Chapter 4: Spherically Symmetrical Potentials

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Spherical potential cookbook

There are three main problems for spherically symmetric potentials: harmonic oscillators, infinite wells, and the Hydrogen atom/Coulomb potentials. Harmonic oscillators can be solved most easily by switching to Cartersian coordinates and solving 1D problems. The other potentials can be solved using the basic formula:

1. Write $\psi(\vec{r})$ as a product of the radial function, $\phi_{nl}(r)$ and spherical harmonics, $Y_{lm}(\theta, \phi)$.
2. Write down the spherical Schrödinger equation for the radial function.
3. Apply boundary conditions to solve for $\phi_{nl}(r)$.
4. Apply normalization condition.

Problem 1: an infinite spherical well

Part a: Nouredine-Zettili Problem 6.5

Find the $l = 0$ energy and wave function of a particle of mass m in the central potential

$$V(r) = \begin{cases} 0, & a < r < b \\ \infty, & \text{elsewhere} \end{cases} . \tag{1}$$

Solution

We only care about the region with zero potential because outside the well, the wavefunction must be zero for the infinite well. Because this is a region with zero potential, the solution must be spherical Bessel functions, $j_0(kr)$, and Neumann functions, $n_0(kr)$, for the $l = 0$ case. If we translate the functions $r \to r - a$ (valid only for $l = 0$, where there is no centrifugal term in the differential equation), we can quickly eliminate the n_0 term, however, because $\phi_{n0}(0) = 0$, while $n_0(0) \to \infty$. Then

$$\phi_{n0}(r) = Aj_0(k(r-a)) = \frac{A\sin(k(r-a))}{k(r-a)}, \tag{2}$$

where A is the normalization. Note that we can also directly solve the differential equation to find the same result. The radial equation in spherical coordinates is given by

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right] u_{nl}(r) = Eu_{nl}(r), \tag{3}$$

where $u_{nl}(r) = kr\phi_{nl}(r)$ and $\psi_{nlm}(r) = \phi_{nl}(r)Y_{lm}(\theta, \phi)$, as usual. We are concerned only with the region $r \in (a, b)$ because $\psi = 0$ elsewhere. Additionally, we are focusing on the $l = 0$ case, so we can simplify Eq. 3:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} u_{n0}(r) = Eu_{n0}(r) \tag{4}$$

We note that this potential is similar to that of an infinite square well in one-dimension, with bounds at a and b. By the spherical symmetry here, the Schrödinger equation behaves as that of a one dimensional case where the salient variable is the radial component. This is solved as a one dimensional infinite square well:

$$\frac{d^2 u_{n0}(r)}{dr^2} + k^2 u_{n0}(r) = 0 \tag{5}$$

Where the constants of the Schrödinger equation have been consolidated as $k^2 = 2mE/\hbar^2$ for the potential $V_0(r) = 0$ within the well.

with continuity at the boundaries $r = a$ and $r = b$:

1. $u_{n0}(a) = 0$
2. $u_{n0}(b) = 0$

Note that there is no tunnelling through the infinite potential, so we need not consider continuity of the derivatives at the boundaries in this case.

To solve the second order ordinary differential equation that the simplified Schrödinger equation presents, we apply Eq. 2 which gives $\phi_{nl}(r)$ and $u_{nl}(r) = kr\phi_{nl}(r)$ to get:

$$u_{n0}(r) = A \sin\left(k(r-a)\right) \tag{6}$$

Since this is only for the wave function in the well, we can then write the global $u_{nl}(r)$ piece-wise as:

$$u_{n0}(r) = \begin{cases} A\sin\left[k(r-a)\right], & r \in (a,b) \\ 0, & \text{elsewhere} \end{cases} . \tag{7}$$

Because $u = kr\phi$, we see that we get the correct form of the wavefunction by either using Bessel functions or solving directly. Using the second boundary condition, we can constrain the allowed values k_n:

$$u_{n0}(r=b) = A\sin\left[k(b-a)\right] = 0, \tag{8}$$

which can only be true if

$$k_n = \frac{n\pi}{b-a}, \qquad n = 1, 2, 3, \ldots \tag{9}$$

Therefore, the allowed energies E_n are

$$\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2m(b-a)^2}.} \tag{10}$$

Finally, we just need to find the normalization A:

$$\begin{aligned} 1 = \int_a^b A^2 \sin^2\left[k(r-a)\right]\, dr &= \frac{A^2}{2}\int_a^b \left(1 - \cos\left[2k(r-a)\right]\right) dr \\ &= \frac{(b-a)}{2}A^2 \Rightarrow A = \sqrt{\frac{2}{b-a}} \end{aligned} \tag{11}$$

