Moderne Theoretische Physik I
Grundlagen der Quantenmechanik

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Exercise Sheet 7

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The problems whose solutions you need to upload are designated with stars.

⋆ Problem 1 ⋆ Reflection and transmission for a Dirac delta potential

Consider a particle of mass m subject to the potential

$$V(x) = V_0\,\delta(x) \tag{1}$$

where V_0 can be positive or negative.

1. Assume that the particle is coming from the left ($x < 0$) with a momentum $\hbar k$, i.e., assume that $\psi(x)$ has a $\mathrm{e}^{\mathrm{i}kx}$ component as $x \to -\infty$, but does not have a $\mathrm{e}^{-\mathrm{i}kx}$ component as $x \to +\infty$. Find the energy and the corresponding wavefunction $\psi(x)$.

2. Define the reflection coefficient as

$$R \equiv \lim_{x\to-\infty} \left| \frac{j_{\text{reflected}}}{j_{\text{incoming}}} \right| \tag{2}$$

   and the transmission coefficient as

$$T \equiv \lim_{x\to\infty} \left| \frac{j_{\text{transmitted}}}{j_{\text{incoming}}} \right|, \tag{3}$$

   where j is the current ($\partial_t \left|\psi\right|^2 + \partial_x j = 0$). Calculate them for the $\psi(x)$ of part 1. Check that $R + T = 1$.

Next, let us put a wall a distance L in front of the Dirac delta well:

$$V(x) = \begin{cases} V_0\,\delta(x), & \text{when } x \le L, \\ \infty, & \text{when } x > L. \end{cases} \tag{4}$$

3. For this new potential, find the wavefunction $\psi(x)$ for a particle incoming from the left with momentum $\hbar k$.

4. Explicitly calculate the reflection coefficient for the $\psi(x)$ of part 3. Discuss.

Solution 1

1. The energy is simply given by

$$E = \frac{\hbar^2 k^2}{2m}.$$

The wavefunction has the form

$$\psi(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + r\mathrm{e}^{-\mathrm{i}kx}, & \text{for } x < 0, \\ t\mathrm{e}^{\mathrm{i}kx}, & \text{for } x > 0, \end{cases}$$

where we have rescaled the solution so that the incoming $\mathrm{e}^{\mathrm{i}kx}$ has a unity prefactor. The kinetic energy density is finite only when $\psi(x)$ is continuous:

$$1 + r = t.$$

Integrating

$$\frac{-\hbar^2}{2m}\psi''(x) + V_0\,\delta(x)\psi(x) = E\psi(x)$$

from $x = -\epsilon$ to $+\epsilon$ in the usual way gives

$$\begin{aligned} \frac{-\hbar^2}{2m}[\psi'(+\epsilon) - \psi'(-\epsilon)] + V_0\psi(0) = 0, \\ \frac{-\hbar^2}{2m}\mathrm{i}k(t - 1 + r) + V_0 t = 0. \end{aligned}$$

Solving for r, t yields:

$$\begin{aligned} r &= \frac{-1}{1 - \mathrm{i}\dfrac{\hbar^2 k}{mV_0}}, \\ t &= \frac{1}{1 + \mathrm{i}\dfrac{mV_0}{\hbar^2 k}}. \end{aligned}$$

2. The current is in general given by

$$j(x) = \frac{\hbar}{m}\,\mathrm{Im}\,\psi^*(x)\partial_x\psi(x).$$

For the $\psi(x)$ of part 1, this gives

$$j(x) = \begin{cases} j_{\text{incoming}} + j_{\text{reflected}}, & \text{for } x < 0, \\ j_{\text{transmitted}}, & \text{for } x > 0, \end{cases}$$

where

$$\begin{aligned} j_{\text{incoming}} &= \frac{\hbar k}{m}, \\ j_{\text{reflected}} &= |r|^2\,\frac{-\hbar k}{m}, \\ j_{\text{transmitted}} &= |t|^2\,\frac{\hbar k}{m}. \end{aligned}$$

Hence

$$R = |r|^2 = \frac{1}{1 + \left(\dfrac{\hbar^2 k}{mV_0}\right)^2},$$
$$T = |t|^2 = \frac{1}{1 + \left(\dfrac{mV_0}{\hbar^2 k}\right)^2}.$$

This indeed satisfies $R + T = 1$, as it must.

