Project II

Codes and Results are due electronically as Pr2.tar in your directory Homework.

Project is due : Thursday, 12/08/2016 9:00 am

Include analytical derivations or setup of equations you want to share with me either as scans of handwritten notes or as pdf file(s) if you do not incorporate them into a latex file.
Please make those extra files easy to recognize by their names.

1. Coordinate-space Schrödinger Equation for ^{13}C *(10 pts)*

A short-range nuclear potential can be approximated by a so-called Wood-Saxon potential, which has the form

$$V(r) = -V_r \, f_{ws}(r,a,R) - V_{so}\left(\frac{-2}{r}\right)\frac{d}{dr}\, f_{ws}(r,a,R)\, \mathbf{l}\cdot\sigma. \tag{1}$$

The Woods-Saxon functions have the form

$$f_{ws}(r,a,R) = \left[1+\exp\left(\frac{r-R}{a}\right)\right]^{-1}, \tag{2}$$

where $R = r_0 A^{1/3}$ with A being the mass number of the nucleus. Let us consider here for ^{13}C the neutron in the Wood-Saxon well given by ^{12}C. In Eq. (1) r is the distance between the neutron and the center-of-mass of the ^{12}C nucleus. Though it is a relative coordinate, the center-of-momentum is not needed in this problem. The relative orbital angular momentum is given by $\mathbf{l}$, and the spin of the neutron by σ. Use the following constants

$$\begin{aligned} V_r &= 52.45 \text{ MeV} \\ R &= 1.15 * 12^{1/3} \text{ fm} \\ a &= 0.69 \text{ fm} \\ \hbar c &= 197.32705 \text{ MeV fm}. \end{aligned} \tag{3}$$

Use as average nuclear mass $m_N = 938.9$ MeV.

1. Write down explicitly the radial Schrödinger equation for $l = 0$, i.e. the s-wave, and pay attention to units.

2. Plot the potential as function of r.

3. Derive the analytic form of the matching condition for $r \to \infty$ and describe the algorithm you plan to use to find the ground state energy, e.g. a bisection or Newton-Raphson-Secant strategy.

4. Choose either a Runge-Kutta or Numerov algorithm to solve the differential equation, and apply your search algorithm for the energy.

5. The potential of Eq. (1) supports one s-wave bound state. Calculate its energies and convince yourself (and me) with an error analysis that your numerically obtained value is accurate to 3 significant figures.

6. Plot the normalized ground state wave function $u_1(r)$.

2. Momentum-space Schrödinger Equation with Delta-Shell Potential *(10 pts)*

The radial part of the momentum space Schrödinger equation for two particles is given by (see Landau-Paez, Ch. 16 or M. Hjort-Jensen Ch. 12.8)

$$\frac{q^2}{2\mu}\psi_n(q) + \frac{2}{\pi}\int_0^\infty dp' p'^2 V(q,p')\psi_n(p') = E_n\psi_n(q), \tag{4}$$

where μ represent the reduced mass of the two-body system. The potential $V(q,p)$ is the momentum space representation (double Fourier transform) of the coordinate-space potential

$$V(q,p) = \frac{1}{qp}\int_0^\infty dr \sin(qr)V(r)\sin(pr). \tag{5}$$

Consider the local delta-shell potential

$$V(r) = \frac{\lambda}{2\mu}\delta(r-b). \tag{6}$$

This might be a good model for an interaction that occurs when two particles are predominantly a fixed distance b apart. Applying Eq. (5) leads to the momentum space representation

$$\begin{aligned} V(p',p) &= \int_0^\infty dr \frac{\sin(p'r')}{p'p}\frac{\lambda}{2\mu}\delta(r-b)\sin(pr) \\ &= \frac{\lambda}{2\mu}\frac{\sin(p'b)\sin(pb)}{p'p}. \end{aligned} \tag{7}$$

This potential is easy to evaluate in momentum space. However, its singular nature in coordinate space leads to Eq. (7) having a very slow fall-off in momentum space, and thus causes the integrals to converge slowly so that the numerics may be a little more tricky.

Set the scale of the problem by setting $2\mu = 1$, $b = 10$, and $\lambda = -8$.

1. Write down explicitly the integral equation you are going to solve. State clearly which numerical procedure you are using for solving the equation, and include details on the discretization of the integral.

2. Set up the eigenvalue problem and solve it using LAPACK routines:

- Set up the potential and Hamiltonian matrices $V(i,j)$ and $H(i,j)$ for the Gaussian quadrature integration with at least $N = 48$ grid points.
- Either set up the eigenvalue problem to find eigenstates for which the determinant vanishes or directly find the eigenvalues and eigenvectors for this H with a routine like *dgeev* from LAPACK.
  Note: The eigenenergy solver may return several eigenenergies. The true bound state will be at negative energy and will change little as the number of grid points changes. The others are most likely numerical artefacts.
- Increase the number of grid points and see how the energy stabilizes. Extract the best value for the bound-state energy and estimate its precision by documenting how it changes with the number of grid points.
- Determinate the momentum-space wave function $\psi_n(k)$ using an eigenvalue solver from LAPACK. Plot the wave function and check is fall off for $k \to \infty$, and if it is well behaved for $q \to 0$.

3. Check your solution by comparing the RHS and LHS in the matrix multiplication $[H][\psi_n] = E_n[\psi_n]$ of the Schrödinger equation.

4. Using the same points and weights as used to evaluate the kernel of the integral equation, determine the coordinate-space wave function via the Bessel transform

$$\psi_n(r) = \int_0^\infty dk\, k^2 \frac{\sin(kr)}{kr} \psi_n(k). \tag{8}$$

   Plot the $\psi_n(r)$ as well as $\ln \psi_n(r)$, and check if your calculated function obeys the expected exponential fall-off for large r.