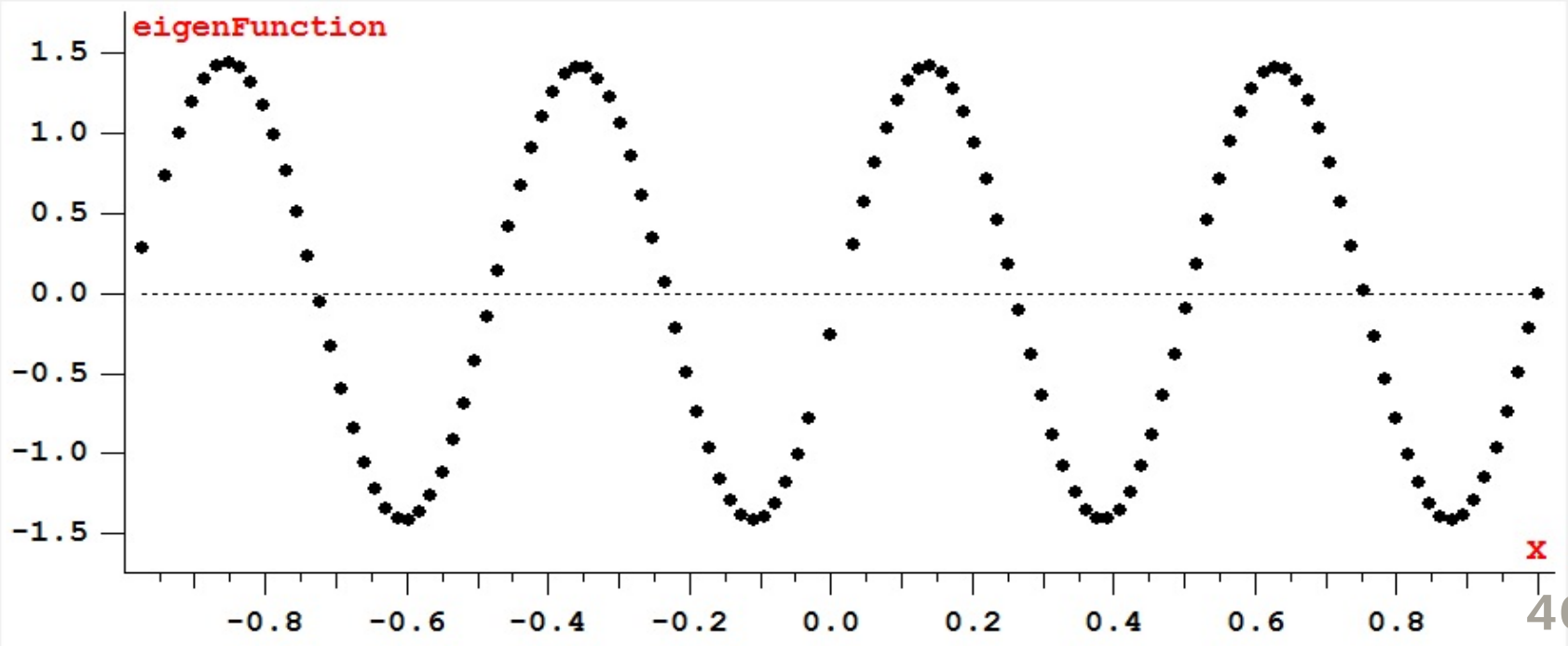
Interval: $x = 0 \dots 1$

Boundary Conditions ...

Number of Eigen Value = 7 +
-

Solve

eigen value = 651.2373046875



Problem:

A WEAKLY REGULAR EQUATION

EQUATION: $-(p(x) \cdot y'(x))' + q(x) \cdot y(x) = \text{Eigen_Value} \cdot w(x) \cdot y(x)$

$p(x) = \text{sqrt}(\text{abs}(x))$

$q(x) = 0$

$w(x) = 1/\text{sqrt}(\text{abs}(x))$

Interval:

x = 0

..

1

Boundary Conditions ...