3. This time, the wavefunction has the form

$$\psi(x) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + r\mathrm{e}^{-\mathrm{i}kx}, & \text{for } x < 0, \\ a\mathrm{e}^{\mathrm{i}kx} + b\mathrm{e}^{-\mathrm{i}kx}, & \text{for } 0 < x < L, \\ 0, & \text{for } L < x. \end{cases}$$

The continuity conditions are

$$1 + r = a + b,$$
$$a\mathrm{e}^{\mathrm{i}kL} + b\mathrm{e}^{-\mathrm{i}kL} = 0,$$

and integrating the stationary Schrödinger equation around x gives:

$$\frac{-\hbar^2}{2m}\mathrm{i}k(a - b - 1 + r) + V_0(a + b) = 0.$$

Solving for r, a, b yields

$$r = -\frac{1 - \left(1 + \mathrm{i}\dfrac{\hbar^2 k}{mV_0}\right)\mathrm{e}^{\mathrm{i}2kL}}{1 - \mathrm{i}\dfrac{\hbar^2 k}{mV_0} - \mathrm{e}^{\mathrm{i}2kL}},$$
$$a = -\mathrm{e}^{-\mathrm{i}2kL} b = \frac{1}{1 + \mathrm{i}\dfrac{mV_0}{\hbar^2 k}(1 - \mathrm{e}^{\mathrm{i}2kL})}.$$

4. For the $\psi(x)$ of part 3:

$$j(x) = \begin{cases} j_{\text{incoming}} + j_{\text{reflected}}, & \text{for } x < 0, \\ 0, & \text{for } x > 0, \end{cases}$$

where

$$j_{\text{incoming}} = \frac{\hbar k}{m},$$
$$j_{\text{reflected}} = |r|^2 \frac{-\hbar k}{m}.$$

Since there is no transmission now, we expect $R = 1$. Indeed, if we define

$$r_0 \equiv \frac{-1}{1 - \mathrm{i}\dfrac{\hbar^2 k}{mV_0}},$$

then

$$r = \mathrm{e}^{\mathrm{i}2kL} \frac{r_0}{r_0^*} \frac{1 + r_0^* \mathrm{e}^{-\mathrm{i}2kL}}{1 + r_0 \mathrm{e}^{\mathrm{i}2kL}}$$

from which it is obvious that

$$R = |r|^2 = 1.$$

⋆ Problem 2 ⋆ Orbital angular momentum

In Hamiltonian mechanics, the Poisson bracket between two phase-space functions $f(q_i, p_i)$ and $g(q_i, p_i)$ is defined as

$$\{f, g\} \equiv \sum_i \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}. \tag{5}$$

1. Calculate the Poisson bracket $\{L_i, L_j\}$ between the orbital angular momentum operators $L_i = \sum_{jk} \epsilon_{ijk} x_j p_k$, that is $\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$. (Hint: use $\{f, gh\} = \{f, g\}h + g\{f, h\}$.)
2. Next, evaluate $\{L_i, \boldsymbol{L}^2\}$, $\{L_\pm, L_z\}$, and $\{L_+, L_-\}$, where $\boldsymbol{L}^2 \equiv L_x^2 + L_y^2 + L_z^2$ and $L_\pm \equiv L_x \pm \mathrm{i}L_y$.
3. If L_x and L_y are conserved quantities relative to some Hamiltonian H, show that L_z must also be conserved. (Hint: exploit a fundamental property of the Poisson bracket.)

According to the canonical quantization procedure, if $f(x_i, p_i)$ is a function on phase space, then in quantum mechanics it becomes the operator $\hat{f} \equiv f(\hat{x}_i, \hat{p}_i)$, with the Poisson brackets moreover mapping onto commutators according to

$$[\hat{f}, \hat{g}] = \mathrm{i}\hbar\,\widehat{\{f, g\}}. \tag{6}$$

Thus $[\hat{x}_i, \hat{p}_j] = \mathrm{i}\hbar\,\widehat{\{x_i, p_j\}} = \mathrm{i}\hbar\delta_{ij}\hat{1} = \mathrm{i}\hbar\delta_{ij}$, for instance.

