Problem 4.11

A particle of mass m is placed in a *finite* spherical well:

$$V(r) = \begin{cases} -V_0, & r \leq a; \\ 0, & r > a. \end{cases}$$

Find the ground state, by solving the radial equation with $\ell = 0$. Show that there is no bound state if $V_0 a^2 < \pi^2 \hbar^2 / 8m$.

Solution

The governing equation for the wave function is Schrödinger's equation. (Use M for the mass.)

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

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 ($0 \leq r < \infty$, $0 \leq \theta \leq \pi$, $0 \leq \phi \leq 2\pi$) for $t > 0$. Since Schrödinger's equation is linear and homogeneous, the method of separation of variables can be used to solve it. Assuming a product solution of the form $\Psi(r, \theta, \phi, t) = R(r)\Theta(\theta)\xi(\phi)T(t)$ and plugging it into the PDE results in four ODEs—one in r, one in θ, one in ϕ, and one in t.

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

The third and fourth eigenvalue problems were solved in Problem 4.4: $F = \ell(\ell + 1)$, $G = m^2$, $\xi(\phi) = C_1 e^{im\phi}$, 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 becomes

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

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

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

E is negative ($E < 0$) for bound states, and for the ground state in particular, $\ell = 0$.

$$r^2 R''(r) + 2rR'(r) - \frac{2Mr^2}{\hbar^2}[V(r) - E]R(r) = 0 \tag{1}$$

Make the substitution $u(r) = rR(r)$ to obtain the radial equation.

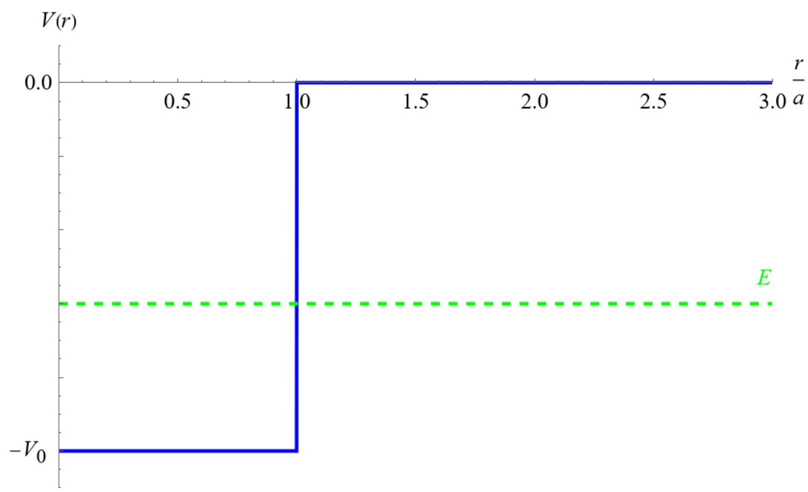
$$r^2 \left[\frac{u(r)}{r}\right]'' + 2r\left[\frac{u(r)}{r}\right]' - \frac{2Mr^2}{\hbar^2}[V(r) - E]\frac{u(r)}{r} = 0$$

$$r^2 \left[\frac{r^2 u''(r) - 2ru'(r) + 2u(r)}{r^3}\right] + 2r\left[\frac{ru'(r) - u(r)}{r^2}\right] - \frac{2Mr^2}{\hbar^2}[V(r) - E]\frac{u(r)}{r} = 0$$

$$r^2 u''(r) - \cancel{2ru'(r)} + \cancel{2u(r)} + \cancel{2ru'(r)} - \cancel{2u(r)} - \frac{2Mr^2}{\hbar^2}[V(r) - E]u(r) = 0$$

$$u''(r) = \frac{2M}{\hbar^2}[V(r) - E]u(r) \tag{2}$$

What's special about the radial equation is that it's really the TISE, and everything we know from Chapter 2 applies here. Based on Problem 2.2, E must exceed the minimum value of $V(x)$ in order for the solution to be normalized: $-V_0 < E < 0$, that is, $V_0 + E > 0$. Below is a graph of the potential energy function $V(r)$ versus r/a.



