INFINITE SPHERICAL WELL - NUMERICAL SOLUTIONS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Section 4.1.3 & Problem 4.8.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 12, Exercise 12.6.8.

In the radial equation for the infinite spherical well, we found the solutions to involve the spherical Bessel functions j_l and the spherical Neumann functions n_l. We saw in the last post that the general solution was

$$u(r) = Arj_l(kr) + Brn_l(kr) \tag{1}$$

We can verify this explicity for $l = 1$ and $u(r) = rj_1(r)$ by using the derivative formula

$$\begin{aligned} j_1(x) &= -x\frac{1}{x}\frac{d}{dx}\left(\frac{\sin x}{x}\right) && (2)\\ &= \frac{\sin x}{x^2} - \frac{\cos x}{x} && (3)\\ rj_1(kr) &= \frac{\sin kr}{k^2 r} - \frac{\cos kr}{k} && (4) \end{aligned}$$

The radial equation for $l = 1$ is

$$\frac{d^2u}{dr^2} - \left(\frac{2}{r^2} - k^2\right)u = 0 \tag{5}$$

So we get (using Maple)

$$\begin{aligned} \frac{d^2u}{dr^2} &= \frac{1}{k^2r^3}\left[\sin kr\left(2 - k^2r^2\right) + \cos kr\left(k^3r^3 - 2\right)\right] && (6)\\ -\left(\frac{2}{r^2} - k^2\right)u &= -\frac{1}{k^2r^3}\left(k^2r^2 - 2\right)\left(kr\cos kr - \sin kr\right) && (7) \end{aligned}$$

Thus the first term cancels the second and the equation is satisfied.

For $l = 0$, the equation actually has a simple solution. We could either solve the original ODE in this case, or use the formula for j_0. From the latter, we get

$$u(r) = Arj_0(kr) \tag{8}$$
$$= \frac{A}{k}\sin kr \tag{9}$$

One of the properties of the spherical Neumann functions is that they all become infinite as $x \to 0$, so they have to be excluded from our general solution. From the continuity of the wave function at the boundary $r = a$, we must have

$$u(a) = 0 \tag{10}$$
$$\sin ka = 0 \tag{11}$$

from which we get

$$k = \frac{n\pi}{a} \tag{12}$$
$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \tag{13}$$
$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{14}$$

This is the same set of energies as in the one dimensional infinite square well.

For higher values of l, as before, we have to exclude the n_l as they become infinite, so the general solution is

$$u(r) = Arj_l(kr) \tag{15}$$

To find the energies requires finding the zeroes of j_l, which has to be done numerically, since the condition $j_l(kr) = 0$ gives rise to transcendental equations (involving both r and a trigonometric function of r). Rough solutions can be found graphically, but a more accurate solution can be found using software such as Maple.

Maple has a BesselJZeros function which will find the zeroes of the Bessel functions of the first kind J_l (that's a capital J). As noted in the last post, these are *not* the same as the spherical Bessel functions we are using here. However, the two functions are related by a simple formula:

$$j_l(x) = \sqrt{\frac{\pi}{2x}}J_{l+\frac{1}{2}}(x) \tag{16}$$

This means that the zeroes of $j_1(x)$ are also the zeroes of $J_{n+1/2}(x)$. With this proviso, the first few zeroes can be found by calling Maple's BesselJZeroes(index, number), where 'index' is $l+\frac{1}{2}$ and 'number' is the ordinal number of the required zero (first, second, third, etc). The first three zeroes of $J_{\frac{3}{2}}$ are at $ka = 4.493,\ 7.725,\ 10.904$. If we denote the n^{th} zero as z_{1n}, then $ka = z_n$; $E_{1n} = \hbar^2 z_{1n}^2/2ma^2$. Thus the energies are $E_{11} = 20.187\frac{\hbar^2}{2ma^2}$; $E_{12} = 59.676\frac{\hbar^2}{2ma^2}$; $E_{13} = 118.897\frac{\hbar^2}{2ma^2}$. The same method can obviously be used to find the energy levels for larger l, where the graphical method becomes a lot more difficult due to the complexity of the equations.

The function for which we are finding the zeroes is

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \tag{17}$$

where $x \equiv ka$. Thus the zeroes are at

$$\frac{\sin x}{x} - \cos x = 0 \tag{18}$$

$$\tan x = x \tag{19}$$

For large n, we are looking at large x, so the first term becomes negligible, and we are essentially looking for the zeroes of $\cos x$, which occur at $ka = (2n+1)\pi/2 = \pi(n+\frac{1}{2})$. Thus the energies are approximately $E_{1n} \approx \hbar^2\pi^2(n+1/2)^2/2ma^2$.