Problem 4.9

(a) From the definition (Equation 4.46), construct $n_1(x)$ and $n_2(x)$.

(b) Expand the sines and cosines to obtain approximate formulas for $n_1(x)$ and $n_2(x)$, valid when $x \ll 1$. Confirm that they blow up at the origin.

[TYPOS: $n_0(x) \approx 1/x$ on page 140 should be $n_0(x) \approx -1/x$, and in Figure 4.2 on page 141 the labels should be $\ell = 0$, $\ell = 1$, $\ell = 2$, and $\ell = 3$.]

Solution

The governing equation for the wave function is Schrödinger's equation.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2M}\nabla^2\Psi + V\Psi$$

If the potential energy function is spherically symmetric $V = V(r)$, then the Laplacian operator is expanded in spherical coordinates (r, θ, ϕ), where θ is the angle from the polar axis.

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2M}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right] + V(r)\Psi(r,\theta,\phi,t)$$

The aim is to solve for $\Psi = \Psi(r, \theta, \phi, t)$ in all of space ($0 \le r < \infty$, $0 \le \theta \le \pi$, $0 \le \phi \le 2\pi$) for $t > 0$. Since Schrödinger's equation is linear and homogeneous, the method of separation of variables can be used to solve it: Assume a product solution of the form $\Psi(r, \theta, \phi, t) = R(r)\Theta(\theta)\xi(\phi)T(t)$ and plug it into the PDE.

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}[R(r)\Theta(\theta)\xi(\phi)T(t)] = -\frac{\hbar^2}{2M}&\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}[R(r)\Theta(\theta)\xi(\phi)T(t)]\right)\right. \\ &+ \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}[R(r)\Theta(\theta)\xi(\phi)T(t)]\right) \\ &\left.+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}[R(r)\Theta(\theta)\xi(\phi)T(t)]\right] + V(r)[R(r)\Theta(\theta)\xi(\phi)T(t)] \end{aligned}$$

$$\begin{aligned} i\hbar R(r)\Theta(\theta)\xi(\phi)T'(t) = -\frac{\hbar^2}{2M}&\left[\frac{\Theta(\theta)\xi(\phi)T(t)}{r^2}\frac{d}{dr}\left(r^2R'(r)\right)\right. \\ &+ \frac{R(r)\xi(\phi)T(t)}{r^2\sin\theta}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) \\ &\left.+\frac{R(r)\Theta(\theta)T(t)}{r^2\sin^2\theta}\xi''(\phi)\right] + V(r)[R(r)\Theta(\theta)\xi(\phi)T(t)] \end{aligned}$$

In order to separate variables, divide both sides by $R(r)\Theta(\theta)\xi(\phi)T(t)$.

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2M}\left[\frac{1}{r^2R(r)}\frac{d}{dr}\left(r^2R'(r)\right) + \frac{1}{r^2\Theta(\theta)\sin\theta}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{1}{r^2\xi(\phi)\sin^2\theta}\xi''(\phi)\right] + V(r)$$

The only way a function of t can be equal to a function of r, θ, and ϕ is if both are equal to a constant.

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2M}\left[\frac{1}{r^2R(r)}\frac{d}{dr}\left(r^2R'(r)\right) + \frac{1}{r^2\Theta(\theta)\sin\theta}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{1}{r^2\xi(\phi)\sin^2\theta}\xi''(\phi)\right] + V(r) = E$$

Multiply both sides by $-2Mr^2/\hbar^2$.

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2R'(r)\right) + \frac{1}{\Theta(\theta)\sin\theta}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{1}{\xi(\phi)\sin^2\theta}\xi''(\phi) - \frac{2Mr^2}{\hbar^2}[V(r) - E] = 0$$

Bring the θ- and ϕ-dependent terms to the right side.

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2R'(r)\right) - \frac{2Mr^2}{\hbar^2}[V(r) - E] = -\frac{1}{\sin^2\theta}\left[\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{\xi''(\phi)}{\xi(\phi)}\right]$$

The only way a function of r can be equal to a function of θ and ϕ is if both are equal to a constant.