4. Use this to find $[\hat{L}_i, \hat{L}_j]$, $[\hat{L}_i, \hat{\boldsymbol{L}}^2]$, $[\hat{L}_\pm, \hat{L}_z]$, and $[\hat{L}_+, \hat{L}_-]$ from the previous parts of this problem.
5. If a state $|\phi\rangle$ has

$$\hat{\boldsymbol{L}}^2 |\phi\rangle = \alpha |\phi\rangle, \qquad L_z |\phi\rangle = \mu |\phi\rangle, \tag{7}$$

what are the corresponding eigenvalues of $|\phi_+\rangle \equiv \hat{L}_+ |\phi\rangle$ and $|\phi_-\rangle \equiv \hat{L}_- |\phi\rangle$?

Solution 2

1. By using

$$\{x_i, p_j\} = \delta_{ij}$$

and the linearity of the Poisson bracket (product differentiation rule), we find that

$$\begin{aligned}
\{L_i, L_j\} &= \sum_{abcd} \epsilon_{iab}\epsilon_{jcd}\{x_a p_b, x_c p_d\} = \sum_{abcd} \epsilon_{iab}\epsilon_{jcd}[\{x_a p_b, x_c\}p_d + x_c\{x_a p_b, p_d\}] \\
&= \sum_{abcd} \epsilon_{iab}\epsilon_{jcd}[x_a\{p_b, x_c\}p_d + \{x_a, x_c\}p_b p_d + x_c x_a\{p_b, p_d\} + x_c\{x_a, p_d\}p_b] \\
&= \sum_{abcd} \epsilon_{iab}\epsilon_{jcd}[-x_a\delta_{bc}p_d + x_c\delta_{ad}p_b] = \sum_{abc} \epsilon_{iab}\epsilon_{jcb}[x_a p_c - p_a x_c] \\
&= \sum_{abc}(\delta_{ij}\delta_{ac} - \delta_{ic}\delta_{ja})[x_a p_c - x_c p_a] = x_i p_j - x_j p_i = \sum_k \epsilon_{ijk} L_k.
\end{aligned}$$

2. By exploiting the product rule again we get

$$\begin{aligned}
\{L_i, \boldsymbol{L}^2\} &= \sum_j \{L_i, L_j L_j\} = \sum_j L_j\{L_i, L_j\} + \{L_i, L_j\}L_j \\
&= \sum_{jk} L_j \epsilon_{ijk} L_k + \epsilon_{ijk} L_k L_j = \sum_{jk} \epsilon_{ijk}(L_j L_k - L_j L_k) = 0.
\end{aligned}$$

Moreover

$$\begin{aligned}
\{L_\pm, L_z\} &= \{L_x, L_z\} \pm \mathrm{i}\{L_y, L_z\} = -L_y \pm \mathrm{i}L_x = \pm\mathrm{i}(L_x \pm \mathrm{i}L_y) = \pm\mathrm{i}L_\pm, \\
\{L_+, L_-\} &= \{L_x + \mathrm{i}L_y, L_x - \mathrm{i}L_y\} = \mathrm{i}\{L_y, L_x\} - \mathrm{i}\{L_x, L_y\} = -2\mathrm{i}L_z.
\end{aligned}$$

3. The Jacobi identity states that

$$\{\{f,g\},h\}+\{\{g,h\},f\}+\{\{h,f\},g\}=0$$

and applied to L_x, L_y, H it gives the desired result:

$$\frac{\mathrm{d}}{\mathrm{d}t}L_z=\{L_z,H\}=\{\{L_x,L_y\},H\}=-\{\{L_y,H\},L_x\}-\{\{H,L_x\},L_y\}=-\{0,L_x\}-\{0,L_y\}=0.$$

4. By applying the prescription (6), one readily finds that

$$\begin{aligned}[\hat{L}_i,\hat{L}_j]&=\mathrm{i}\hbar\sum_k\epsilon_{ijk}\hat{L}_k,\\ [\hat{L}_i,\hat{\boldsymbol{L}}^2]&=0,\\ [\hat{L}_\pm,\hat{L}_z]&=\mp\hbar\hat{L}_\pm,\\ [\hat{L}_+,\hat{L}_-]&=2\hbar\hat{L}_z.\end{aligned}$$

One can prove this directly too. The algebraic manipulations are analogous to the classical ones since $[\hat{A},\hat{B}\hat{C}]=[\hat{A},\hat{B}]\hat{C}+\hat{B}[\hat{A},\hat{C}]$.

