Phys 3810, Fall 2009
Computer Calculation Notes

0.1 Setting Up the Problem

The goal here is to calculate the radial wave function for a bound state of a particle trapped in some thing like a finite spherical "square well", which is basically posed in Problem 4.9. Of course, with a computer we can solve for a more complicated binding potential than the simple square well. And the "exact" solution will involve some messy combinations of spherical Bessel functions; we want to flat out solve it numerically for any ℓ.

First, write out the DE for the reduced radial function $u_\ell(r)$. This is what we will solve for the eigenfunctions and eigenvalues; (4.37) is easily rewritten as:

$$\frac{d^2u_\ell}{dr^2} - \left[\frac{2mV(r)}{\hbar^2} + \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = Eu_\ell(r) \tag{1}$$

The boundary conditions[1] are $u(0) = 0$ and $u(\infty) = 0$. Satisfying these will give solutions for the possible energies E for each ℓ. Of course, what we really do is to try to satisfy $u_\ell(\infty) = 0$ by searching on E.

The first thing to do is to get the equation into a form so that it can be programmed up easily and we can input and receive numbers that we can *understand*. We will be dealing with atomic or nuclear–sized systems but we certainly don't want to deal with a lot of incomprehensible numbers in scientific notation. We want to use *sensible units*. These will depend on the scales in the problem, but here we will solve a problem on nuclear scales, for which the energies are or the order of MeV's and the length scales are of the order of fermis (1 fm $= 10^{-15}$ m.) In particular, the bound particle will be a proton, which has rest energy 938.3 MeV. For definiteness, we'll say that the depth of the well is 60.0 MeV and its radius is 4.00 fm.

It is most convenient to rewrite 1 as

$$\frac{d^2u_\ell}{dr^2} - \left[\frac{2(mc^2)V(r)}{(\hbar c)^2} + \frac{\ell(\ell+1)}{r^2} - \frac{2(mc^2)E}{(\hbar c)^2}\right] u_\ell(r) = 0 \tag{2}$$

With the very useful fact (which you are encouraged to show)

$$\hbar c = 197.33 \text{ MeV} \cdot \text{fm}$$

and $mc^2 = 938.3$ MeV, the radial equation is now

$$\frac{d^2u_\ell}{dr^2} - \left[(0.04819)(V(r) - E) + \frac{\ell(\ell+1)}{r^2}\right] u_\ell(r) = 0 \tag{3}$$

[1] To be a correct radial wave function, u_ℓ also needs to be normalized, but if we only want the energies, we won't worry about that.

In using this equation you *must* use V and E in MeV and r in fermis. Then the units of the bracket in 3 are fm^{-2}.

Eq. 3 is of the form

$$\frac{d^2u_\ell}{dr^2} - \mathcal{V}(r)u_\ell(r) = 0 \tag{4}$$

but of course if we don't know E then $\mathcal{V}(r)$ isn't fully known. (It is known provisionally if we're searching on E.)

At this point there are several ways to go. Maple provides a way of solving the DE directly while giving the eigenvalue E and we can use this, at worst searching on E by hand.

One can vary E until one gets a solution that is small at large r or equivalently which goes through a large change in sign at large r when E is varied. For this, we want to take as the two boundary conditions:

$$u_\ell(0) = 0 \qquad\qquad u'_\ell(0) = 1.$$

We can give the second condition because as the function $u_\ell(x)$ does not need to be normalized (in our problem) u'_ℓ does not have a definite value; it varies in proportion to the normalization. Since I know that u_ℓ is something like a sine function, $u'_\ell(0) = 1.$ is a reasonable choice. Regardless, we are still looking for a (dramatic) change in the sign of u_ℓ at large r when we vary E.

0.2 Maple

Maple has some fairly convenient routines for solving differential equations and plotting the results. I will give the steps which will let you do the most basic and clumsy calculation. I hope you will do more than that.

