Lecture 2

Finding roots of a function, Λ hypernuclei

We start the course with a standard numerical problem: finding the roots of a function. This exercise is meant to get you started with programming in gcc or ROOT, and hopefully also in using latex. We will apply a method to finding the energy levels of a Λ particle bound in a nucleus. First we discuss an algorithm, then the physics.

Finding the roots of a Function

Often in Physics one has to solve an algebraic equation that does not have a simple form. One can usually cast the equation into the form

$$f(x) = 0 \tag{1}$$

The goal is to find the value(s) of x that satisfy this equation, i.e. the roots of $f(x)$. If there is no analytic solution, then numerical methods can be used to find a solution to the desired accuracy. In lecture I will describe a method we call the "Bracket and Half". In the appendix I also describe two more standard algorithms: the Bisection Method, and Newton's method. In each method, an algorithm is developed for producing a series of $x's$, x_i. The algorithm is designed such that the series x_i converges to a root of $f(x)$.

Bracket and Half Method

The bracket and half method is best explained by describing the algorithm. One choses an initial starting value, x_1, and an initial step size δ. The next value of x, $x_2 = x_1 + \delta$. If $f(x_2)f(x_1) > 0$, then we have not passed a root. This is because if the product is greater than zero, the sign of $f(x_2)$ and $f(x_1)$ is the same. We keep the same value of δ and continue with $x_3 = x_2 + \delta$. We keep increasing x_i by δ until $f(x_{i+1})f(x_i) < 0$. When this occurs, we have steped over the root, because now the signs of $f(x_i)$ and $f(x_{i+1})$ are different. Now we halve the step size and reverse its direction by changing δ to $-\delta/2$. The process is continued until we have reached the desired accuracy.

Below is an example code for the bracket and half method:

```
a=starting value
del=initial step size
for (i = 1; i < imax; i++)
{
b = a + del;
if (f(b) * f(a) < 0) then del=-del/2;
a = b;
}
```

Another possibility is:

```
a=starting value
xtol=0.00001
del=initial step size
while (del > xtol)
{
b = a + del;
if (f(b) * f(a) < 0) then del=-del/2;
a = b;
}
```

The bracket and half method is useful for finding the zeros above (or below) a certain value of x. It is also useful in finding the bound state energy levels of the non-relativistic Schroedinger equation, which we will consider in the next assignment. For this application, the algorithm is refered as the "shooting method".

The particular equation that we will solve is

$$tan(\sqrt{\alpha(x-1)}\ ) + \sqrt{x-1} = 0 \tag{2}$$

where $x > 1$. Since α will be greater than zero, the solution for x will occur when the tan function is negative, i.e. when the argument of the tangent is in second quadrant. You should start your initial value at $x_1 > 1$. Let me discuss the physics behind this equation.

Lambda Hypernuclei

When particles are confined to a region of space, the energies that they can have are quantized. For our first example, we will examine the energies that a lambda (Λ) particle can have when it is "trapped" inside of a nucleus. The Λ particle is similar to a neutron and proton, and is a member of their "baryon octet":

baryon	mass(MeV/c^2)	charge	lifetime (sec)	quarks	spin
proton	938.3	+e	∞	uud	1/2
neutron	939.7	0	880	udd	1/2
Λ	1115.7	0	2.63×10^{-10}	uds	1/2
Σ^+	1189.4	+e	8.02×10^{-11}	uus	1/2
Σ^0	1192.6	0	7.4×10^{-20}	uds	1/2
Σ^-	1197.4	-e	1.48×10^{-10}	dds	1/2
Ξ^0	1314.9	0	2.9×10^{-10}	uss	1/2
Ξ^-	1321.7	-e	1.6×10^{-10}	dss	1/2

Although the Λ particle has a short lifetime, it can exist long enough to be "trapped" within a nucleus. Nuclei that have a Λ particle trapped inside are called Lambda-hypernuclei.

The Λ is neutral, so it does not experience the electrostatic force. However, it is attacted to neutrons and protons via the strong force. The Λ "lives" long enough for experimentalists to measure the quantized energy levels of the Λ when it is in the nucleus. If one wanted to put a Λ particle in say a ^{12}C nucleus, one would collide K^- particles on a ^{13}C nucleus. One of the neutrons in the ^{13}C carbon nucleus would be converted into a Λ and a pion would be emitted:

$$K^- + n \rightarrow \Lambda + \pi^- \tag{3}$$

By measuring the energy of the π^- one can determine the binding energy of the Λ within the ^{12}C nucleus.

