

## Discussion 6 - Finite Spherical Well

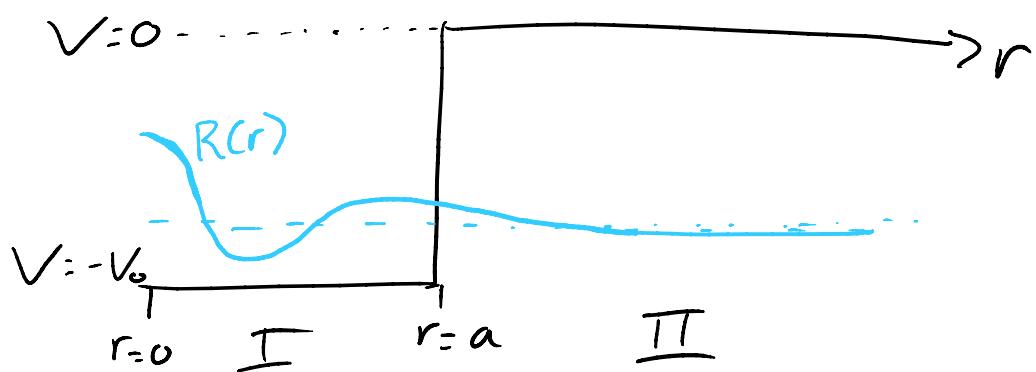
Wednesday, October 18, 2017 1:40 PM

Suppose a particle of mass 'm' is trapped in a finite spherical well.

$$V(r) = \begin{cases} -V_0, & r \leq a \\ 0, & r > a \end{cases}$$

(Very simple model  
for an impurity in  
a material)

This is a 3D, spherically symmetric potential, but here is what it looks like as a function of the radius:



Since the potential is spherically symmetric, we can immediately write the energy eigenstates as separable solutions:

$$\Psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$$

where the angular wavefunctions are given by the spherical harmonics.

$$Y(\theta, \phi) = Y_e^m(\theta, \phi)$$

So all we have to work on is the

## Radial Equation

$$\frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} [V(r) - E] R = l(l+1)R$$

Or, if we change variables to  $u(r) = rR(r)$ ,

$$-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[ V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u = Eu$$

Keep in mind the normalization condition in spherical coordinates:

$$\int_0^\infty |R(r)|^2 r^2 dr = \int_0^\infty |u(r)|^2 dr = ?$$

If the potential is constant in a region, then the radial equation is

$$-\frac{\hbar^2}{2m} \frac{d^2u}{dr^2} + \left[ V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u = Eu$$

$$\frac{d^2u}{dr^2} = \left[ -\frac{2m}{\hbar^2}(E-V) + \frac{l(l+1)}{r^2} \right] u$$

★  $\frac{d^2u}{dr^2} = \left[ \frac{l(l+1)}{r^2} - K^2 \right] u \rightsquigarrow K = \sqrt{\frac{2m(E-V)}{\hbar^2}}$

This is very similar to the Finite Square Well! When  $E > V$ ,  $K$  will be real and we expect an oscillating solution (region I). When  $E < V$ ,  $K$  will be  $0 \dots$  or next a decaying solution.

Solution (region I). When  $E < V$ ,  $k$  will be imaginary and we expect a decaying solution.

## General Solution

Compare to the finite square well. There, we get:

$$\frac{d^2\psi}{dx^2} = -k^2 \psi$$

And the general solutions are:

$$\left. \begin{array}{l} \psi = A \cos(kx) + B \sin(kx) \\ \text{or} \\ \psi = C e^{ikx} + D e^{-ikx} \end{array} \right\} E > V$$

$$\left. \begin{array}{l} \psi = E e^{kx} + F e^{-kx} \end{array} \right\} E < V$$

And we choose the coefficients to obey boundary conditions and make the wavefunction smooth.

For the finite spherical well, the same idea applies but the functions that satisfy ~~A~~ are just a bit more complicated.