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2R'(r)\right) - \frac{2Mr^2}{\hbar^2}[V(r) - E] = -\frac{1}{\sin^2\theta}\left[\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{\xi''(\phi)}{\xi(\phi)}\right] = F$$

Multiply both sides by $-\sin^2\theta$.

$$\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + \frac{\xi''(\phi)}{\xi(\phi)} = -F\sin^2\theta$$

Bring the θ-dependent terms to the left side.

$$\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + F\sin^2\theta = -\frac{\xi''(\phi)}{\xi(\phi)}$$

The only way a function of θ can be equal to a function of ϕ is if both are equal to a constant.

$$\frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + F\sin^2\theta = -\frac{\xi''(\phi)}{\xi(\phi)} = G$$

As a result of using the method of separation of variables, Schrödinger's equation has reduced to four ODEs—one in r, one in θ, one in ϕ, and one in t.

$$\left.\begin{aligned} i\hbar\frac{T'(t)}{T(t)} &= E \\ \frac{1}{R(r)}\frac{d}{dr}\left(r^2R'(r)\right) - \frac{2Mr^2}{\hbar^2}[V(r) - E] &= F \\ \frac{\sin\theta}{\Theta(\theta)}\frac{d}{d\theta}\left(\Theta'(\theta)\sin\theta\right) + F\sin^2\theta &= G \\ -\frac{\xi''(\phi)}{\xi(\phi)} &= G \end{aligned}\right\}$$

The strategy is to solve the fourth eigenvalue problem first to get G, then to solve the third eigenvalue problem for F, then to solve the second eigenvalue problem for E, and then finally to solve the first eigenvalue problem to get $T(t)$. In Problem 4.4 it was found that $F = \ell(\ell+1)$, $G = m^2$, $\xi(\phi) = C_1 e^{im\phi}$, and $\Theta(\theta) = C_2 P_\ell^m(\cos\theta)$, where $\ell = 0, 1, 2, \ldots$ and $m = -\ell, -\ell+1, \ldots, -1, 0, 1, \ldots, \ell-1, \ell$. As a result, the second eigenvalue problem is

$$\frac{1}{R(r)}\frac{d}{dr}\left(r^2 R'(r)\right) - \frac{2Mr^2}{\hbar^2}[V(r) - E] = \ell(\ell+1).$$

Multiply both sides by $R(r)$.

$$\frac{d}{dr}\left(r^2 R'(r)\right) - \frac{2Mr^2}{\hbar^2}[V(r) - E]R(r) = \ell(\ell+1)R(r) \tag{1}$$

For the infinite spherical well in particular,

$$V(r) = \begin{cases} 0 & \text{if } r \leq a \\ \infty & \text{if } r > a \end{cases}.$$

If $r > a$, then equation (1) becomes

$$\frac{d}{dr}\left(r^2 R'(r)\right) - \frac{2Mr^2}{\hbar^2}(\infty - E)R(r) = \ell(\ell+1)R(r), \quad r > a.$$

The only way both sides of this equation can be satisfied is if $R(r) = 0$. The wave function is required to be continuous at $r = a$, so $R(a) = 0$ is a boundary condition. If $r \leq a$, then equation (1) becomes

$$\frac{d}{dr}\left(r^2 R'(r)\right) - \frac{2Mr^2}{\hbar^2}(0 - E)R(r) = \ell(\ell+1)R(r), \quad r \leq a$$

$$r^2 R''(r) + 2rR'(r) + \left[\frac{2ME}{\hbar^2}r^2 - \ell(\ell+1)\right]R(r) = 0.$$

This is the spherical Bessel equation, which has the general solution,

$$R(r) = C_3 j_\ell\left(\frac{\sqrt{2ME}}{\hbar}r\right) + C_4 n_\ell\left(\frac{\sqrt{2ME}}{\hbar}r\right).$$

$j_\ell(x)$ and $n_\ell(x)$ are spherical Bessel functions of the first and second kind, respectively, which can be obtained from

$$j_\ell(x) = (-x)^\ell\left[\left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}\right]$$

$$n_\ell(x) = -(-x)^\ell\left[\left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x}\right].$$

