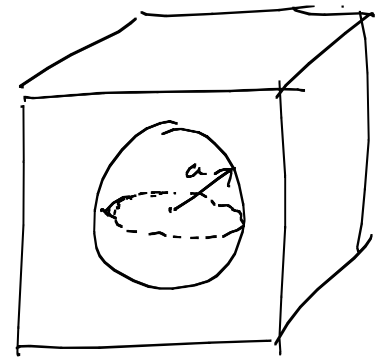
3D Infinite spherical well

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



Solve: $$-\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial r^2} + \left(V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}\right)u = Eu \quad , \quad R(r) = \frac{u(r)}{r}$$

$r<a$: $$\frac{\partial^2 u}{\partial r^2} = \left(\frac{l(l+1)}{r^2} - \frac{2mE}{\hbar^2}\right)u \quad , \quad l = 0, 1, 2 \ldots$$

For simplest case, $l=0$:

$$\frac{\partial^2 u}{\partial r^2} = -\frac{2mE}{\hbar^2}u = -k^2 u \longrightarrow \begin{array}{l} u(r) = A\sin kr + B\cos kr \\ R(r) = \frac{u(r)}{r} = A\frac{\sin kr}{r} + B\frac{\cos kr}{r} \end{array}$$

Boundary conditions:

$R(r=0)$ must be finite to normalize Ψ! $B=0$.

$R(r=a)=0 \longrightarrow \frac{A\sin ka}{a} = 0 \longrightarrow ka = n\pi$ so $k_n = \frac{n\pi}{a}$, $n = 1, 2, 3, \ldots$

$E_{n00} = \frac{\hbar^2 n^2\pi^2}{2ma^2}$, $\Psi_{n00}(r,\theta,\phi) = R_{n0}(r)Y_{00}(\theta,\phi) = A\frac{\sin k_n r}{r}Y_{00} = A'\frac{\sin k_n r}{r}$

Normalization

$$\iiint \psi^* \psi \, d^3r = \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} \psi^*(r,\theta,\phi)\,\psi(r,\theta,\phi)\, r^2 \sin\theta \, dr\, d\theta\, d\phi = 1$$

By convention, we normalize angular and radial parts separately:

$$\int_0^{2\pi}\int_0^{\pi} Y_{lm}^*(\theta,\phi)\, Y_{lm}(\theta,\phi) \sin\theta \, d\theta\, d\phi = 1$$

$$\int_0^{\infty} R_{nl}^*(r)\, R_{nl}(r)\, r^2 dr = 1$$

TABLE 2.1 SPHERICAL HARMONICS

$l = 0$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$l = 1$

$$Y_{1,\pm1} = \mp\sqrt{\frac{3}{8\pi}} \sin\theta\, e^{\pm i\phi}$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$l = 2$

$$Y_{2,\pm2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta\, e^{\pm 2i\phi}$$

$$Y_{2,\pm1} = \mp\sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta\, e^{\pm i\phi}$$

$$Y_{20} = \sqrt{\frac{5}{16\pi}} (2\cos^2\theta - \sin^2\theta)$$

$l = 3$

$$Y_{3,\pm3} = \mp\sqrt{\frac{35}{64\pi}} \sin^3\theta\, e^{\pm 3i\phi}$$

$$Y_{3,\pm2} = \sqrt{\frac{105}{32\pi}} \sin^2\theta \cos\theta\, e^{\pm 2i\phi}$$

$$Y_{3,\pm1} = \mp\sqrt{\frac{21}{64\pi}} (4\cos^2\theta \sin\theta - \sin^3\theta)\, e^{\pm i\phi}$$

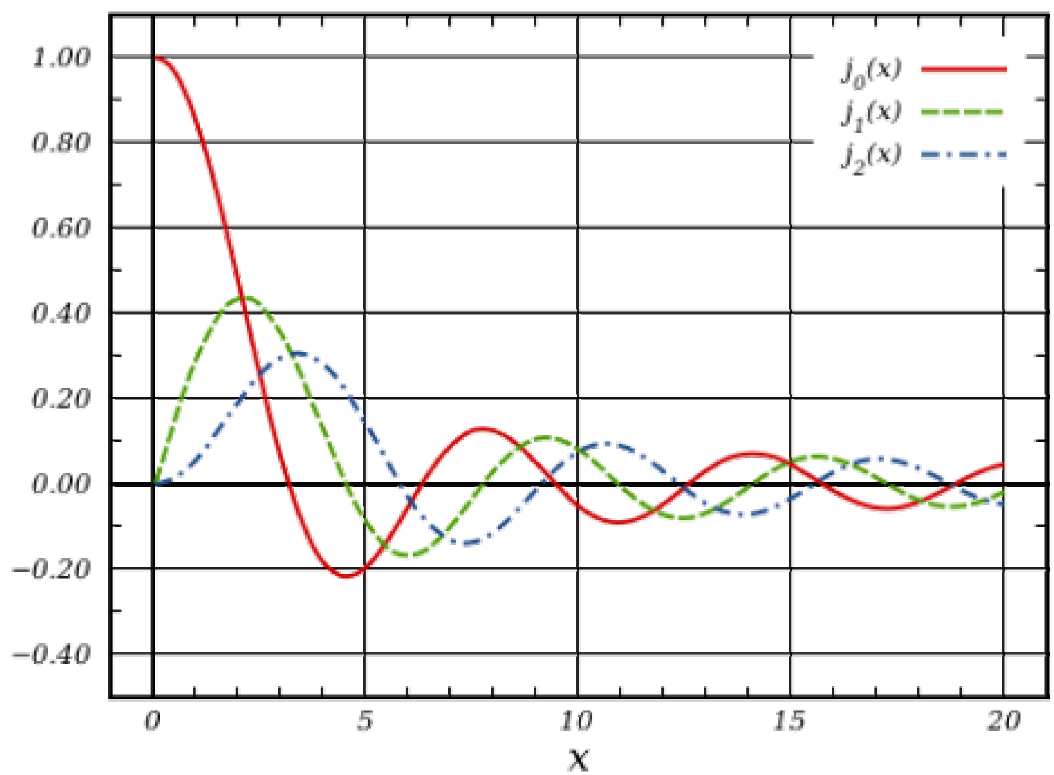
$$Y_{30} = \sqrt{\frac{7}{16\pi}} (2\cos^3\theta - 3\cos\theta \sin^2\theta)$$

$\ell \neq 0$ solutions to spherical well

Bessel function of order ℓ

$$R_{n\ell}(r) = A_{n\ell}\, j_\ell(k_{n\ell}\, r)$$

n^{th} zero of the ℓ^{th} Bessel function $\beta_{n\ell}$ satisfies B.C.'s: $k_{n\ell} = \frac{\beta_{n\ell}}{a}$



Numerical Results