5. Since $\hat{\boldsymbol{L}}^2$ commutes with $\hat{L}_\pm$:

$$\hat{\boldsymbol{L}}^2\left|\phi_\pm\right\rangle=\hat{\boldsymbol{L}}^2\hat{L}_\pm\left|\phi\right\rangle=\hat{L}_\pm\hat{\boldsymbol{L}}^2\left|\phi\right\rangle=\hat{L}_\pm\alpha\left|\phi\right\rangle=\alpha\hat{L}_\pm\left|\phi\right\rangle=\alpha\left|\phi_\pm\right\rangle.$$

On the other hand:

$$L_z\left|\phi_\pm\right\rangle=\hat{L}_z\hat{L}_\pm\left|\phi\right\rangle=(\hat{L}_\pm L_z\pm\hbar L_\pm)\left|\phi\right\rangle=(\hat{L}_\pm\mu\pm\hbar\hat{L}_\pm)\left|\phi\right\rangle=(\mu\pm\hbar)\left|\phi_\pm\right\rangle.$$

Problem 3 Particle in a finite-depth well in 3 dimensions

Consider a particle described by the Hamiltonian

$$\hat{H}=\frac{\hat{p}_x^2+\hat{p}_y^2+\hat{p}_z^2}{2m}+V_0\Theta(\hat{x}^2+\hat{y}^2+\hat{z}^2-R^2) \tag{8}$$

where $\boldsymbol{r}=(x,y,z)$ are the Cartesian coordinates, $\hat{p}_x=-\mathrm{i}\hbar\partial_x$, $\hat{p}_y=-\mathrm{i}\hbar\partial_y$, and $\hat{p}_z=-\mathrm{i}\hbar\partial_z$ are the momentum operators, and $\Theta(x)$ is the Heaviside step function. $V_0>0$ is the potential well depth and $R>0$ is its radial size.

1. Write the Hamiltonian as a differential operator in spherical coordinates (in the position representation). Express the angular part in terms of the differential operator $\hat{\boldsymbol{L}}^2=\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2$, where $\hat{\boldsymbol{L}}=\hat{\boldsymbol{r}}\times\hat{\boldsymbol{p}}$ is the angular momentum operator.

2. Next, assume that you are given a wavefunction $Y(\theta,\phi)$ that depends on the spherical angles θ and ϕ and that is an eigenvector of the $\hat{\boldsymbol{L}}^2$ operator with an eigenvalue $\lambda>0$:

$$\hat{\boldsymbol{L}}^2Y(\theta,\phi)=\hbar^2\lambda Y(\theta,\phi). \tag{9}$$

If a stationary state of energy E has the form $\psi(\boldsymbol{r})=\psi(r,\theta,\phi)=\varphi(r)Y(\theta,\phi)$, how does the corresponding radial stationary Schrödinger equation for $\varphi(r)$ look like?

3. Now consider the special case when $Y(\theta,\phi)=1$. What is the value of λ? Solve the radial stationary Schrödinger equation for this case and find all the bound states that do not depend on the spherical angles. If any transcendental equations arise, formulate their solutions graphically.