The first few spherical Bessel functions of the first kind are

$$j_0(x) = (-x)^0 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^0 \frac{\sin x}{x}\right] = (1)\left[(1)\frac{\sin x}{x}\right] = \frac{\sin x}{x}$$

$$j_1(x) = (-x)^1 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^1 \frac{\sin x}{x}\right] = -x\left[\frac{1}{x}\frac{d}{dx}\left(\frac{\sin x}{x}\right)\right] = -x\left[\frac{1}{x}\frac{(\cos x)x - (1)(\sin x)}{x^2}\right] = -x\left(\frac{x\cos x - \sin x}{x^3}\right)$$

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

$$j_2(x) = (-x)^2 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^2 \frac{\sin x}{x}\right] = x^2\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{x\cos x - \sin x}{x^3}\right] = x^2\left[\frac{1}{x}\frac{(-x\sin x)(x^3) - (3x^2)(x\cos x - \sin x)}{x^6}\right]$$

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

$$j_3(x) = (-x)^3 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^3 \frac{\sin x}{x}\right] = -x^3\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{(-x^2+3)\sin x - 3x\cos x}{x^5}\right]$$

$$= -x^3\left[\frac{1}{x}\frac{x(15-x^2)\cos x + 3(2x^2-5)\sin x}{x^6}\right]$$

$$= \frac{x(x^2-15)\cos x + 3(5-2x^2)\sin x}{x^4}$$

$$j_4(x) = (-x)^4 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^4 \frac{\sin x}{x}\right] = x^4\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{1}{x}\frac{x(15-x^2)\cos x + 3(2x^2-5)\sin x}{x^6}\right]$$

$$= \frac{5x(2x^2-21)\cos x + (x^4-45x^2+105)\sin x}{x^5}$$

$$j_5(x) = (-x)^5 \left[\left(\frac{1}{x}\frac{d}{dx}\right)^5 \frac{\sin x}{x}\right] = -x^5\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{5x(2x^2-21)\cos x + (x^4-45x^2+105)\sin x}{x^9}\right]$$

$$= \frac{-x(x^4-105x^2+945)\cos x + 15(x^4-28x^2+63)\sin x}{x^6}.$$

If $x \ll 1$, then sine and cosine can be expanded in Taylor series about $x = 0$.

$$j_0(x) = \frac{1}{x}\sin x = \frac{1}{x}\left(x - \frac{x^3}{6} + \frac{x^5}{120} - \cdots\right) = 1 - \frac{x^2}{6} + \frac{x^4}{120} - \cdots \approx 1$$

$$j_1(x) = \frac{1}{x^2}\sin x - \frac{1}{x}\cos x = \frac{1}{x^2}\left(x - \frac{x^3}{6} + \frac{x^5}{120} - \cdots\right) - \frac{1}{x}\left(1 - \frac{x^2}{2} + \frac{x^4}{24} - \cdots\right) = \frac{x}{3} - \frac{x^3}{30} - \cdots \approx \frac{x}{3}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x = \left(\frac{3}{x^3} - \frac{1}{x}\right)\left(x - \frac{x^3}{6} + \frac{x^5}{120} - \cdots\right) - \frac{3}{x^2}\left(1 - \frac{x^2}{2} + \frac{x^4}{24} - \cdots\right)$$

$$= \frac{x^2}{15} - \frac{x^4}{120} - \cdots \approx \frac{x^2}{15}$$

The first few spherical Bessel functions of the second kind are

$$n_0(x) = -(-x)^0\left[\left(\frac{1}{x}\frac{d}{dx}\right)^0\frac{\cos x}{x}\right] = -(1)\left[(1)\frac{\cos x}{x}\right] = -\frac{\cos x}{x}$$

$$n_1(x) = -(-x)^1\left[\left(\frac{1}{x}\frac{d}{dx}\right)^1\frac{\cos x}{x}\right] = x\left[\frac{1}{x}\frac{d}{dx}\left(\frac{\cos x}{x}\right)\right] = x\left[\frac{(-\sin x)x-(1)(\cos x)}{x^3}\right] = x\left(-\frac{x\sin x+\cos x}{x^3}\right)$$

