1 2-particle bound state problem in configuration space

Exercise 1 *Provided code estimates matrix elements for a given potential (IPOT), fills Hamiltonian matrix and calculates negative eigenvalues (bound state binding energies). As the basis functions defined on Lagrange-Laguerre mesh are used. Matrix elements of the potential are calculated in two ways:*

1. *'Exactly' using a Gauss-Laguerre quadrature e.q.(1) with many knots.*
2. *Approximately using Lagrange-mesh method (formulae's (19))*

   Your goals are:

- *To calculate binding energies obtained using two methods variational (1) and Lagrange-mesh(2). Compare obtained results.*
- *Try to optimize the grid to reduce number of points (NMAX), by varying scaling parameter HAV.*
- *Print the wave function, by setting proper values of the grid size (RBMAX) and number of points (NB_points). Compare obtained wave functions: accurate (many basis functions, 30<NMAX<80) and optimized (NMAX<15)*

To run the code: control the parameters in the input file 'input_matrix_elem.para' then execute ./Run_2bbs_exercise.

Binding energies are printed on screen. Shape of the potential is printed into the file 'Potential.txt'. Calculated bound-state wave function is printed into the file 'bs_wave_function.txt'.

#	***NMAX***	*TYPE*	*ALPHA*	*BETA*	*N_REG*	*COOR_TR*	***HAV***	*R_MIN*	*R_MAX*
	30	*5*	*1.0*	*0.0*	*0.5*	*1*	***0.4***	*0.*	*1.*
#	*IPOT*	*L_2C*	*ENERGY*						
	5	*0*	*1.0*						
#	*RB_MAX*	*NB_PNT*							
	20.0	*100*							

Parameter IPOT is 1...6 and corresponds your group/session number!

2 2-particle scattering problem in configuration space

Exercise 2 *Provided code calculates for a given potential (IPOT) and angular momentum L_2C scattering phaseshifts at provided energy (ENERGY). Lagrange-Laguerre mesh method ans Kohn variational principle are used.*
Your goals are:

- *To calculate scattering phaseshifts at several energies (0.001<ENERGY<10). How they evolve with energy?*
- *Try to optimize the grid by reducing number of points (NMAX) and by varying scaling parameter (HAV).*
- *Print the wave function, by setting proper values of the grid size (RBMAX) and number of points (NB_points). Compare obtained scattering wave functions: accurate (many basis functions, 30<NMAX< 80) and optimized (NMAX<15).*
- *Wave functions at different energies, how they evolve?*
- *Compare obtained wave function to one obtained for the bound state! To run the code: control the parameters*

in the input file 'input_matrix_elem.para' then execute ./Run_2bsc_exercise

Phaseshifts are printed on screen. Calculated scattering wave function is printed into the file sc_wave_function.txt'.

#	NMAX	TYPE	ALPHA	BETA	N_REG	COOR_TR	HAV	R_MIN	R_MAX
	30	5	1.0	0.0	0.5	1	**0.4**	0.	1.
#	IPOT	**L_2C**	**ENERGY**						
	5	**0**	**1.0**						
#	RB_MAX	NB_PNT							
	20.0	100							

Parameter IPOT is 1...6 and corresponds your group/session number!

2.1 Short overview of the formalism

2.1.1 Gaussian quadrature

Possible meshes: [1]

$Type$	$Kind$	$w(x)$	$Interval$
Gauss − Legendre	1	1	$[-1,1]$
$Chebychev 1^{st} kind$	2	$\frac{1}{\sqrt{(1-x^2)}}$	$(-1,1)$
Gegenbauer	3	$(1-x^2)^\alpha$	$[-1,1]$
Jacobi	4	$(1-x)^\alpha(1+x)^\beta$	$[-1,1]$
GeneralizedLaguerre	5	$x^\alpha \exp(-x)$	$[0,\infty)$
GeneralizedHermite	6	$x^\alpha \exp(-x^2)$	$(-\infty,\infty)$
Exponential	7	$\left[\frac{x}{2}\right]^\alpha$	$[-1,1]$
Rational	8	$x^\alpha x^\beta$	$[0,\infty)$
Cosh	−	$\frac{1}{\cosh(x)}$	$(-\infty,\infty)$

Approximation of an integral using a Gauss quadrature:

$$\boxed{\int_a^b f(x)w(x)dx \approx \sum_{i=1}^{N_g} w_i f(x_i)} \tag{1}$$

where w_i are special weights, $w(x)$ a well chosen weighting function, whereas x_i are knots of the Gaussian quadrature.

