Lecture 3

Last lecture we were in the middle of deriving the energies of the bound states of the Λ in the nucleus. We will continue with solving the non-relativistic Schroedinger equation for a spherically symmetric potential.

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:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi = E\Psi \tag{1}$$

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

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

A further simplification is obtained by writing $R(r)$ as $R(r) = u(r)/r$. The radial part of the Schrödinger equation finally becomes

$$-\frac{\hbar^2}{2m}(\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)) + V(r)u(r) = Eu(r) \tag{3}$$

For Ψ to be finite, $u(0)$ equals 0, and for bound states, $u(r)$ goes to zero as $r \to \infty$. The integer l is related to the particles *orbital angular momentum.*

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

$$-\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + V(r)u(r) = Eu(r) \tag{4}$$

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

$$u(r) = Asin(k'r) \tag{5}$$

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

$$u(r) = Be^{-kr} \tag{6}$$

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

$$Asin(k'R) = Be^{-kR} \tag{7}$$

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

$$Ak'cos(k'R) = -Bke^{-k'R} \tag{8}$$

Dividing these two equations yields:

$$\frac{tan(k'R)}{k'} = -\frac{1}{k} \tag{9}$$

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.

In your homework assignment you are given the following data, and asked to determine V_0.

Nucleus	^{13}C	^{16}O	^{28}Si	^{40}Ca	^{51}V	^{89}Y
Mass Number (A):	13	16	28	40	51	89
ℓ=0 binding energy (in MeV):	10.5	12.1	17.1	18.5	18.0	23.0

For each nucleus determine α, solve the equation

$$tan(\sqrt{\alpha(x-1)}\ ) + \sqrt{x-1} = 0 \tag{10}$$

for x. Then $V_0 = x|E|$.

Solving the Schroedinger Equation Numerically

In our second assignment, we will solve the Schroedinger equation numerically. It will be necessary to solve it numerically, since the potential V(r) will yield a simple analytic solution.

As derived previously, the radial part of the Schroedinger is:

$$-\frac{\hbar^2}{2m}(\frac{d^2u(r)}{dr^2} - \frac{l(l+1)}{r^2}u(r)) + V(r)u(r) = Eu(r) \tag{11}$$

where l is the orbital angular momentum of the particle about the center of the potential.

We will solve this differential equation numerically by using a simple "finite difference" method. There are other algorithms, but here we can obtain accurate results using the simplest of methods. The main idea is to make the continuous variables and functions, r, $V(r)$, and $u(r)$ discrete. We do this by making the radial coordinate r discrete with a step size Δ. That is, $r \to r(i) = i{*}\Delta$ where i is an integer. The variable r and the functions $V(r)$ and $u(r)$ become arrays: $r \to r(i)$, $V(r) \to V(r(i)) \to V(i)$, and $u(r) \to u(r(i)) \to u(i)$.

The first derivative of u with respect to r is approximately

$$\frac{du}{dr} \approx \frac{u(i+1) - u(i)}{\Delta} \tag{12}$$

from the definition of the derivative. Actually the limit as $\Delta \to 0$ gives the derivative. Taking Δ small enough will give a good approximation. We need the second derivative in the Schroedinger equation. Using the finite difference approximation once again with the first derivative yields:

$$\begin{aligned} \frac{d^2u}{dr^2} &\approx \frac{\frac{u(i+1)-u(i)}{\Delta} - \frac{u(i)-u(i-1)}{\Delta}}{\Delta} \\ \frac{d^2u}{dr^2} &\approx \frac{u(i+1) + u(i-1) - 2u(i)}{\Delta^2} \end{aligned}$$

After substituting these expressions into the differential equation and doing some algebra, one obtains a discrete version of the Schrödinger equation:

$$u(i+1) = 2u(i) - u(i-1) + \Delta^2 \frac{l(l+1)}{r^2} u(i) + \frac{2m\Delta^2}{\hbar^2}(V(i) - E)u(i) \tag{13}$$

This "discrete Schrödinger equation" allows one to determine all values of $u(i)$ if $u(0)$ and $u(1)$ are known. This can be done by iteration, since $u(i)$ is completely determined from $u(i-1)$ and $u(i-2)$.

