Homework 4; due Thursday, October 24

PY 502, Computational Physics, Fall 2024

Department of Physics, Boston University

Instructor: Anders Sandvik

The deuteron, the nucleus of which consists of a neutron and a proton, constitutes the simplest composite nuclear system. In this assignment you are to solve the radial Schrödinger equation for the bound state of the neutron-proton system, using a Yukawa potential supplemented by a hard-core short-range repulsion. You will adjust the width and depth parameters of this potential to fit the known binding energy and radius of the deuteron.

Radial Schrödinger equation for the neutron-proton system

The wave function for a two-particle system with a central potential $V(r)$ can be written in the form

$$\Psi_{L,L_z,n}(\vec{x}) = R_{L,n}(r)Y_{L,L_z}(\phi,\Theta), \tag{1}$$

where $Y_{L,L_z}(\phi,\Theta)$ are the spherical harmonics and the radial function satisfies the equation

$$\left(-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{L(L+1)\hbar^2}{2mr^2} + V(r)\right)R_{L,n}(r) = E_{L,n}R_{L,n}(r), \tag{2}$$

where m is the reduced mass,

$$m = \frac{M_1 M_2}{M_1 + M_2}. \tag{3}$$

Defining the function

$$U_{L,n}(r) = rR_{L,n}(r), \tag{4}$$

a simpler radial equation is obtained;

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{L(L+1)\hbar^2}{2mr^2} + V(r)\right)U_{L,n}(r) = E_{L,n}U_{L,n}(r). \tag{5}$$

This is of the same form as the one-dimensional Schrödinger equation, apart from the fact that there $-\infty < x < \infty$ but here $r \geq 0$, and the presence of the repulsive "centrifugal barrier" which effectively contributes to the potential energy.

For the deuteron $L = 0$,[1] and the radial function $U(r) = U_{0,0}(r)$ can be written as

$$\frac{d^2U(r)}{dr^2} = \alpha\left(\frac{V(r)}{E} - 1\right)U(r), \tag{6}$$

where we have defined

$$\alpha = E\frac{2m}{\hbar^2}. \tag{7}$$

The deuteron has only one bound state, with energy $E = -2.226$ MeV. The neutron and proton masses are almost equal; $M_p = 1.6726 \cdot 10^{-27}$ kg and $M_p = 1.6749 \cdot 10^{-27}$ kg. Using these values,

[1] Actually, due to a small non-central nuclear force component, L is strictly not a conserved quantum number for the deuteron; a small amount of $L = 2$ wave function is mixed with the $L = 0$ state. We will here neglect this.

we get $\alpha = -5.3667 \cdot 10^{28}$ m^{-2}. In order not to have to work with the very small numerical values corresponding to the short inter-nuclear distances expressed in meters, we change the unit of length from m to fm (1 fm $= 10^{-15}$ m) in Eq. (6), leading to

$$\frac{d^2U(r)}{dr^2} = \beta\left(\frac{V(r)}{E} - 1\right)U(r), \quad \beta = -0.053667. \tag{8}$$

Nuclear potential

A description of nuclear systems in terms of point particles governed by static central potentials is not completely correct, but nevertheless is important as a first approximation. Several types of model potentials are used, among them the Yukawa potential

$$V_{\mathrm{Y}}(r) = -V_0\frac{\mathrm{e}^{-r/a}}{r/a}. \tag{9}$$

At very short distances the potential should become strongly repulsive, which is not a feature of the Yukawa potential. A hard-core (infinite barrier) repulsion can be included to accomplish this. Then the full potential is

$$V(r) = \infty, \ \ \text{for } r < r_0, \qquad V(r) = V_{\mathrm{Y}}(r) = -V_0\frac{\mathrm{e}^{-r/a}}{r/a}, \ \ \text{for } r \geq r_0. \tag{10}$$

This potential will be used here. The three parameters—the hard-core radius r_0, the range a, and the depth parameter V_0—can be adjusted so that known properties of the deuteron are reproduced. Here we shall consider a simplification, fixing the hard-core radius at

$$r_0 = 0.1 \text{ fm}. \tag{11}$$

The results are in fact not very sensitive to the exact value of r_0. To fix the remaining two parameters, we will use the binding energy and the radius of the deuteron. The radius is defined in terms of the expectation value of its square

$$\langle r^2\rangle = \frac{1}{4}\langle\Psi|r^2|\Psi\rangle. \tag{12}$$

Here the factor 1/4 comes from the fact that for two particles of equal mass, the distance between them correspond to the diameter of a circular orbit, not the radius (we can here neglect the small mass difference between the neutron and the proton). Experimentally, one cannot measure the radius directly; different radia can be defined depending on what physical scattering process is measured. All of the estimates are, however, close to $r = 2$ fm, which we will use here.