Remark 3 *Of course the* (w_i, x_i) *depends on the choice of the quadrature type and* N_g.

[1] Here a column Kind represent an integer index used as argument in subroutine cdgqf to pick between different Gauss-quadratures.

2.1.2 How one gets an optimal (w_i, x_i)?

Let consider characteristic polynomial $L_{N_g}(x)$ of the order N_g for the integral with a given weight function $w(x)$:

$$\int_a^b L_{N_g}(x)w(x)dx \tag{2}$$

By definition

$$\int_a^b L_i(x)L_j(x)w(x)dx = \delta_{i,j} \tag{3}$$

For any polynomial $p_n(x)$ of the order $n < N_g$:

$$\int_a^b p_n(x)L_{N_g}(x)w(x)dx \equiv 0; \qquad \text{if } n < N_g \tag{4}$$

since any $p_n(x)$ might be expressed as a linear combination of $L_i(x)$ with $i = 0, 1, ..., N_g - 1$.

Theorem 4 *If we pick the N_g nodes x_i to be the zeros of $L_{N_g}(x)$, then there exist N_g weights w_i which make the Gauss-quadrature computed integral exact for all polynomials $h_n(x)$ of degree $n = 2N_g - 1$ or less. Furthermore, all these nodes x_i will lie in the open interval (a, b).*

So let find the N_g roots x_i of the $L_{N_g}(x)$, i.e.

$$L_{N_g}(x) = c\prod_{i=1}^{N_g}(x - x_i) \tag{5}$$

and from these roots construct N_g independent polynomials $f_i(x)$ of order $N_g - 1$:

$$f_{i,N_g}(x) = c_i \frac{L_{N_g}(x)}{(x - x_i)}, \tag{6}$$

thus by definition $f_{i,N_g}(x)$ are orthogonal to $L_{N_g}(x)$ in the interval (a, b). Then any polynomial $p_n(x)$ of order $n \leq N_g - 1$ is easily expressed by $f_{i,N_g}(x)$ using Lagrange interpolation:

$$p_n(x) = \sum_{i=1}^{N_g} \frac{p_n(x_i)}{f_{i,N_g}(x_i)} f_{i,N_g}(x) \tag{7}$$

Now let take any polynomial $h_n(x)$ of order $n \leqslant 2N_g - 1$. One may always express:

$$h_n(x) = a_{n-N_g}(x)L_{N_g}(x) + r_{n-N_g-1}(x) \tag{8}$$

Then:

$$\int_a^b h_n(x)w(x)dx = \int_a^b r_{n-N_g-1}(x)w(x)dx = \sum_{i=1}^{N_g} \frac{r_{n-N_g-1}(x_i)}{f_{i,N_g}(x_i)} \int_a^b f_{i,N_g}(x)w(x)dx \tag{9}$$

Let see that gives Gauss quadrature rule with knots x_i :

$$\begin{aligned}
\int_a^b h_n(x)w(x)dx &= \int_a^b \left[a_{n-N_g}(x)L_{N_g}(x) + r_{n-N_g-1}(x)\right] w(x)dx \\
&\approx \sum_{i=1}^{N_g} w_i a_{n-N_g}(x_i)L_{N_g}(x_i) + \sum_{i=1}^{N_g} w_i r_{n-N_g-1}(x_i) \\
&= \sum_{j=1}^{N_g} w_i r_{n-N_g-1}(x_i)
\end{aligned}$$

