WEEK2: 3D Wood-Saxon potential for ^{208}Pb.

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CONSIDER FOLDER NAMED COULOMB, THE FOLDER WITHOUT COULOMB IS OUTDATED.

1 Structure

This program calculates the eigenvalues and wavefunctions of each given nlj orbital, with Wood-Saxon and spin-orbit potentials. In addition we have put the Coulomb potential when studying protons. The program consists in a loop over isospin (ipart=1,2 first neutrons, then protons), and calculates for each possible nlj (up to the limit put in the input file) the corresponding eigenvalue and wavefunction.

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.

When all possible orbitals are calculated, we rearrange the energy in ascending order, in order to find the correct order in the levels.

After, the density profiles are calculated.

1.1 Functions and Subroutines

- Function Vpot(xy, mm, ip) : xy: point in the mesh to study, mm: spin, ip: neutrons/protons. Function that calculates the total potential. Includes the Wood-Saxon potential, the Spin-Orbit contributions and the Coulomb potential when studying the protons. For the equations in order to calculate each potential, refer to manuale_hf.pdf.

- Subroutine simpson(N, dx, f, res) : 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 integrate. Output:res value of the integration.

- Subroutine arrange_energy (matrix, numorb, wavef): Subroutine that arranges the energy in ascending order. As the energy is given as an input inside matrix (includes energy and quantum numbers), all is arranged according to the value of the energy. Also the matrix that contains all the wavefunctions (wavef) is arranged according to the same pattern in the energies. Numorb is the number of orbitals calculated.

2 Files

- 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.
- arrange.f90: file that contains the subroutine that arranges the energy in ascending order.

3 Input file

- NN and ZZ = number of neutrons and protons of the nucleus to study.
- epsi= epsilon error to find the solution.
- h2m = value of $\hbar^2/2m$.
- e= value of e^2, value of the charge for the Coulomb potential.
- 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.
- n_max, l_max = maximum n and l quantum numbers to calculate.
- r0 = parameter to calculate R0 in Wood-Saxon potential.
- a = difusivity of the Wood-Saxon potential.
- out_wave_func = logical parameter to output all the wavefunctions calculated in files or not.

4 Output

- Energy levels of neutrons (energy_level_n.dat) and protons (energy_level_p.dat).
- Density profiles of neutrons (density_N.dat), protons(density_P.dat) and total (density_T.dat)
- If wanted, output with all wavefunctions calculated. (out_wave_func =.true.)

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.**