Programming tasks

Write a program that solves the radial wave function written in the form (8) with the given value of β. For a bound state, with a potential decaying exponentially to zero at long distances, the asymptotic form of the wave function is given by

$$U(r) \propto \mathrm{e}^{-\sqrt{|\beta|}r}, \qquad (r \to \infty). \tag{13}$$

The second boundary condition is simple, due to the hard-core;

$$\Psi(r_0) = 0. \tag{14}$$

In this case, it is best to start the integration from the outside, at some longest distance $r_{\max}$ from the center (where $r_{\max}$ is an input value to be read in by the program, and you have to figure out by experimentation what a suitable value is), at which the wave function is well approximated by the form (13). The integration is done inward, and at the last point r_0 the second boundary condition (14) should be satisfied. Actually, provided that $r_{\max}$ is sufficiently large, the initial condition at this distance plays a very minor role (i.e., the resulting wave function in the region where it is large depends very little on it). Instead of using (13) for the two starting values $U(r_{\max})$ and $U(r_{\max} - \Delta_r)$, it is therefore also fine to choose two arbitrary (preferably small, $\ll 1$) values with $U(r_{\max}) < U(r_{\max} - \Delta_r)$.

Normally, when solving the Schrödinger equation we are interested in finding the energy eigenvalues. Here we are considering the corresponding inverse problem; we know the binding energy $E = -2.226$ MeV [given in the form of the constant β and in the ratio with the potential in Eq. (8)] and the radius $r = \sqrt{\langle r^2 \rangle} = 2$ fm. We want to find the potential that gives rise to a ground state with this energy (and no excited bound states).

For a given value of the Yukawa range parameter a in Eq. (10), your program should extract the ratio V_0/E for which a bound state is obtained. The energy of the bound state is negative (relative to the potential at $r = \infty$, which here is 0), and hence the ratio $-V_0/E = V_0/|E|$ has to be positive. Using values $V_0/|E| = 0, \Delta_V, 2\Delta_V, ...$, first search for two values between which $U(r_0)$ changes sign. Then use bisection to find the $V_0/|E|$ for which the boundary condition $U(r_0) = 0$ is satisfied. Knowing $|E| = 2.226$ MeV, you then have the potential depth parameter V_0 that gives the correct binding energy for the range parameter a used.[2] You can then calculate the radius using the wave function corresponding to these parameters, according to (12). Here you should keep in mind Eqs. (1) and (4) and note that the angular part Y of the wave function is normalized and does not enter explicitly in an expectation value of an operator not involving the angles.

Write the program in such a way that a number of different range parameters $a = a_0 + n\Delta_a$ can be processed and a file 'vr.dat' is produced which contains rows with a, V_0, r for all the values of a. Produce graphs showing V_0 and r versus a for a between 0.5 fm and 3 fm. Find the value of a for which the radius r is equal to 2 fm (in practive, very close to this value), and produce a graph of the radial wave function $U(r)$ for these potential parameters.

As always, you should do some testing to confirm that the results you present are converged, i.e., that you use a sufficiently small Δ_r as well as a sufficiently large $r_{\max}$ (by comparing results for several values of Δ_r and $r_{\max}$). You should also test the influence of the boundary condition used for the initial values $U(r_{\max})$ and $U(r_{\max} - \Delta_r)$, i.e., try some different choices, using the correct asymptotic form (13) or arbitrary values and discuss (with a graph or graphs for illustration) to what degree the boundary condition is important.

[2] Clearly, the procedure of first gradually reducing $-V_0$ from 0 implies, provided that Δ_V is sufficiently small, that the potential you find is the shallowest one for the given a that can have a bound state; hence there will be no excited bound states for this potential, in accord with the case of the actual deuteron.