It is obvious that one can adjust N_g weights w_i to make calculation of N_g integrals $\int_a^b f_{i,N_g}(x)w(x)dx$ exact. Comparing the last two equations one can see that the last equation becomes exact, if w_i is chosen to be:

$$w_i = \frac{\int_a^b f_{i,N_g}(x)w(x)dx}{f_{i,N_g}(x_i)} \tag{10}$$

Since $f_{i,N_g}(x)$ are polynomials of order $N_g - 1$ and $f_{i,N_g}(x)f_{j,N_g}(x)$ are the polynomials of order $2N_g - 2$:

$$\begin{aligned}\int_a^b f_{i,N_g}(x)f_{j,N_g}(x)w(x)dx &= \sum_{i=1}^{N_g} w_i f_{i,N_g}(x_i)f_{j,N_g}(x_j) = \delta_{i,j} w_i \left[f_{i,N_g}(x_i)\right]^2 \\ &= \delta_{i,j} f_{i,N_g}(x_i) \int_a^b f_{i,N_g}(x)w(x)dx\end{aligned}$$

3 Langrange mesh method

Based on the Gauss quadrature and the Lagrange interpolation one can construct a very efficient numerical method to solve integro-differential equations, called Lagrange mesh method [1].

We start by constructing a square-integrable basis in the domain $[a, b]$:

$$\boxed{f_i(x) = c_i \left(\frac{x}{x_i}\right)^n \frac{L_{N_g}(x)}{(x-x_i)} \sqrt{w(x)}} \tag{11}$$

with $L_{N_g}(x)$

$$L_{N_g}(x) = c \prod_{i=1}^{N_g} (x - x_i) \tag{12}$$

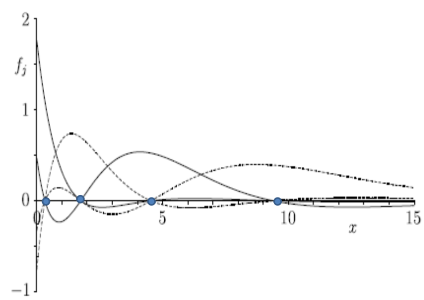

Fig. 2. Lagrange–Laguerre functions (3.52) for $\alpha = 0$ and $N = 4$.

Figure 1:

as previously eq.(3) characteristic polynomial associated with a weighting function $w(x)$; c_i are chosen in such a way that:

$$\int_a^b f_i(x) f_i(x) dx = 1. \tag{13}$$

If the Gauss-quadrature approximation is used with N_g points and weighting function $w(x)$:

$$\int_a^b f_i(x) f_j(x) dx \approx \sum_{k=1}^{N_g} w_k \frac{f_i(x_k) f_j(x_k)}{w(x_k)} = \delta_{i,j} w_i \left[\frac{f_i(x_i)}{\sqrt{w(x_i)}}\right]^2 \tag{14}$$

The last approximation becomes an exact expression if $2N_g - 1 - 2(N_g - 1 + n) \geq 0$; i.e. $n \leq 1/2$. For this case:

$$\boxed{w_i = \left[\frac{f_i(x_i)}{\sqrt{w(x_i)}}\right]^{-2}} \tag{15}$$

and the defined basis functions $f_i(x)$ are orthogonal:

$$\boxed{\int_a^b f_i(x) f_j(x) dx = \delta_{i,j}} \tag{16}$$

4 Evaluation of the matrix elements using Langrange mesh method

In order to construct the matrix elements corresponding to the Operator $\widehat{O}(x)$ one has to estimate:

$$O_{ij} = \left\langle f_i \left| \widehat{O} \right| f_j \right\rangle = \int_a^b f_i(x)\widehat{O}(x)f_j(x)dx \tag{17}$$

By using Gauss-quadrature approximation with N_g points and weighting function $w(x)$, one has:

$$\begin{aligned} O_{ij} &= \int_a^b f_i(x)\widehat{O}(x)f_j(x)dx \\ &\approx \sum_{k=1}^{N_g} w_k \frac{f_i(x_k)\left[\widehat{O}(x_k)f_j(x_k)\right]}{w(x_k)} = w_i \frac{f_i(x_i)\left[\widehat{O}(x_i)f_j(x_i)\right]}{w(x_i)} \end{aligned}$$