Number of Eigen Value =

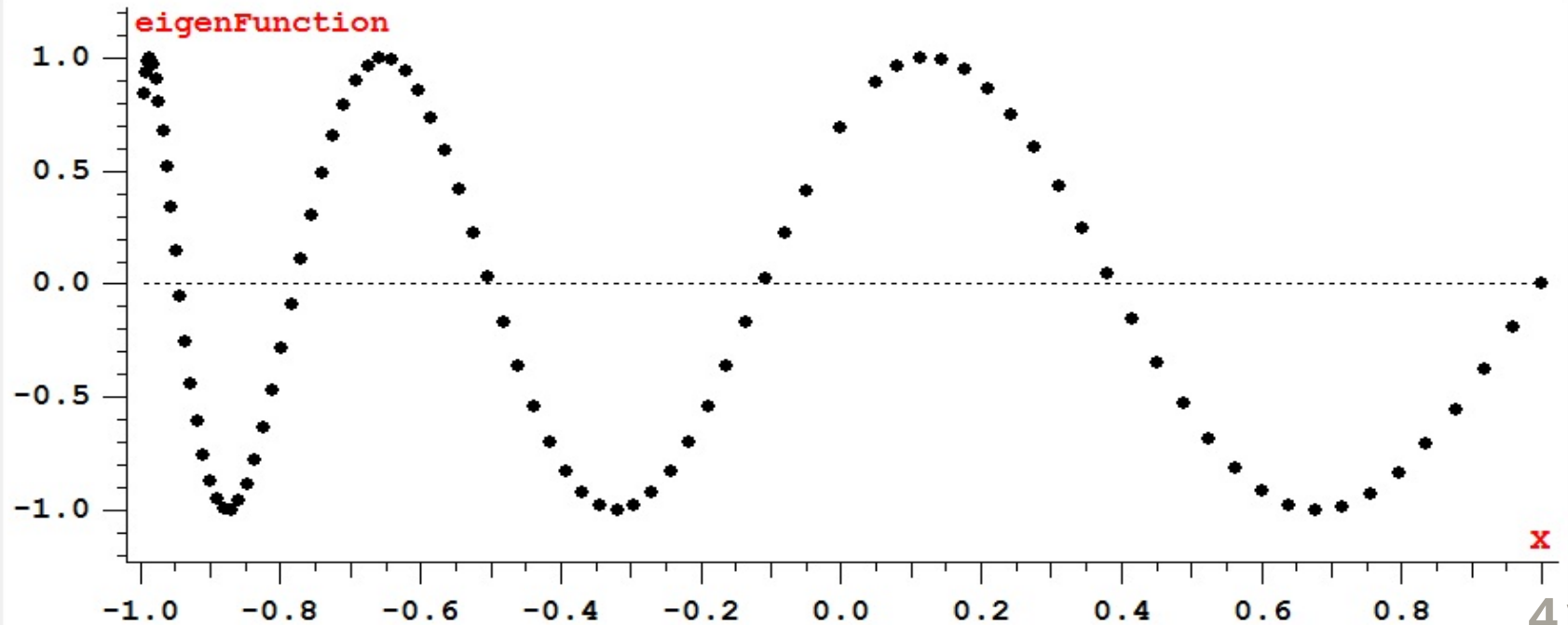
5



Solve

eigen value =

88.8362655639648



The comparison between SLEIGN2 and well known mathematical packages (Mathematica, Maple, COMSOL Multiphysics) shows that SLEIGN2 is more efficient from the point of view time of computation and numerical errors. Moreover, is not possible to solve problem with coupled conditions in Maple and Mathematica.

References and resources:

1. Werner O. Amrein, Andress M. Hinz, David B. Pearson "Sturm - Liouville Theory. Past an Present"
2. J.D. Pryce "Numerical solution of Sturm-Liouville Problems" (Oxford University Press; 1993)
3. <http://www.docstoc.com/docs/2594692/SLEIGN2>
4. <http://www.math.niu.edu/SL2>
5. A. Devdariani, E. Dalimier "Dipole transition-matrix elements of the one-electron heterodiatomic quasimolecules"



Thank you for attention!