Boundary Conditions

The Schrödinger equation will describe both bound state and scattering situations. In both cases, the "boundary condition" on $u(r)$ at $r = 0$ is the same, namely $u(0) = 0$. For a bound state solution the other boundary condition is that $u(i \to \infty) \to 0$. Only certain values of E will allow this limit to be satisfied. These values of E are the allowed "bound state" energies that the particle can have.

Bound States

$$\begin{aligned} u(0) &= 0 \\ u(r \to \infty) &\to 0 \end{aligned}$$

For a scattering situation, $u(r)$ will oscillate as $r \to \infty$. We will consider scattering problems later on in the course. Now lets see how we can solve for the energies of any bound states.

Scattering state

$$\begin{aligned} u(0) &= 0 \\ u(r \to \infty) &\to \mathit{oscillatory} \end{aligned}$$

Solving for the bound state energies

We can determine the bound-state energies using a "bracket and half" method. First a trial energy E_t is chosen which lies below the ground state energy. In the discrete Schrödinger equation, $u(i+1)$ is determined from the values of $u(i)$ and $u(i-1)$. We assign $u(0)$ a value of 0, and $u(1)$ is assigned a non-zero value (e.g. $u(1) = 1.0$). The discrete Schroedinger equation can then be used to iterate $u(i)$ to a large value of $i = imax$, well outside the range of the potential. We assign $u(imax)$ the value $u(imax) \equiv test0$. Next, the trial energy is increased by an amount δE and the process is repeated. The function $u(imax)$ will now have a different value which we call $test1$. If $test0$ and $test1$ have the same sign, then the trial energy is changed again by an amount δE, $test1 \rightarrow test0$, and the process is repeated. If $test0$ and $test1$ have opposite signs, then the wave function at $r = imax * \Delta$ has changed sign and the trial energy has passed over the ground state energy. The energy step is reversed and halved, $\delta E \rightarrow -\delta E/2$, $test1 \rightarrow test0$, and the process is repeated to the desired accuracy.

To determine the energy of the next excited state, one starts with a trial energy just above the ground state energy. The trial energy is stepped up in a similar manner until the energy converges. The next higher allowed energy is found in a similar manner. For our homework problem, you will solve for the bound state energies of a valance neutron and a valance proton in different nuclei.

Nuclear Shell Model

The independent particle model, or shell model, of the nucleus has been successful in understanding many properties of nuclei. In this model, the nucleons are treated as independent particles that move in an average potential due to the other nucleons in the nucleus.

The mean field potential consists of a "strong force" part that both the neutrons and protons experience. Since the protons possess charge, they will have an electrostatic Coulomb potential in addition to the strong force.