Projection of a given wave function $\phi(r) = F(r)/r$ on the Lagrange-mesh basis:

$$\begin{aligned} F(r) &\approx \sum_{i=1}^{N_g} C_i f_i(r) \\ C_i &= \langle f_i \,| F \rangle = \int_0^\infty \frac{F(r)}{r}\frac{f_i(r)}{r} r^2 dr \approx \sum_{k=1}^{N_g} w_k \frac{f_i(x_k)F(x_k)}{w(x_k)} = w_i \frac{f_i(x_i)F(x_i)}{w(x_i)} = \frac{F(x_i)}{f_i(x_i)} \end{aligned}$$

Example: to solve radial Schrődinger equation one needs to estimate matrix elements of the potential V_{ij} as well as of the total energy E_{ij}.For this problem it is practical to use Lagrange meshes defined on the infinite domain [0,∞) like Lagrange-Laguerre one.

Using Gauss-quadrature approximation with N_g points:

$$E_{ij} = \int_0^\infty \frac{f_i(r)}{r} E \frac{f_j(r)}{r} r^2 dr \approx \sum_{k=1}^{N_g} w_k \frac{f_i(x_k)\left[E f_j(x_k)\right]}{w(x_k)} = \delta_{i,j} E \tag{18}$$

Local potential:

$$V_{ij} = \int_0^\infty \frac{f_i(r)}{r} V(r) \frac{f_j(r)}{r} r^2 dr \approx \sum_{k=1}^{N_g} w_k \frac{f_i(x_k)\left[V(x_k) f_j(x_k)\right]}{w(x_k)} = \delta_{i,j} V(x_i) \tag{19}$$

4.1 Calculation of the scattering phase-shifts by Lagrange-mesh method:

One has to solve Schrödinger equation for a provided potential V and at a given scattering energy E_{cm}. It is:

$$(E_{cm} - \widehat{H}_l(r) - V_l(r))\psi_{l,k}(r) = 0$$

where

$$\widehat{H}_l(r) = \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}$$

One knows, that radial wave-function should satisfy the boundary condition:

$$\begin{aligned} \psi_{l,k}(r) &\underset{r\to 0}{\longrightarrow} 0 \\ \psi_{l,k}(r) &\underset{r\to\infty}{\longrightarrow} \widehat{j}_l(kr) + \tan(\delta)\widehat{n}_l(kr) \quad , \end{aligned}$$

where $k = \frac{2\mu}{\hbar^2} E_{cm}$ is scatttering momentum, whereas $\widehat{j}_l(kr)$ and $\widehat{n}_l(kr)$ are respectively Riccati-Bessel and Riccati-Neumann functions.

We search wave function in the form:

$$\psi_{l,k}(r) = \sum_{i=1}^{Ng} C_i f_i(r) + \widehat{j}_l(kr) + \tan(\delta)\widehat{n}_l(kr)F_{cut}(r) \tag{20}$$

where $F_{cut}(r)$ is some smooth function used to regularize divergence of $\widehat{n}_l(kr)$ at $r \to 0$, such that:

$$\begin{aligned} F_{cut}(r)\widehat{n}_l(kr) &\quad \underset{r\to 0}{\longrightarrow} 0 \\ F_{cut}(r)\widehat{n}_l(kr) &\quad \underset{r\to \infty}{\longrightarrow} \widehat{n}_l(kr) \end{aligned} \quad ,$$

Solution: By plugging expression eq.(20) into radial Schrödinger equation and projecting on each of Lagrange-mesh functions $f_i(r)$,

$$\boxed{\int dr f_i(r) \quad (E_{cm} - \hat{H}_l(r) - V_l(r))\psi_{l,k}(r) = 0} \tag{21}$$

we get Ng equations for $Ng + 1$unknowns (Ng coefficients C_i and $\tan(\delta)$). These Ng equations are supplemented by the Kohn-variational principle:

$$\boxed{\tan(\delta) = -\frac{2\mu}{\hbar^2 k} \int \widehat{j}_l(kr) V_l(r) \psi_{l,k}(r) dr} \tag{22}$$

References

[1] D. Baye, Phys. Rep. **565** (2015) 1.