# INFINITE SPHERICAL WELL - SPHERICAL BESSEL FUNCTIONS

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The solution of the 3-d Schrödinger equation for a radial potential splits into two parts; one involving spherical harmonics that is independent of the potential, and the other being the radial equation, which does. The radial equation has the general form

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

where $u(r)=rR(r)$, and the wave function is $\Psi(r,\theta\phi)=R(r)Y_l^m(\theta,\phi)$.

The radial equation is usually not solvable in terms of standard functions, but one special case is that of the infinite spherical well. It is a spherical equivalent of the infinite square well, in that its potential is

$$V(r)=\begin{cases}0 & r<a\\ \infty & r>a\end{cases} \tag{2}$$

For $r>a$, we must have $\Psi=0$, and for $r<a$, we can write the radial equation as

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

$$\frac{d^2u}{dr^2}-\left(\frac{l(l+1)}{r^2}-k^2\right)u=0 \tag{4}$$

where

$$k\equiv\frac{\sqrt{2mE}}{\hbar} \tag{5}$$

It turns out that the general solution of this equation for arbitrary $k$ involves *spherical Bessel functions*, (denoted by $j_l(r)$ and $n_l(r)$) which are defined as solutions of the differential equation

$$x^2\frac{d^2y}{dx^2}+2x\frac{dy}{dx}+\left[x^2-n(n+1)\right]y=0 \tag{6}$$

Clearly these two differential equations aren't the same, so the solutions to our problem aren't straight Bessel functions, but if we try the solution

$$u=rj_l(kr) \tag{7}$$

in our ODE, we get

$$\frac{d}{dr}\left(j_l(kr)+r\frac{d}{dr}j_l(kr)\right)-r\left(\frac{l(l+1)}{r^2}-k^2\right)j_l(kr)=0 \tag{8}$$

$$2\frac{d}{dr}j_l(kr)+r\frac{d^2}{dr^2}j_l(kr)-r\left(\frac{l(l+1)}{r^2}-k^2\right)j_l(kr)=0 \tag{9}$$

$$r^2\frac{d^2}{dr^2}j_l(kr)+2r\frac{d}{dr}j_l(kr)-\left(l(l+1)-k^2r^2\right)j_l(kr)=0 \tag{10}$$

If we let $x=kr$ we get

$$x^2\frac{d^2}{dx^2}j_l(x)+2x\frac{d}{dx}j_l(x)+\left(x^2-l(l+1)\right)j_l(x)=0 \tag{11}$$

which is exactly the Bessel ODE above. The same derivation works for the other spherical Bessel function $n_l$, so the general solution is

$$u(r)=Arj_l(kr)+Brn_l(kr) \tag{12}$$

The $n_l$ are sometimes called *spherical Neumann functions*.

The two types of spherical Bessel function can also be written as derivatives:

$$j_l(x)=(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\sin x}{x} \tag{13}$$

$$n_l(x)=-(-x)^l\left(\frac{1}{x}\frac{d}{dx}\right)^l\frac{\cos x}{x} \tag{14}$$

A note of caution is needed here. If you look up Bessel functions (say, in Wikipedia) you'll discover that there are a bewildering number of different types. The solutions of the radial equation here are specifically **spherical** Bessel functions, and *not* 'ordinary' Bessel functions of the first, second *or* third kind, nor are they Hankel functions. This is especially important to remember if you are looking up solutions in mathematical tables (or, more likely these days, using software to find the solutions).

The first two spherical Neumann functions can be found from the derivative formula:

$$n_1(x) = -(-x)\frac{1}{x}\frac{d}{dx}\frac{\cos x}{x} \tag{15}$$

$$= \frac{-x\sin x - \cos x}{x^2} \tag{16}$$

$$n_2(x) = -x\frac{d}{dx}\frac{-x\sin x - \cos x}{x^3} \tag{17}$$

$$= -x\frac{-x^3(x\cos x) + 3x^2(x\sin x + \cos x)}{x^6} \tag{18}$$

$$= \frac{x^2\cos x - 3x\sin x - 3\cos x}{x^3} \tag{19}$$

As $x \to 0$, $\sin x \to x$ and $\cos x \to 1$ so $n_1(x) \to -(x^2+1)/x^2$, which blows up. Also, $n_2(x) \to -(2x^2+3)/x^3$ which also blows up.

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