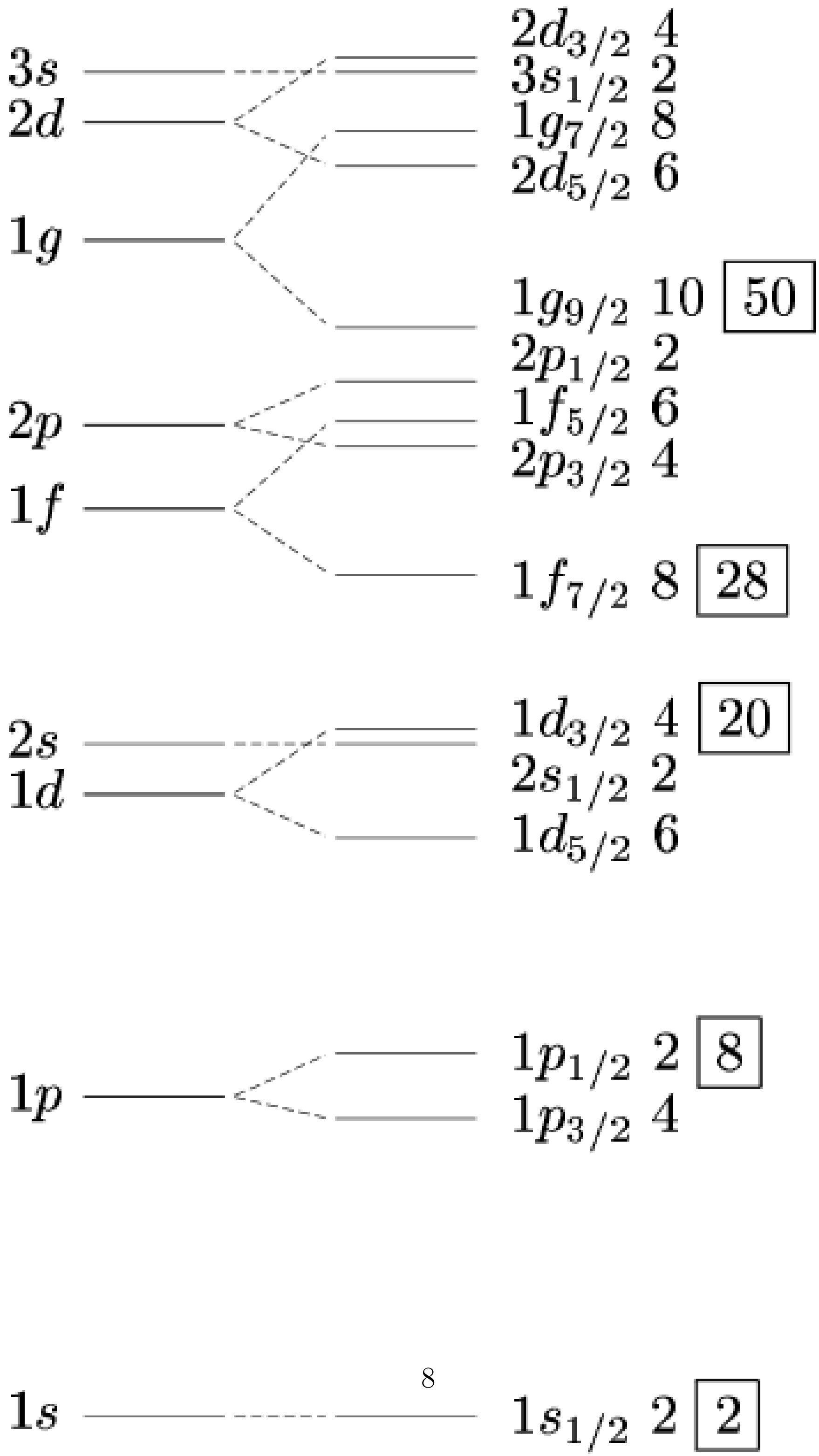
A common potential that is used to represent the strong interaction between a nucleon and the rest of the nucleus is the "Woods-Saxon" potential:

$$V(r) = \frac{-V_0}{1 + e^{(r-c)/a}} \tag{14}$$

This potential is a smoothed out square well, and the potential strength V_0 is the same for both neutrons and protons.

For your homework exercise, you will calculate the bound state energies for neutrons and protons in various nuclei. To reduce the number of parameters, we will take use a simple model for the potential. For the strong potential we will use a *spherical square well potential* as we did for the Λ particle. For the electrostatic potential that the proton experiences, we will use the potential from a uniformly charged sphere of radius R and total charge Ze:

$$\begin{aligned} V_{Coulomb}(r) &= Ze^2 \frac{3R^2 - r^2}{2R^3} \qquad if\ r \leq R \\ &= \frac{Ze^2}{r} \qquad if\ r > R \end{aligned}$$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