WEEK 1: Infinite square well potential, finite square well potential, Wood-Saxon potential

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1 Structure

The three programs have the same structure in order to find the eigenvalues and eigenvectors of the considered system.
The main file contains the code that finds the eigenvalues between 0 and 100 MeV (E_{plus}). The eigenvalues are found with the bissection method, which includes the numerov method in order to calculate the eigenfunction for each eigenvalue. For each eigenfunction found, we calculate its nodes, and we modify the extremes of the bissection method according to them. When the extremes are closer than epsi, we exit the loop, and put the eigenvalue as the right extreme of the bissection method. Then we recalculate the eigenfunction with the shooting method, with right hand side equal to 0, in order to find the convergence, and we normalize it.

The only thing that changes between the different programs is the potential.

1.1 Functions and Subroutines

- Function Vpot(xy) : potential used in each case.
- Subroutine Simpson : subroutine to integrate the densities, in order to normalize the eigenfunctions. Inputs: N number of points in the mesh, dx space between the points in the mesh,f array to integrare. Output:res value of the integration.

2 Files

2.1 Infinite

- global.f90: module that includes the global variables.
- infinite.input: input file (see below).
- main.f90: main file that includes the code to find the eigenvalues and eigenfunctions.
- Makefile : makefile to compile the code (see below).

2.2 Finite

- global.f90: module that includes the global variables.
- finite.input: input file (see below).
- main.f90: main file that includes the code to find the eigenvalues and eigenfunctions.
- Makefile : makefile to compile the code (see below).
- Simpson.f90: file that contains the subroutine that integrates using the Simpson method.

2.3 WS

- global.f90: module that includes the global variables.
- WS.input: input file (see below).
- main.f90: main file that includes the code to find the eigenvalues and eigenfunctions.
- Makefile : makefile to compile the code (see below).
- Simpson.f90: file that contains the subroutine that integrates using the Simpson method.

3 Input file

- epsi= epsilon error to find the solution.
- h2m = value of $\hbar^2/2m$.
- R_{max} = in coordinate space, up to where the potential acts.
- R_{box} = size of our considered and studied system.
- h= space between two points in the mesh.
- E_{minus}= left value of the energy when finding the eigenvalues using the bissection method.
- E_{plus} = right value of the energy when finding the eigenvalues using the bissection method.
- V0 = depth of the potential. (used for finite square and WS).
- a = difusivity of the Wood-Saxon potential.

4 Output

- XYZ.dat files: Output that setore the wavefunctions, where XYZ is the number of the nodes of each wavefunction.
- Console: Output of the eigenvalues according to the number of nodes of the wavefunction, and the name of the file where the wavefunction is.

5 Makefile

To run the program, there is a Makefile, that compiles all files that form the code. To compile, type **make**, and an executable **main** is created. To run the code, type **./main**. And to delete all exectuables and outputs, type either **make clean or make clear. Makefile has to be changed with vi or vim programs.**