Split up the radial equation over the intervals where $V(r)$ is defined.

$$u''(r) = \begin{cases} \frac{2M}{\hbar^2}(-V_0 - E)u(r) & \text{if } r \le a \\ \frac{2M}{\hbar^2}(0 - E)u(r) & \text{if } r > a \end{cases}$$

$$= \begin{cases} -\frac{2M(V_0 + E)}{\hbar^2}u(r) & \text{if } r \le a \\ \frac{-2ME}{\hbar^2}u(r) & \text{if } r > a \end{cases}$$

For $r \leq a$, the general solution is written in terms of sine and cosine. For $r > a$, the general solution is written in terms of exponential functions,

$$u(r) = \begin{cases} C_3 \cos lr + C_4 \sin lr & \text{if } r \leq a \\ C_5 e^{-\kappa r} + C_6 e^{\kappa r} & \text{if } r > a \end{cases},$$

where

$$l = \frac{\sqrt{2M(V_0 + E)}}{\hbar} \quad \text{and} \quad \kappa = \frac{\sqrt{-2ME}}{\hbar}.$$

Boundary conditions are necessary to determine C_3, C_4, C_5, and C_6. Since $0 \leq r < \infty$, there are conditions as $r \to 0$ and $r \to \infty$. Ψ must be finite as $r \to 0$, and Ψ and its derivatives with respect to r tend to zero as $r \to \infty$. After separating variables, these conditions pass along to $R(r)$.

$$\text{finite} = \lim_{r\to 0} \Psi(r,\theta,\phi,t) = \lim_{r\to 0} R(r)\Theta(\theta)\xi(\phi)T(t) = \Theta(\theta)\xi(\phi)T(t) \lim_{r\to 0} R(r) \quad \Rightarrow \quad \lim_{r\to 0} R(r) = \text{finite}$$

$$0 = \lim_{r\to \infty} \Psi(r,\theta,\phi,t) = \lim_{r\to \infty} R(r)\Theta(\theta)\xi(\phi)T(t) = \Theta(\theta)\xi(\phi)T(t) \lim_{r\to \infty} R(r) \quad \Rightarrow \quad \lim_{r\to \infty} R(r) = 0$$

As a result,

$$\begin{cases} \lim_{r\to 0} u(r) = \lim_{r\to 0} rR(r) = 0 \\ \lim_{r\to \infty} u(r) = \lim_{r\to \infty} rR(r) = 0 \end{cases}.$$

Set $C_3 = 0$ and $C_6 = 0$ to satisfy these boundary conditions.

$$u(r) = \begin{cases} C_4 \sin lr & \text{if } r \leq a \\ C_5 e^{-\kappa r} & \text{if } r > a \end{cases}$$

Note that the solution for $r \leq a$ could have been found from equation (1), the spherical Bessel equation with $\ell = 0$.

$$R(r) = C_7 j_0(lr) + C_8 n_0(lr).$$

Because $R(0)$ is finite, $C_8 = 0$.

$$\begin{aligned} R(r) &= C_7 j_0(lr) \\ &= C_7 \left(\frac{\sin lr}{lr}\right) \\ &= C_9 \left(\frac{\sin lr}{r}\right) \end{aligned}$$

In order to determine C_4 and C_5, require $u(r)$ and its derivative to be continuous at $r = a$.

$$\lim_{r\to a^-} u(r) = \lim_{r\to a^+} u(r) : \quad C_4 \sin la = C_5 e^{-\kappa a} \tag{3}$$

$$\lim_{r\to a^-} \frac{du}{dr} = \lim_{r\to a^+} \frac{du}{dr} : \quad C_4 l \cos la = -C_5 \kappa e^{-\kappa a} \tag{4}$$

Substitute equation (3) into equation (4). Assume $C_4 \neq 0$.

$$C_4 l \cos la = -\kappa (C_4 \sin la)$$

$$l \cos la = -\kappa \sin la$$

$$-la \cot la = \kappa a$$

$$-\frac{\sqrt{2M(V_0+E)}}{\hbar} a \cot \left[\frac{\sqrt{2M(V_0+E)}}{\hbar} a\right] = \frac{\sqrt{-2ME}}{\hbar} a$$

$$= \left[\sqrt{\frac{2MV_0}{\hbar^2} - \frac{2M(V_0+E)}{\hbar^2}}\right] a$$

$$= \sqrt{\frac{2MV_0}{\hbar^2} a^2 - \frac{2M(V_0+E)}{\hbar^2} a^2}$$

$$= \sqrt{\left(\frac{\sqrt{2MV_0}}{\hbar} a\right)^2 - \left[\frac{\sqrt{2M(V_0+E)}}{\hbar} a\right]^2}$$