Theoreticians can calculate the binding energies of the Λ by describing the interaction of the Λ with the rest of the nucleus with a potential $V(\vec{r})$. The potential function $V(\vec{r})$ is the potential energy due to the strong interaction between the Λ and the rest of the nucleus, where $\vec{r}$ is the position vector of the Λ from the center of the nucleus. There are some properties that we believe $V(\vec{r})$ should have:

1. $V(\vec{r})$ should be spherically symmetric. That is, $V(\vec{r}) = V(r)$ where $r = |\vec{r}|$.

2. Since the range of the interaction between the Λ and a nucleon is very short, $V(r)$ should go to zero just outside the nucleus.

3. Since the $\Lambda - nucleon$ interaction is very short range, the Λ is only affected by its nearest neighbor nucleons. Thus, $V(r)$ should be fairly constant for $r < R$, where R is the radius of the nucleus.

These three properties guide us in choosing a spherical square well potential as $V(r)$:

$$
\begin{aligned}
V(r) &= -V_0 \qquad\qquad r < R \\
&= 0 \qquad\qquad\quad r > R
\end{aligned}
$$

where R is the radius of the nucleus, and V_0 is the "depth" of the potential.

To solve for the energy levels that the Λ can have, one uses $V(r)$ as the potential in the Schroedinger equation. Solving the Schroedinger equation for the spherical square well potential (we will show this later), one obtains for $l = 0$:

$$
tan\Big(\sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}\, R\Big) = -\sqrt{\frac{V_0 - |E|}{|E|}} \tag{4}
$$

where m is the mass of the Λ, and the binding energy is $|E|$.

To solve this equation for $|E|$, we need to choose the appropriate units and cast the equation into its simplest form.

In particle physics a common unit for mass is MeV/c^2, or GeV/c^2. One ususally leaves off the c^2. A common unit for length is the Fermi, fm, where $1\ fm = 10^{-15}m$. The Fermi is roughly the radius of a neutron or proton. Another important constant that enters in quantum mechanics is Plank's constant, h, or $\hbar = h/(2\pi)$. Usually $\hbar$ can be coupled with c, as $\hbar c$. $\hbar c$ has units of (energy)(distance). In particle physics units, $\hbar c \approx 197.33\ MeV - fm$.

To solve for the potential strength V_0, it is easiest to express the equation in unitless quantities. This can be done as follows:

$$\begin{aligned} tan\Big(\sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}\ R\Big) &= -\sqrt{\frac{V_0 - |E|}{|E|}} \\ tan\Big(\sqrt{\frac{2mc^2(V_0/|E| - 1)}{\hbar^2 c^2}}\ R\Big) &= -\sqrt{V_0/|E| - 1} \end{aligned}$$

If we let $\alpha = 2mc^2|E|R^2/(\hbar c)^2$ and $x = V_0/|E|$, the equation becomes

$$tan(\sqrt{\alpha(x-1)}\ ) = -\sqrt{x-1} \tag{5}$$

or

$$tan(\sqrt{\alpha(x-1)}\ ) + \sqrt{x-1} = 0 \tag{6}$$

Solving the Non-Relativistic Schroedinger Equation
for a spherically symmetric potential

If the energy of a particle is non-relativistic, and its interaction is described by a potential energy function, the "physics" is described by solutions to the the time independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi \tag{7}$$

Whether one is performing a scattering experiment or measuring the bound state energies, will determine the boundary conditions of the solution $\Psi(\vec{r})$.
For bound state solutions, the wavefunction Ψ and the integral $\int \Psi^*\Psi dV$ over all space must be finite. Thus the "boundary conditions" at infinity are: $r \to \infty$, Ψ must approach zero faster than $1/r$. Since the potential is spherically symmetric, the angular dependence can be separated from the radial. Writing $\Psi = R(r)Y_{lm}(\theta, \phi)$ as a product of a radial part times a *spherical harmonic* ($Y_{lm}(\theta, \Phi)$), the above equation reduces to

$$-\frac{\hbar^2}{2m}(\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{l(l+1)}{r^2}R(r)) + V(r)R(r) = ER(r) \tag{8}$$

The integer l is related to the particles *orbital angular momentum.* A further simplification is obtained by writing $R(r)$ as $u(r) = R(r)/r$. The radial part of the Schrödinger equation finally becomes the somewhat simple form:

$$-\frac{\hbar^2}{2m}(\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)) + V(r)u(r) = Eu(r) \tag{9}$$

For Ψ to be finite, $u(0)$ equals 0, and for bound states, $u(r)$ goes to zero as $r \to \infty$.