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

$$n_2(x) = -(-x)^2\left[\left(\frac{1}{x}\frac{d}{dx}\right)^2\frac{\cos x}{x}\right] = -x^2\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{-x\sin x-\cos x}{x^3}\right]$$

$$= -x^2\left[\frac{1}{x}\frac{(-x\cos x)(x^3)-(3x^2)(-x\sin x-\cos x)}{x^6}\right]$$

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

$$n_3(x) = -(-x)^3\left[\left(\frac{1}{x}\frac{d}{dx}\right)^3\frac{\cos x}{x}\right] = x^3\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{(3-x^2)\cos x+3x\sin x}{x^5}\right]$$

$$= x^3\left[\frac{1}{x}\frac{x(x^2-15)\sin x+3(2x^2-5)\cos x}{x^6}\right]$$

$$= \frac{x(x^2-15)\sin x+3(2x^2-5)\cos x}{x^4}$$

$$n_4(x) = -(-x)^4\left[\left(\frac{1}{x}\frac{d}{dx}\right)^4\frac{\cos x}{x}\right] = -x^4\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{1}{x}\frac{x(x^2-15)\sin x+3(2x^2-5)\cos x}{x^6}\right]$$

$$= -\frac{5x(21-2x^2)\sin x+(x^4-45x^2+105)\cos x}{x^5}$$

$$n_5(x) = -(-x)^5\left[\left(\frac{1}{x}\frac{d}{dx}\right)^5\frac{\cos x}{x}\right] = x^5\left[\left(\frac{1}{x}\frac{d}{dx}\right)\frac{5x(21-2x^2)\sin x+(x^4-45x^2+105)\cos x}{x^9}\right]$$

$$= -\frac{x(x^4-105x^2+945)\sin x+15(x^4-28x^2+63)}{x^6}$$

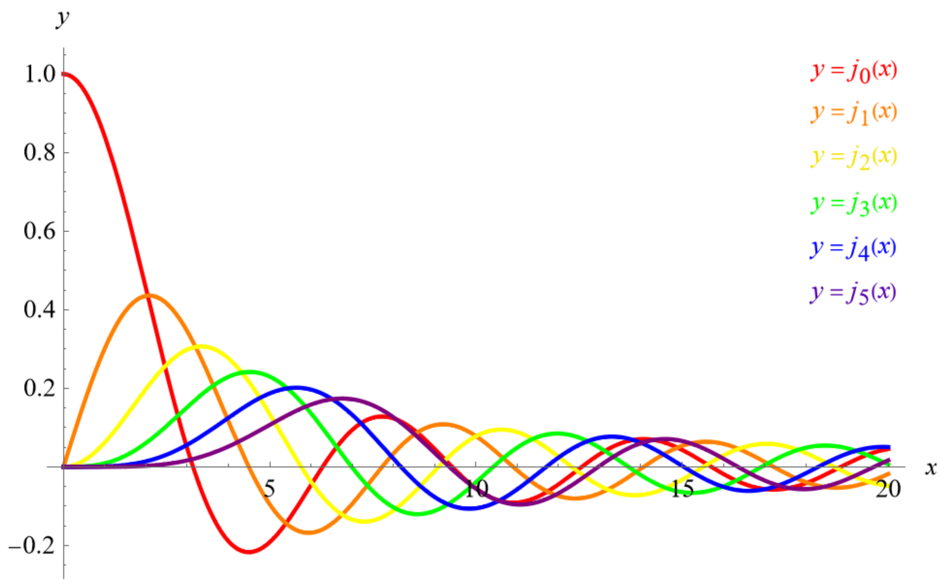
If $x \ll 1$, then sine and cosine can be expanded in Taylor series about $x=0$.

