Problem 4.51

In Section 2.6 we noted that the finite square well (in one dimension) has at least one bound state, no matter how shallow or narrow it may be. In Problem 4.11 you showed that the finite *spherical* well (three dimensions) has no bound state, if the potential is sufficiently weak. *Question:* What about the finite circular well (two dimensions)? Show that (like the one-dimensional case) there is always at least one bound state. *Hint:* Look up any information you need about Bessel functions, and use a computer to draw the graphs.

Solution

The governing equation for the wave function of a particle with mass M is Schrödinger's equation.

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

For the finite circular well,

$$V(r) = \begin{cases} -V_0 & \text{if } 0 \le r \le a \\ 0 & \text{if } r > a \end{cases},$$

and the appropriate expansion of the laplacian operator is in cylindrical coordinates (r, ϕ, z) .

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2M} \left[\frac{1}{r}\frac{\partial}{\partial r} \left(r\frac{\partial\Psi}{\partial r} \right) + \frac{1}{r^2}\frac{\partial^2\Psi}{\partial\phi^2} + \underbrace{\frac{\partial^2\Psi}{\partial z^2}}_{=0} \right] + V(r)\Psi(r,\phi,t), \quad \begin{cases} 0 \le r < \infty\\ 0 \le \phi \le 2\pi\\ t > 0 \end{cases}$$

Here $r = \sqrt{x^2 + y^2}$ represents the radial coordinate. The equation and its associated boundary conditions (to be considered later) are linear and homogeneous, so use the method of separation of variables: Assume a product solution of the form $\Psi(r, \phi, t) = R(r)P(\phi)T(t)$ and plug it into the equation.

$$i\hbar\frac{\partial}{\partial t}[R(r)P(\phi)T(t)] = -\frac{\hbar^2}{2M} \left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}[R(r)P(\phi)T(t)]\right) + \frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}[R(r)P(\phi)T(t)]\right] + V(r)[R(r)P(\phi)T(t)]$$

Evaluate the derivatives.

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

Divide both sides by $R(r)P(\phi)T(t)$ to separate variables.

$$i\hbar \frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2M} \left[\frac{1}{rR(r)} \frac{d}{dr} \left(r\frac{dR}{dr} \right) + \frac{1}{r^2} \frac{P''(\phi)}{P(\phi)} \right] + V(r)$$

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

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2M} \left[\frac{1}{rR(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{1}{r^2}\frac{P''(\phi)}{P(\phi)}\right] + V(r) = E$$

Bring the function of ϕ to the right side exclusively.

$$-\frac{\hbar^2}{2M}\frac{1}{rR(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \left[V(r) - E\right] = \frac{\hbar^2}{2M}\frac{1}{r^2}\frac{P''(\phi)}{P(\phi)}$$

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

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E-V(r)]}{\hbar^2}r^2 = -\frac{P''(\phi)}{P(\phi)}$$

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

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E-V(r)]}{\hbar^2}r^2 = -\frac{P''(\phi)}{P(\phi)} = F$$

As a result of applying the method of separation of variables, the Schrödinger equation has reduced to three ordinary differential equations—one for each independent variable.

$$i\hbar \frac{T'(t)}{T(t)} = E$$
$$-\frac{P''(\phi)}{P(\phi)} = F$$
$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E - V(r)]}{\hbar^2}r^2 = F$$

The strategy is to first determine F from the second equation, then to determine E from the third equation, and then (if we wanted to) determine T(t) from the first equation.

$$\frac{d^2P}{d\phi^2} = -FP\tag{1}$$

F is determined from the boundary conditions involving ϕ in particular. Since the well is circular, the wave function is expected to be the same at $\phi = 0$ and $\phi = 2\pi$. The same is true for its slope in the azimuthal direction. In other words, the boundary conditions are periodic.

$$\begin{cases} \Psi(r,0,t) = \Psi(r,2\pi,t) \\ \frac{\partial\Psi}{\partial\phi}(r,0,t) = \frac{\partial\Psi}{\partial\phi}(r,2\pi,t) \end{cases} \xrightarrow{\rightarrow} \begin{cases} R(r)P(0)T(t) = R(r)P(2\pi)T(t) \\ R(r)P'(0)T(t) = R(r)P'(2\pi)T(t) \end{cases} \xrightarrow{\rightarrow} \begin{cases} P(0) = P(2\pi) \\ P'(0) = P'(2\pi) \end{cases}$$

A solution to equation (1) that satisfies both these boundary conditions only exists if $F = m^2$ is a positive integer.

$$P(\phi) = C_1 e^{im\phi}, \quad m = 0, \pm 1, \pm 2, \dots$$

The third equation then becomes

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \frac{2M[E-V(r)]}{\hbar^2}r^2 = m^2$$
$$\frac{r}{R(r)}\left(\frac{dR}{dr} + r\frac{d^2R}{dr^2}\right) + \frac{2M[E-V(r)]}{\hbar^2}r^2 - m^2 = 0$$
$$r^2\frac{d^2R}{dr^2} + r\frac{dR}{dr} + \left[\frac{2M[E-V(r)]}{\hbar^2}r^2 - m^2\right]R = 0.$$

Split it up over the intervals that the potential energy function is defined on.

$$\begin{cases} r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + \left[\frac{2M(E+V_0)}{\hbar^2} r^2 - m^2 \right] R = 0 & \text{if } 0 \le r \le a \\ \\ r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + \left(\frac{2ME}{\hbar^2} r^2 - m^2 \right) R = 0 & \text{if } r > a \end{cases}$$

For the sake of convenience, use Mr. Griffiths's notation on page 70 and page 71:

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

Note that since we're looking for bound states, energy is assumed to be negative but greater than the potential energy floor: $-V_0 < E < 0$, that is, $E + V_0 > 0$.