Therefore, we can write the wave function now that we know $\phi_{n0} = u_{n0}/r$ and $Y_{00} = 1/\sqrt{4\pi}$ (where $l = 0$ necessitates $m = 0$, giving the necessary Y_{lm}):

$$\boxed{\psi_{n00}(r) = \begin{cases} \frac{1}{r\sqrt{4\pi}}\sqrt{\frac{2}{b-a}}\sin\left[\frac{n\pi(r-a)}{(b-a)}\right], & r \in (a,b) \\ 0, & \text{elsewhere} \end{cases}} \tag{12}$$

Part b: $l = 1$ Eigenenergies

For the same potential, find a transcendental equation for the eigenenergies in the $l = 1$ case. Hint: find a transcendental equation for k; you can then state the eigenenergies in terms of k.

Solution

Beginning with Eq. 3, when we apply $l = 1$, for $r \in (a, b)$, the equation of motion takes the form:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{\hbar^2}{mr^2}\right] u_{n1}(r) = E u_{n1}(r). \tag{13}$$

Because the potential is zero inside the well, the solutions should have the form of spherical Bessel functions and Neumann functions. Because we are only concerned with $l = 1$, this means

$$u_{n1}(r) = kr\left(j_1(kr) + Bn_1(kr)\right), \tag{14}$$

where B is the relative amplitude term. Writing this out explicitly:

$$u_{n1}(kr) = \frac{\sin(kr)}{kr} - \cos(kr) - B\frac{\cos(kr)}{kr} - B\sin(kr). \tag{15}$$

Applying the $u(a) = 0$ condition:

$$\frac{\sin(ka)}{ka} - \cos(ka) = B\left[\frac{\cos(ka)}{ka} + \sin(ka)\right], \tag{16}$$

so we see that

$$B = \frac{\sin(ka) - ka\cos(ka)}{\cos(ka) + \sin(ka)}. \tag{17}$$

We can then apply the $u(b) = 0$ boundary condition to find the (ugly) transcendental equation:

$$\boxed{\sin(kb) - kb\cos(kb) = B\left[\cos(kb) + kb\sin(kb)\right]} \tag{18}$$

where B is defined in Eq. 17.

Problem 2: Hydrogen-like atoms

A generic version of homework problems 4.10 and 4.11

Find the Bohr radius and ground state binding energy of an atom composed of two attracted particles with charges $Z_1 e$ and $-Z_2 e$, and reduced mass μ.

Solution

The Bohr radius for a Hydrogen-like atom is found by defining a characteristic length scale for the Schrödinger equation with a Coulomb potential. If you don't remember how to scale the Bohr radius, you can do this explicitly by inserting the potential into the spherical radial equation,

$$\left[-\frac{\hbar^2}{2\mu}\partial_r^2 + \frac{\hbar^2 l(l+1)}{2\mu r^2} - \frac{Z_1 Z_2 e^2}{r}\right] u_{nl}(r) = -\frac{\hbar^2 k_{nl}^2}{2\mu} u_{nl}(r), \tag{19}$$

where we use the relation $-E = \hbar^2 k^2/2\mu$ on the right-hand side of the equation.[1] Then we can rearrange constants to isolate $-k_{nl}^2 u_{nl}(r)$ on the right-hand side:

$$\left[-\partial_r^2 + \frac{l(l+1)}{r^2} - \left(\frac{\mu Z_1 Z_2 e^2}{\hbar^2}\right)\frac{2}{r}\right] u_{nl}(r) = -k_{nl}^2 u_{nl}(r). \tag{20}$$

In Eq. 20, we see a natural length scale emerge in the group of constants associated with the Coulomb potential term. You can see this via dimensional analysis or by noting that the other terms on the left-hand

[1] Note the sign convention; for a bound state, $E < 0$, so $k^2 \propto -E$ to ensure a positive number.

side of the equation have dimension $1/r^2$, so the Coulomb term must have the same dimension, and group constants accordingly. This is the generic Bohr radius:

$$\boxed{a = \frac{\hbar^2}{\mu Z_1 Z_2 e^2}} \tag{21}$$

With the Bohr radius, we can plug it into the eigenenergy formula for this potential (already solved in the lecture notes) and state the binding energy using $n = 1$:

$$\boxed{E = -\frac{e^2}{2a}} \tag{22}$$