First off, while I hope you will use a more exotic form for the binding potential later on, the "square well" is good to start with. But how to get it into a Maple statement? Yes, could define a function using some "`if`" statement, but Maple does include a step function. The famous Heaviside step function, often denoted $\theta(x)$ is defined by

$$\theta(x) = \begin{cases} 0 & \text{if} \quad x < 0 \\ 1 & \text{if} \quad x \geq 0 \end{cases}$$

except that it's not called $\theta(x)$ (they reserve the `Theta` name for something else), rather it's called `Heaviside(x)`. With this function, our potential function $V(x)$ (given in MeV, with x the radial coordiante in fermis) is

$$(-60.0) * \texttt{Heaviside}(4.0 - \texttt{x})$$

which as you can see will give -60.0 MeV if x is less than 4.0 fm and 0.0 if x is bigger than 4.0 fm.

At very least we would like to get a plot of the function $u_\ell(r)$ that results from a particular choice of E. Maple has the means to solve the radial DE.

```
with (plots);
```

```
ode:=diff(y(x),x,x)= 0.4810((-60.)*Heaviside(4.-x)+50.0)*y(x);
ics:= y(0)=0, D(y)(0)=1.  ;
p:= dsolve ({ode ics}, type=numeric, range=0..8.);
odeplot(p);
```

0.3 Fortran or C or Something

The second approach is to integrate up from the two starting values of $u_\ell(r)$ so that we must discretize the differential equation in 4. All the functions are only defined on the grid points r_i.

The most naive way to do this is to use an approximation for the seond derivative of u_ℓ:

$$\frac{d^2u}{dr^2}(r_i) = \frac{(u(r_i+\Delta r) - 2u(r_i) + u(r_i - \Delta r))}{(\Delta r)^2}$$

If this is put into 4 we can solve for $u(r_i + \Delta r)$ in terms of $u(r_i)$ and $u(r_i - \Delta r)$:

$$\begin{aligned} u(r_i+\Delta r) &= 2u(r_i) - u(r_i - \Delta r) + (\Delta r)^2 \mathcal{V}(r_i) \\ &= (2 + (\Delta r)^2 \mathcal{V}(r_i))u(r_i) - u(r_i - \Delta r) \end{aligned}$$

Or more simply, using the indices:

$$u_{i+1} = (2 + (\Delta r)^2 \mathcal{V}_i)u_i - u_{i-1} \tag{5}$$

And we do have two starting values to get the process rolling, since we demand $u_0 = u_\ell(0) = 0$ and again from the arbitrariness of normalization we can assume that $u_1 = u(dr)$ is any small number. Then the first value our program determines is u_2.

That would be good enough for beginning study of a full numerical solution, but in fact we can do much better. A professional would *not* use 5 but rather would use a more sophisticated algorithm for getting u_{i+1} from the two preceding points and the values $\mathcal{V}_i$.

Most commonly used is something often called the **Numerov algorithm**. It is useful when the DE does not have a term with a first derivative (as ours, in 4 does not). To solve:

$$\left(\frac{d^2}{dx^2} + \mathcal{V}(x)\right) u = 0$$

the following algorithm is better:

$$u_{i+1} = \frac{\left(2 - \frac{5h^2}{6}\mathcal{V}_i\right) u_i - \left(1 + \frac{h^2}{12}\mathcal{V}_{i-1}\right) u_{i-1}}{1 + \frac{h^2}{12}\mathcal{V}_{i+1}} \tag{6}$$

which has more terms and some other numbers, but which is *just as easy to use* because it just comes from the previous values u_i and u_{i-1}. Note the denominator has $\mathcal{V}_{i+1}$ but that is no problem because the function $\mathcal{V}(x)$ is known at all points.

(This algorithm is widely known as "Numerov" among those who have had to use a quick and powerful technique for integrating the Schrödinger equation, but I don't find that name in any numerical analysis books and that's probably because it's a special case of some other method. I've never tracked down the official name for the algorithm in 6.)