When  $E > V$ , the solutions are Bessel ( $j_\ell(\rho)$ ) and Neumann ( $n_\ell(\rho)$ )

$$u(r) = r R(r) = A r j_\ell(kr) + B r n_\ell(kr)$$

$$\hookrightarrow R(r) = A j_\ell(kr) + B n_\ell(kr)$$

$$j_\ell(\rho) = (-\rho)^\ell \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^\ell \frac{\sin(\rho)}{\rho}; \quad n_\ell(\rho) = -(-\rho)^\ell \left( \frac{1}{\rho} \frac{d}{d\rho} \right)^\ell \frac{\cos(\rho)}{\rho}$$

$\swarrow$  finite as  $\rho \rightarrow 0$        $\searrow$  blows up as  $\rho \rightarrow 0$

These are analogous to the  $\sin$  &  $\cos$  functions, and just like for the finite square well we can <sup>also</sup> express the general solution in terms of new linear combinations of the Bessel & Neumann functions, called Hankel ( $h_\ell^{(1)}, h_\ell^{(2)}$ ) functions.

$$h_\ell^{(1)}(\rho) = j_\ell(\rho) + i n_\ell(\rho); \quad h_\ell^{(2)}(\rho) = j_\ell(\rho) - i n_\ell(\rho)$$

$\swarrow$  'first kind'       $\searrow$  'second kind'

[compare with  $e^{ikr} = \cos(kr) + i \sin(kr)$ ]

A nice thing about Hankel functions of the first kind ( $h_\ell^{(1)}(kr)$ ), is what they decay exponentially as  $r \rightarrow \infty$  if you give them an imaginary argument, i.e. if  $k = i|k| \leftrightarrow E < V$ !

Putting all this together, we would expect the solution in region I to be a Bessel function (since the Neumann function blows up at the origin) and a Hankel function of the first kind for region II (since the wavefunction should decay there)

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$$R_I(r) = A j_e(kr)$$

$$k = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

-  $V_0$

$$R_{II}(r) = B h_e^{(1)}(ik'r)$$

$$k' = \frac{\sqrt{2m/E}}{\hbar}$$

$$\text{BCs: } R_I(r=a) = R_{II}(r=a)$$

$$\left. \frac{dR_I}{dr} \right|_{r=a} = \left. \frac{dR_{II}}{dr} \right|_{r=a}$$

Plugging the solutions into the BCs yields:

$$A j_e(z) = B h_e^{(1)}(z') \quad z = ka$$

$$A K \frac{d}{dz} j_e(z) = B i k' \frac{d}{dz'} h_e^{(1)}(z') \quad z' = ik'a$$

Dividing these equations yields a single transcendental function that is only a function of  $E$ .

$$\left. \frac{iK \frac{d}{dz} j_e(z)}{j_e(z)} \right|_{z=ka} = \left. \frac{i k' \frac{d}{dz'} h_e^{(1)}(z')}{h_e^{(1)}(z')} \right|_{z'=ik'a}$$

Any energy that satisfies this equation is an eigen-energy, and the corresponding wavefunction is an eigen-state.

Once we know a correct energy  $E$ , we can then plug it into the continuity equation to find the

Once we know a correct energy, we can then plug it into the continuity equation to find the coefficients.

$$\frac{A}{B} = \left. \frac{h_\ell^{(1)}(ik'a)}{j_\ell(ka)} \right|_E$$

So

$$R(r) = \begin{cases} \left. \frac{B h_\ell^{(1)}(ik'a)}{j_\ell(ka)} \right|_E \cdot j_\ell(kr), & r \leq a \\ B \cdot h_\ell^{(1)}(ik'r), & r > a \end{cases}$$

And then finally we find B by normalizing:

$$\int_0^\infty |R|^2 r^2 dr = 1$$

## Computational Details

- In order to do all this on a computer, you need some way of getting the values of  $j_\ell(z)$  and  $h_\ell^{(1)}(z)$ . The best way to do this is by making use of the Scipy library. For example, in order to calculate the first derivative of  $j_\ell(z)$  at  $z=z_0$ , you can call

`scipy.special.spherical_jn(l, z0, 1)`

which derivative  
do you want?

- In unfortunate the Hankel functions are not

do you want:

- Unfortunately, the hankel functions are not so easy, because what we really need are the spherical hankel functions,  $h_e^{(1)}(z)$ , but Scipy only provides routines for the regular Hankel functions,  $H_e^{(1)}(z)$ .