For $l = 0$, no orbital angular momentum, the equation further simplifies to

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r) \tag{10}$$

For the spherical square well potential, we can solve the Schrödinger equation exactly for $r < R$, and for $r > R$. Then, we can require that $u(r)$ and it's derivative are continuous at $r = R$.

For $r < R$, $V(r) = -V_0$, and for bound states $E = -|E| < 0$. Thus, we have

$$\begin{aligned} \frac{d^2u(r)}{dr^2} &= -\frac{2m(V_0 - |E|)}{\hbar^2}u(r) \\ \frac{d^2u(r)}{dr^2} &= -k'^2u(r) \end{aligned}$$

where $k' = \sqrt{2m(V_0 - |E|)/\hbar^2}$. The solution to this equation that has $u(0) = 0$ is

$$u(r) = Asin(k'r) \tag{11}$$

for $r < R$. The cos function is not allowed, since $cos(0) \neq 0$.

For $r > R$, $V(r) = 0$, and we have

$$\begin{aligned} \frac{d^2u(r)}{dr^2} &= \frac{2m|E|}{\hbar^2}u(r) \\ \frac{d^2u(r)}{dr^2} &= k^2u(r) \end{aligned}$$

where $k = \sqrt{2m|E|/\hbar^2}$. The solution to this equation that has $u(r \to \infty) \to 0$ is

$$u(r) = Be^{-kr} \tag{12}$$

Requiring $u(r)$ to be continuous at R gives:

$$Asin(k'R) = Be^{-kR} \tag{13}$$

and requiring $u'(r)$ to be continuous at R gives:

$$Ak'cos(k'R) = -Bke^{-k'R} \tag{14}$$

Dividing these two equations yields:

$$\frac{tan(k'R)}{k'} = -\frac{1}{k} \tag{15}$$

Expressing this equation with our original variables gives

$$\begin{aligned} tan(k'R) &= -\frac{k'}{k} \\ tan\Big(\sqrt{\frac{2m(V_0 - |E|)}{\hbar^2}}\,R\Big) &= -\sqrt{\frac{V_0 - |E|}{|E|}} \end{aligned}$$

which is the equation that we are solving numerically.

Appendix
Bisection Method

The bisection method finds roots in the interval between the values a and b, where $a < b$. If $f(a)$ and $f(b)$ have opposite signs, then there is at least one root of $f(x)$ between a and b. Another way of stating that $f(a)$ and $f(b)$ have opposite signs is $f(a)f(b) < 0$. The next point in the series is the mid-point of a and b, $c = (a+b)/2$. If $f(c)$ and $f(a)$ have opposite signs, then a root is between a and c. If $f(c)$ and $f(b)$ have opposite signs, then a root is between c and b. Only one of these options will be true, since $f(a)$ and $f(b)$ have themselves opposite signs. The interval that contains the root is bisected again and the procedure repeated.

Below is an example code that carries out the bisection method:

```
for (i = 1; i < imax; i++)
{
c=(a+b)/2;
if (f(c) * f(a) < 0) then b = c;
if (f(c) * f(b) < 0) then a = c;
}
```

One could use an "else" statement instead of the two "if" statements. The approximate root is c, with an estimated error of $(b-a)/2$.

There are some problems to watch out for. Eventually $f(a)$, $f(b)$, and $f(c)$ will be very close to zero. When multiplying two of these quantites, the product can fall below the accuracy of the machine. Instead of a "for" loop, a "while" loop can be used:

```
c = (a+b)/2;
tol=0.0000001;
while (f(c) > tol)
{
c=(a+b)/2;
if (f(c) * f(a) < 0) then b = c;
if (f(c) * f(b) < 0) then a = c;
}
```

where "tol" can be determined from the accuracy desired or the machine tolerance. Instead of $f(c)$ being the condition, the while loop could continue till $|b-a|$ is less than a tolerance.

One limitation of the bisection method is that one needs to choose a and b such that there is a root between them. The next method avoids this requirement, and only needs a starting value and step size.

Newton's Method

Newton's method can be used if the first derivative, $f'(x)$, is known. We will just state the algorithm here. For a derivation as to its validity, refer to a text on numerical methods.

One starts with an initial guess for the root of $f(x)$, x_1. The algorthym is an equation to obtain x_{i+1} from x_i:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \tag{16}$$

Under certain conditions, the series x_i will converge to a root of $f(x)$. Usually in physics applications one does not know the analytic form of $f'(x)$, so Newton's method is not commonly used.