Problem 4.3

(a) Suppose $\psi(r,\theta,\phi) = Ae^{-r/a}$, for some constants A and a. Find E and $V(r)$, assuming $V(r) \to 0$ as $r \to \infty$.

(b) Do the same for $\psi(r,\theta,\phi) = Ae^{-r^2/a^2}$, assuming $V(0) = 0$.

[TYPO: Write the end of footnote 3 on page 134 as "Some authors now switch to M or μ for mass, but I hate to change notation in midstream. And I don't think confusion will arise as long as you are aware of the problem."]

Solution

For a spherically symmetric wave function and a spherically symmetric time-independent potential energy function, Schrödinger's equation becomes

$$\begin{aligned} i\hbar\frac{\partial\Psi}{\partial t} &= -\frac{\hbar^2}{2m}\nabla^2\Psi + V(r)\Psi(r,t) \\ &= -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Psi}{\partial r}\right) + V(r)\Psi(r,t). \end{aligned}$$

Because it's linear and homogeneous, the method of separation of variables can be applied: Assume a product solution of the form $\Psi(r,t) = \psi(r)T(t)$ and plug it into the PDE.

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}[\psi(r)T(t)] &= -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left[r^2\frac{\partial}{\partial r}[\psi(r)T(t)]\right] + V(r)[\psi(r)T(t)] \\ i\hbar\psi(r)T'(t) &= -\frac{\hbar^2}{2m}\frac{T(t)}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + V(r)[\psi(r)T(t)] \end{aligned}$$

Divide both sides by $\psi(r)T(t)$ in order to separate variables.

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + V(r)$$

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

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + V(r) = E$$

As a result of separating variables, the PDE has reduced to two ODEs—one in t and one in r.

$$\left.\begin{aligned} i\hbar\frac{T'(t)}{T(t)} &= E \\ -\frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) + V(r) &= E \end{aligned}\right\}$$

Solve this second equation for the potential energy function.

$$V(r) = E + \frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right)$$

Part (a)

If $\psi(r) = Ae^{-r/a}$, then

$$\begin{aligned}
V(r) &= E + \frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) \\
&= E + \frac{\hbar^2}{2m}\frac{1}{r^2(Ae^{-r/a})}\frac{d}{dr}\left[r^2\frac{d}{dr}(Ae^{-r/a})\right] \\
&= E + \frac{\hbar^2}{2m}\frac{1}{r^2(Ae^{-r/a})}\frac{d}{dr}\left[r^2\left(-\frac{A}{a}e^{-r/a}\right)\right] \\
&= E - \frac{\hbar^2}{2ma}\frac{1}{r^2e^{-r/a}}\frac{d}{dr}\left(r^2e^{-r/a}\right) \\
&= E - \frac{\hbar^2}{2ma}\frac{1}{r^2e^{-r/a}}\left(2re^{-r/a} - \frac{r^2}{a}e^{-r/a}\right) \\
&= E - \frac{\hbar^2}{2ma^2}\left(\frac{2a}{r} - 1\right).
\end{aligned}$$

Use the fact that $V(r) \to 0$ as $r \to \infty$ to determine E.

$$\lim_{r\to\infty} V(r) = E - \frac{\hbar^2}{2ma^2}(-1) = 0 \quad \to \quad E = -\frac{\hbar^2}{2ma^2}$$

Therefore,

$$\begin{aligned}
V(r) &= -\frac{\hbar^2}{2ma^2} - \frac{\hbar^2}{2ma^2}\left(\frac{2a}{r} - 1\right) \\
&= -\frac{\hbar^2}{mar}.
\end{aligned}$$

Part (b)

If $\psi(r) = Ae^{-r^2/a^2}$, then

$$\begin{aligned}
V(r) &= E + \frac{\hbar^2}{2m}\frac{1}{r^2\psi(r)}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) \\
&= E + \frac{\hbar^2}{2m}\frac{1}{r^2\left(Ae^{-r^2/a^2}\right)}\frac{d}{dr}\left[r^2\frac{d}{dr}\left(Ae^{-r^2/a^2}\right)\right] \\
&= E + \frac{\hbar^2}{2m}\frac{1}{r^2e^{-r^2/a^2}}\frac{d}{dr}\left[r^2\left(-\frac{2r}{a^2}e^{-r^2/a^2}\right)\right] \\
&= E - \frac{\hbar^2}{ma^2}\frac{1}{r^2e^{-r^2/a^2}}\frac{d}{dr}\left(r^3e^{-r^2/a^2}\right) \\
&= E - \frac{\hbar^2}{ma^2}\frac{1}{r^2e^{-r^2/a^2}}\left[r^2\left(3-2\frac{r^2}{a^2}\right)e^{-r^2/a^2}\right] \\
&= E - \frac{\hbar^2}{ma^2}\left(3-2\frac{r^2}{a^2}\right).
\end{aligned}$$

Use the fact that $V(0) = 0$ to determine E.

$$\lim_{r\to 0} V(r) = E - \frac{\hbar^2}{ma^2}(3) = 0 \quad \to \quad E = \frac{3\hbar^2}{ma^2}$$

Therefore,

$$\begin{aligned}
V(r) &= \frac{3\hbar^2}{ma^2} - \frac{\hbar^2}{ma^2}\left(3-2\frac{r^2}{a^2}\right) \\
&= \frac{2\hbar^2}{ma^4}r^2.
\end{aligned}$$