Luckily though, the relationship between  $h_e^{(1)}(z)$  and  $H_e^{(1)}(z)$  is pretty simple:

$$h_e^{(1)}(z) = \sqrt{\frac{\pi}{2z}} H_{l+\frac{1}{2}}^{(1)}(z)$$

and so the derivative is given by

$$\begin{aligned} \frac{d}{dz} h_e^{(1)} &= \frac{1}{2} \left(\frac{\pi}{2z}\right)^{1/2} \left(-\frac{\pi}{2z^2}\right) H_{l+\frac{1}{2}}^{(1)}(z) + \sqrt{\frac{\pi}{2z}} \frac{d}{dz} H_{l+\frac{1}{2}}^{(1)}(z) \\ &= -\frac{1}{2z} \sqrt{\frac{\pi}{2z}} H_{l+\frac{1}{2}}^{(1)}(z) + \sqrt{\frac{\pi}{2z}} \frac{d}{dz} H_{l+\frac{1}{2}}^{(1)}(z) \end{aligned}$$

And derivatives of  $H_e^{(1)}(z)$  come from

scipy.special.h1vp( $l, z_0, n$ )  
 $\text{C } n^{\text{th}}$  derivative

- Here's the equation from the boundary conditions:

$$\left. \frac{k \frac{d}{dz} j_e(z)}{j_e(z)} \right|_{z=ka} = i \left. \frac{k' \frac{d}{dz} h_e^{(1)}(z)}{h_e^{(1)}(z)} \right|_{z=ik'a}$$

Since  $k$  &  $k'$  are just functions of  $E$ , this has the following form

$$f_n(E) = g_n(E)$$

$$f_e(E) = g_e(E)$$

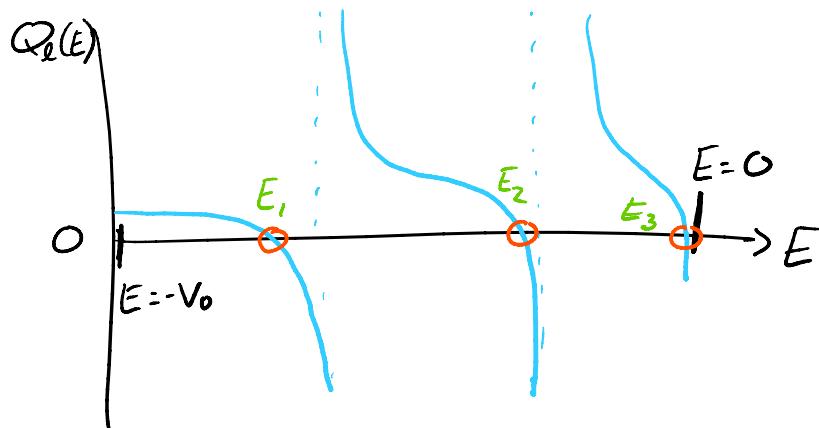
If we define a new function  $Q_e(E)$ ,

$$Q_e(E) = f_e(E) - g_e(E)$$

Then the energies we are searching for are the roots of  $Q_e(E)$ , or where

$$\underline{Q_e(E) = 0}$$

A plot of  $Q_e(E)$  might look like this:



Note that all the bound state energies must be within the well,

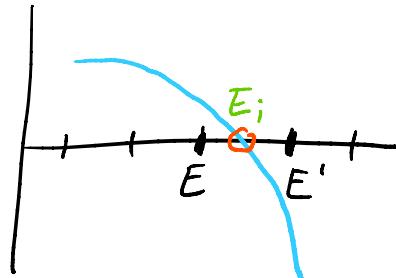
$$\rightarrow \underline{-V_0 \leq E_i \leq 0}$$

We need to find these energies to high precision, so we'll use a two step procedure:

1) Get a rough estimate: find a zero between  $E$  and  $E'$

2) Use the brentg function from Scipy to get the precise value of  $E_i$ .

- 1) Create a discrete grid of energies between  $-V_0$  and 0. Walk through the grid and figure out which grid energies surround a zero.



$E_i$  is between  
 $E$  and  $E'$

- 2) Given the function  $Q_\ell(E)$  and the values  $E + E'$ , use SciPy's brentq function to get the exact value of  $E_i$ .

$$E_i = \text{scipy.optimize.brentq}(Q_\ell, E, E', l)$$

replace with the name  
of the Python function that  
calculates  $Q_\ell(E)$

after  $E, E'$  comes a  
list of all the other  
variables needed by  
the function  $Q_\ell(E)$ .