TALENT School@MITP 2022
Numerov exercise

1/8/2022 and 2/8/2022

1 Numerov method

Starting with Schrödinger equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r}) \tag{1}$$

and defining

$$\psi(\boldsymbol{r}) = \frac{1}{r}Y_{lm}(\hat{r})u_l(r) \tag{2}$$

one obtains the radial equation

$$\frac{d^2}{dr^2}u_l(r) = \frac{2\mu}{\hbar^2}\left[-E + V(r) + \frac{\hbar^2}{2\mu}\frac{l(l+1)}{r^2}\right]u_l(r) \tag{3}$$

The radial equation is subject to the boundary condition $u_l(0) = 0$ Furthermore for $r \to 0$ the radial wave function behaves as $u_l(r) = Ar^{(l+1)}$.

In order to apply the Numerov method it is convinient to write the radial equation in the form

$$u_l''(r) + k(r)u_l(r) = 0 \tag{4}$$

with

$$k(r) = 2\mu\left[E - V(r) - \frac{1}{2\mu}\frac{l(l+1)}{r^2}\right], \tag{5}$$

where from now on we assume $\hbar = c = 1$.

The Eq. 4 can be solved using the Numerov method:

$$\frac{1}{2}[u(r+h)+u(r-h)] = u + \frac{h^2}{2}u'' + \frac{h^4}{4!}u^{(4)} + \frac{h^6}{6!}u^{(6)} + \dots \tag{6}$$

differentiating twice we get

$$\frac{1}{2}[u''(r+h)+u''(r-h)] = u'' + \frac{h^2}{2}u^{(4)} + \frac{h^4}{4!}u^{(6)} + \dots \tag{7}$$

Multiplying Eq. (7) by $\frac{1}{12}h^2$ and subtracting the result from Eq. (6) eliminates the h^4 term, yielding the result

$$u_{i+1} + u_{i-1} = 2u_i + \frac{h^2}{12}(u''_{i+1} + 10u''_i + u''_{i-1}) + O(h^6) \tag{8}$$

substituting into the Numerov expansion we get

$$u_{i+1} = \frac{[2 - \frac{5h^2}{6}k_i]u_i - [1 + \frac{h^2}{12}k_{i-1}]u_{i-1}}{1 + \frac{h^2}{12}k_{i+1}}. \tag{9}$$

Bound state solution :

The Numerov method requires the initial conditions u_0 , u_1 and the energy E. However, for a bound state problem the energy is the observable one wants to calculate. Remember that for a bound state with the negative energy it follows that the physical solution has to vanish as $r \to \infty$. Clearly, it is not possible to calculate all steps up to infinity, but since the wave function has an exponential decrease it is sufficient to set the r_{max} such that $u(r_{\max}) \approx 0$. Thus one has to solve Eq. (9) for all energies in a given energy interval $\langle E_{\min}, E_{\max}\rangle$ with spacing dE and pick out the energy satisfying the $u(r_{\max}) \approx 0$.

Scattering solution :

Scattering solution $u(r)$ for a given positive energy $E > 0$ is obtained quite easily using Eq. 9. Scattering phase shifts are then determined using the matching condition which can be done either via the logarithmic derivative or using the value of the numerical solution $u(r)$ at two different points r_1 and r_2 at large distances beyond the range of the potential. We will use the latter method in order to avoid calculating derivatives. In this case the phase shift $\delta(k)$ at the momentum $k = \sqrt{2\mu E}$ is given by

$$\tan[\delta(k)] = \frac{\beta j_l(kr_1) - j_l(kr_2)}{\beta n_l(kr_1) - n_l(kr_2)}, \tag{10}$$

where

$$\beta = \frac{r_1 u(r_2)}{r_2 u(r_1)} \tag{11}$$

and j_l, n_l are spherical Bessel functions.

2 Python exercise

Open the python script `central_nomerov.py`. This script is prepared for an implementation of the Numerov method employed to solve single-channel two-body Schrödinger equation with a local short-range interaction.

Two-body bound state exercise :

In the script you can find function `numerov_wf(E,potential)` which takes as an input two-body energy E, potential function and returns normalized $u(r)$ wave function ($u_i(r_i)$ grid array).

1. Complete the `numerov_wf(E,potential)` function calculating the wave function $u(r)$ via Numerov method.

2. After completion of `numerov_wf(E,potential)` function use the python script to calculate the deuteron bound state energy and wave function $u(r)$ using Volkov and Minnesota NN potential. Use the result for Volkov potential given in Tab. 1 as a benchmark.

Potential	Volkov	Minnesota
$E_b(^2\mathrm{H})$	-0.5458	

Table 1: Bound state energies in MeV.

Two-body scattering exercise :

The function `calc_phaseshifts(u,k)` takes as an input $u_i(r_i)$ grid array for some positive energy $E = k^2/(2\mu)$ and the corresponding two-body relative momentum k. Matching calculated $u(r)$ wave function to the free scattering solution the `calc_phaseshifts(u,k)` function calculates phase shifts $\delta(k)$ which are subsequently returned in a form of $k\mathrm{cot}[\delta(k)]$.

1. Complete the `calc_phaseshifts(u,k)` function writting a short code which calculates the phase shifts using the matching condition.

2. Use the python script to calculate $NN(^3S_1)$ scattering phaseshift using Volkov or Minnesota NN interaction.

Calculated phaseshifts can be parametrize using effective range expansion (ERE)

$$k\mathrm{cot}[\delta(k)] = -\frac{1}{a} + \frac{1}{2} r_{\mathrm{eff}} k^2 + \mathcal{P} r_{\mathrm{eff}}^3 k^4 + \ldots$$

Corresponding scattering parameters - scattering length a, effective range r_{eff}, and shape parameter $\mathcal{P}$ are then extracted fitting the phaseshifts with ERE. This fit is expected to be performed in the `ere_param(phsf)` function which takes as an input a grid of calculated phashifts in the $k\text{cot}[\delta(k)]$ form and returns the scattering perameters a, r_{eff}, $\mathcal{P}$ with the correspong error induced by the fit.

3. Complete the `ere_param(phsf)` function and extract the $NN(^3S_1)$ scattering parameters for Volkov or Minnesota potential. Use the result for Volkov potential given in Tab. 2 as a benchmark.

Potential	a	r_{eff}	$\mathcal{P}$
Volkov	10.0832	2.3739	0.0322
Minnesota			

Table 2: Scattering parameters in fm.

Extra :

1. Use the two-body bound state wave function $u(r)$ to calculate the corresponding rms radius $\sqrt{< r^2 >}$, $< r^2 >= \int_0^\infty |u(r)|^2 r^2 \text{d}r$. Note that rms radius should be calculated in a function `rms_radius(u)`.

2. Solving Schrödinger equation for a potential $V(r) = -8e^{-0.16r^2} + 4e^{-0.04r^2}$ and particle masses $m_1 = m_2 = 2(\hbar c)^2$ yields one s-wave ($l = 0$) bound state and one p-wave ($l = 1$) bound state which are followed by a series of resonances. Implement the potential into your Numerov python script. As a benchmark calculate bound state energies and compare them to results given in Tab. 3. In the last step calculate corresponding s-wave and p-wave phaseshifts up to 2.1 MeV. How many resonances do you see and at which energies ? Try to plot $u_l(r)$ at the resonance energy. How it differes from a bound state wave function or a scattering wave function at energies far from the resonance position ?

Channel	E
s-wave ($l = 0$)	-1.928
p-wave ($l = 1$)	-0.675

Table 3: Bound state energies in MeV.