

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

$$u(r) = Arj_l(kr) + Brn_l(kr) \quad (1)$$

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

$$j_1(x) = -x \frac{d}{dx} \left(\frac{\sin x}{x} \right) \quad (2)$$

$$= \frac{\sin x}{x^2} - \frac{\cos x}{x} \quad (3)$$

$$rj_1(kr) = \frac{\sin kr}{k^2 r} - \frac{\cos kr}{k} \quad (4)$$

The radial equation for $l = 1$ is

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

So we get (using Maple)

$$\frac{d^2 u}{dr^2} = \frac{1}{k^2 r^3} [\sin kr (2 - k^2 r^2) + \cos kr (k^3 r^3 - 2)] \quad (6)$$

$$- \left(\frac{2}{r^2} - k^2 \right) u = - \frac{1}{k^2 r^3} (k^2 r^2 - 2) (kr \cos kr - \sin kr) \quad (7)$$

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

$$u(r) = Arj_0(kr) \quad (8)$$

$$= \frac{A}{k} \sin kr \quad (9)$$

One of the properties of the spherical Neumann functions is that they all become infinite as $x \rightarrow 0$, 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

$$u(a) = 0 \quad (10)$$

$$\sin ka = 0 \quad (11)$$

from which we get

$$k = \frac{n\pi}{a} \quad (12)$$

$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{a} \quad (13)$$

$$E = \frac{n^2\pi^2\hbar^2}{2ma^2} \quad (14)$$

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

$$u(r) = Arj_l(kr) \quad (15)$$

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:

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

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 `BesselJZeros(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

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

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

$$\frac{\sin x}{x} - \cos x = 0 \quad (18)$$

$$\tan x = x \quad (19)$$

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 $E_{1n} \approx \hbar^2 \pi^2 (n + 1/2)^2 / 2ma^2$.