$$n_0(x) = -\frac{1}{x}\cos x = -\frac{1}{x}\left(1-\frac{x^2}{2}+\frac{x^4}{24}-\cdots\right) = -\frac{1}{x}+\frac{x}{2}-\frac{x^3}{24}+\cdots \approx -\frac{1}{x}$$

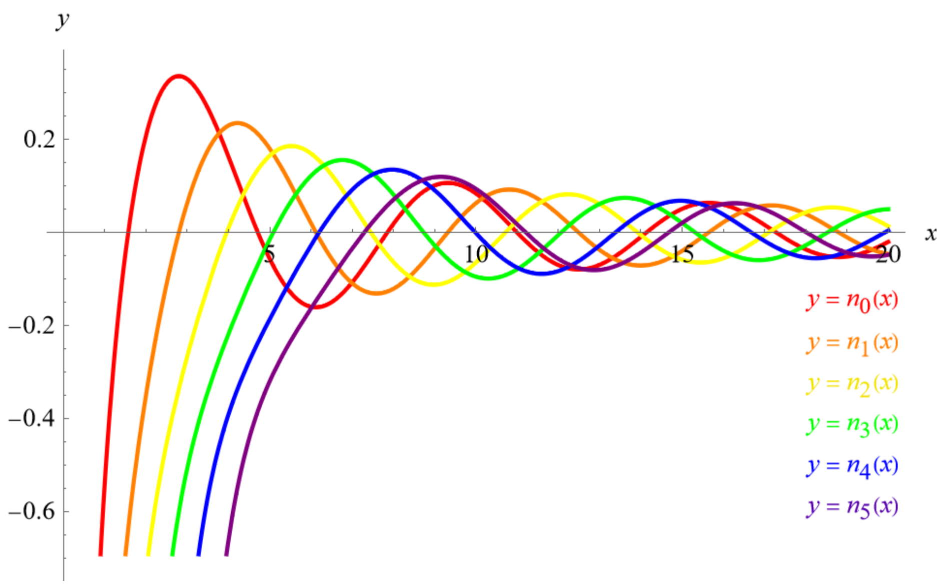
$$n_1(x) = -\frac{1}{x}\sin x-\frac{1}{x^2}\cos x = -\frac{1}{x}\left(x-\frac{x^3}{6}+\cdots\right)-\frac{1}{x^2}\left(1-\frac{x^2}{2}+\frac{x^4}{24}-\cdots\right) = -\frac{1}{x^2}-\frac{1}{2}+\frac{x^2}{8}+\cdots \approx -\frac{1}{x^2}$$

$$n_2(x) = \left(\frac{1}{x}-\frac{3}{x^3}\right)\cos x-\frac{3}{x^2}\sin x = \left(\frac{1}{x}-\frac{3}{x^3}\right)\left(1-\frac{x^2}{2}+\cdots\right)-\frac{3}{x^2}\left(x-\frac{x^3}{6}+\cdots\right) \approx -\frac{3}{x^3}$$

Below are graphs of the first six spherical Bessel functions of the first kind versus x.



Below are graphs of the first six spherical Bessel functions of the second kind versus x.



The spherical Bessel functions of the second kind all diverge as $x \to 0$, so these are physically irrelevant solutions. Set $C_4 = 0$ in the general solution.

$$R(r) = C_3 j_\ell \left(\frac{\sqrt{2ME}}{\hbar} r \right)$$

Apply the boundary condition $R(a) = 0$ to determine E.

$$R(a) = C_3 j_\ell \left(\frac{\sqrt{2ME}}{\hbar} a \right) = 0$$

$$\frac{\sqrt{2ME}}{\hbar} a = \beta_{N\ell}, \quad N = 1, 2, \ldots$$

$$E_{N\ell} = \frac{\hbar^2}{2Ma^2} \beta_{N\ell}^2$$

Here $\beta_{N\ell}$ is the Nth zero of the ℓth spherical Bessel function of the first kind. Therefore,

$$R(r) = C_3 j_\ell \left(\frac{\beta_{N\ell}}{a} r \right),$$

where C_3 is arbitrary and chosen so that

$$\int_0^\infty |R(r)|^2 r^2 \, dr = 1.$$