With this new notation,

$$\begin{cases} r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + (l^2 r^2 - m^2)R = 0 & \text{if } 0 \le r \le a \\ \\ r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + (-\kappa^2 r^2 - m^2)R = 0 & \text{if } r > a \end{cases}$$

The first equation is the parametric form of the Bessel equation of order m, and the second equation is the parametric form of the modified Bessel equation of order m. Their general solutions are linear combinations of Bessel and modified Bessel functions.

$$R(r) = \begin{cases} C_2 J_m(lr) + C_3 Y_m(lr) & \text{if } 0 \le r \le a \\ \\ C_4 I_m(\kappa r) + C_5 K_m(\kappa r) & \text{if } r > a \end{cases}$$



Below are plots of some Bessel functions to illustrate their behavior.

E is determined from the boundary conditions involving *r* in particular. To keep R(r) finite as $r \to 0$, set $C_3 = 0$. To keep R(r) finite as $r \to \infty$, set $C_4 = 0$.

$$R(r) = \begin{cases} C_2 J_m(lr) & \text{if } 0 \le r \le a \\ \\ C_5 K_m(\kappa r) & \text{if } r > a \end{cases}$$

The wave function and its slope in the radial direction are expected to be the same coming from either side of r = a.

$$\begin{cases} \lim_{r \to a^{-}} \Psi(r, \phi, t) = \lim_{r \to a^{+}} \Psi(r, \phi, t) \\ \\ \lim_{r \to a^{-}} \frac{\partial \Psi}{\partial r} = \lim_{r \to a^{+}} \frac{\partial \Psi}{\partial r} \end{cases} \longrightarrow \begin{cases} \lim_{r \to a^{-}} R(r)P(\phi)T(t) = \lim_{r \to a^{+}} R(r)P(\phi)T(t) \\ \\ \\ \lim_{r \to a^{-}} R'(r)P(\phi)T(t) = \lim_{r \to a^{+}} R'(r)P(\phi)T(t) \end{cases} \longrightarrow \begin{cases} R(a^{-}) = R(a^{+}) \\ R'(a^{-}) = R'(a^{+}) \\ \\ R'(a^{-}) = R'(a^{+}) \end{cases}$$

Apply these two boundary conditions.

$$\begin{cases} C_2 J_m(la) = C_5 K_m(\kappa a) \\ C_2 l J'_m(la) = C_5 \kappa K'_m(\kappa a) \end{cases}$$

Divide both sides of the second equation by the respective sides of the first equation to eliminate the constants.

$$\frac{lJ'_m(la)}{J_m(la)} = \frac{\kappa K'_m(\kappa a)}{K_m(\kappa a)}$$

$$\frac{laJ'_m(la)}{J_m(la)} = \frac{\kappa aK'_m(\kappa a)}{K_m(\kappa a)}$$
(2)

Use Mr. Griffiths's notation on page 72 to simplify this equation. Let

$$Z = la$$
 and $Z_0 = \frac{a}{\hbar}\sqrt{2MV_0}.$

Then

$$\kappa a = \sqrt{Z_0^2 - Z^2}$$

so equation (2) becomes

$$\frac{ZJ'_m(Z)}{J_m(Z)} = \frac{\sqrt{Z_0^2 - Z^2}K'_m\left(\sqrt{Z_0^2 - Z^2}\right)}{K_m\left(\sqrt{Z_0^2 - Z^2}\right)}.$$

Consider the ground state m = 0 as in Problem 4.11.

$$\frac{ZJ_0'(Z)}{J_0(Z)} = \frac{\sqrt{Z_0^2 - Z^2}K_0'\left(\sqrt{Z_0^2 - Z^2}\right)}{K_0\left(\sqrt{Z_0^2 - Z^2}\right)}$$

Note that $J'_0(Z) = -J_1(Z)$ and $K'_0(Z) = -K_1(Z)$.

$$\frac{ZJ_1(Z)}{J_0(Z)} = \frac{\sqrt{Z_0^2 - Z^2}K_1\left(\sqrt{Z_0^2 - Z^2}\right)}{K_0\left(\sqrt{Z_0^2 - Z^2}\right)}$$

Now plot the functions on both sides of this equation on the same graph. Let L(Z) represent the function on the left, and let R(Z) represent the function on the right. Solutions (bound states) occur where there are intersections.





Notice that regardless of how small Z_0 is, there's always one intersection.

Therefore, the finite circular well has at least one bound state regardless of the strength of V_0 .