Introduce the variables,

$$z_0 = \frac{\sqrt{2MV_0}}{\hbar} a \quad \text{and} \quad z = \frac{\sqrt{2M(V_0+E)}}{\hbar} a,$$

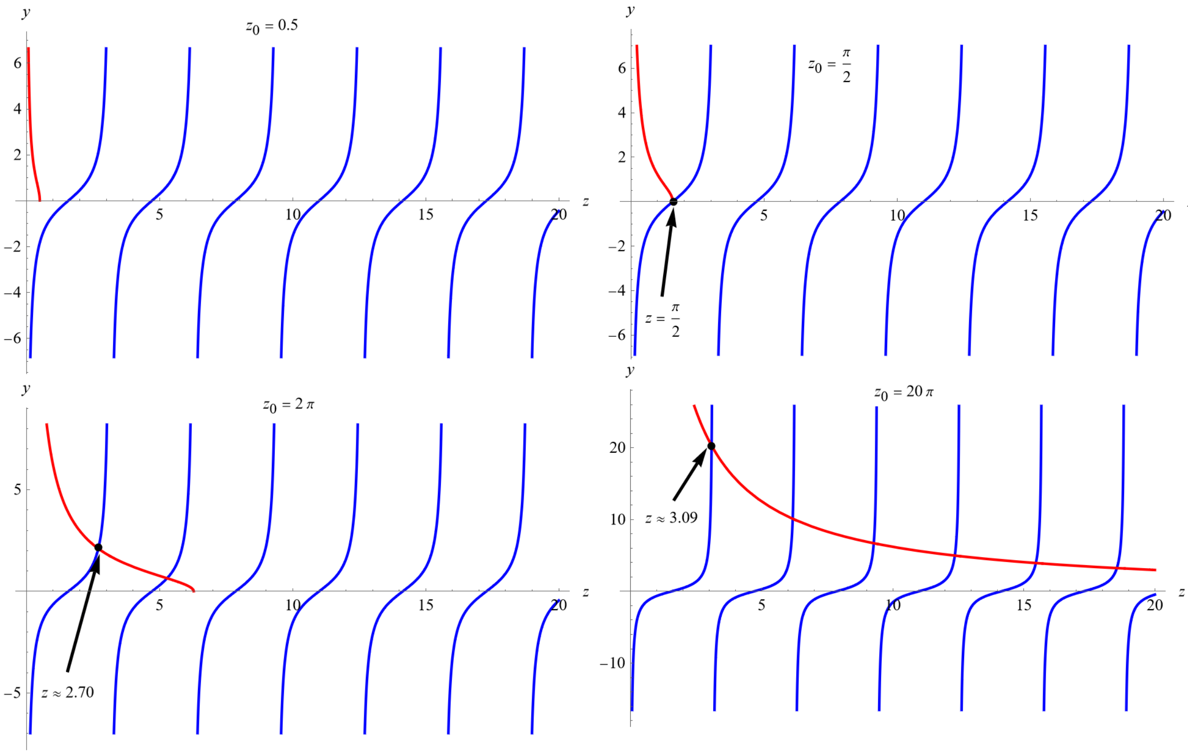
to get a transcendental equation for the eigenvalues.

$$-z \cot z = \sqrt{z_0^2 - z^2}$$

Divide both sides by z to get an equation analogous to Equation 2.159 (page 72) in the textbook.

$$-\cot z = \sqrt{(z_0/z)^2 - 1}$$

Below are plots of $y = -\cot z$ (in blue) and $y = \sqrt{(z_0/z)^2 - 1}$ (in red) versus z for various values of z_0.



There exists a ground state when the red curve intersects the first blue curve, which can occur anywhere between $z = \pi/2$ and $z = \pi$.

$$\frac{\pi}{2} \le z < \pi$$

$$\frac{\pi}{2} \le la < \pi$$

$$\frac{\pi}{2} \le \frac{\sqrt{2M(V_0 + E)}}{\hbar} a < \pi$$

$$\frac{\pi^2\hbar^2}{8Ma^2} \le V_0 + E < \frac{\pi^2\hbar^2}{2Ma^2}$$

There are no intersections below a certain value of z_0. Once z_0 reaches $\pi/2 \approx 1.57$, there is one intersection at $z = \pi/2$. Therefore, if

$$z_0 = \frac{\sqrt{2MV_0}}{\hbar} a < \frac{\pi}{2}$$

$$V_0 a^2 < \frac{\pi^2\hbar^2}{8M},$$

then there is no ground state.