4. Does a bounded state always exist? If not, how large does V_0 have to be?

Solution 3

1. In the position representation

$$\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V_0\Theta(\hat{r} - R).$$

On the other hand

$$\begin{aligned}\hat{\boldsymbol{L}}^2 &= (\hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}) \cdot (\hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}) = \sum_{iabcd} \epsilon_{iab}\epsilon_{icd}\hat{x}_a\hat{p}_b\hat{x}_c\hat{p}_d \\ &= \sum_{iabcd} \epsilon_{iab}\epsilon_{icd}\hat{x}_a(-\mathrm{i}\hbar\delta_{bc} + \hat{x}_c\hat{p}_b)\hat{p}_d = \sum_{abcd}(\delta_{ac}\delta_{bd} - \delta_{ad}\delta_{bc})\hat{x}_a(-\mathrm{i}\hbar\delta_{bc} + \hat{x}_c\hat{p}_b)\hat{p}_d \\ &= \sum_{ad}(\delta_{ad} - 3\delta_{ad})(-\mathrm{i}\hbar\hat{x}_a\hat{p}_d) + \sum_{ab}\hat{x}_a\hat{x}_a\hat{p}_b\hat{p}_b - \hat{x}_a\hat{x}_b\hat{p}_a\hat{p}_b \\ &= 2\mathrm{i}\hbar\sum_a \hat{x}_a\hat{p}_a + \sum_{ab}\hat{x}_a\hat{x}_a\hat{p}_b\hat{p}_b - \hat{x}_a\hat{x}_b\hat{p}_a\hat{p}_b\end{aligned}$$

where all the indices go over $\{1,2,3\}$. Now notice that $\sum_a \hat{x}_a\hat{p}_a = \hat{\boldsymbol{r}} \cdot \hat{\boldsymbol{p}} = -\mathrm{i}\hbar r\partial_r$ isolates the radial gradient. Hence

$$\begin{aligned}\hat{\boldsymbol{L}}^2 &= 2\mathrm{i}\hbar(-\mathrm{i}\hbar r\partial_r) - \hbar^2 r^2\nabla^2 - (-\mathrm{i}\hbar r)^2\partial_r^2 = -\hbar^2 r^2\nabla^2 + \hbar^2(2r\partial_r + r^2\partial_r^2) \\ &= -\hbar^2 r^2\nabla^2 + \hbar^2 r\partial_r^2\, r,\end{aligned}$$

where ∂_r is an operator that acts on everything to the right. The final result is

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{2mr^2}\hat{\boldsymbol{L}}^2 + V_0\Theta(r - R).$$

Since we know the Laplace operator in spherical coordinates:

$$\begin{aligned}\nabla^2\psi &= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2} \\ &= \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2},\end{aligned}$$

if follows that

$$\hat{\boldsymbol{L}}^2 = \frac{-\hbar^2}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{-\hbar^2}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}$$

acts only on the angular coordinates.

2. The stationary Schrödinger equation is

$$\begin{aligned}\hat{H}\psi &= \frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + \frac{1}{2mr^2}\hat{\boldsymbol{L}}^2\psi + V_0\Theta(r - R)\psi \\ &= \frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\varphi Y) + \frac{1}{2mr^2}\hat{\boldsymbol{L}}^2(\varphi Y) + V_0\Theta(r - R)\varphi Y \\ &= \frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\varphi)Y + \frac{1}{2mr^2}(\hat{\boldsymbol{L}}^2 Y)\varphi + V_0\Theta(r - R)\varphi Y \\ &= \left[\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\varphi) + \frac{1}{2mr^2}\hbar^2\lambda\varphi + V_0\Theta(r - R)\varphi\right]Y = [E\varphi]Y,\end{aligned}$$

so its radial part is

$$\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\varphi) + \frac{1}{2mr^2}\hbar^2\lambda\varphi + V_0\Theta(r - R)\varphi = E\varphi.$$

3. Since $Y(\theta, \phi) = 1$ does not depend on the angles, whereas $\hat{\boldsymbol{L}}^2$ differentiates in the angles, it follows that $\lambda = 0$. So we want to solve

$$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial r^2}[r\varphi(r)] + V_0\Theta(r-R)r\varphi(r) = E\,r\varphi(r).$$

The solutions of this equation are given by

$$r\varphi(r) = \begin{cases} A\sin(kr) + B\cos(kr), & \text{for } r \le R, \\ C\mathrm{e}^{-\kappa(r-R)} + D\mathrm{e}^{\kappa(r-R)}, & \text{for } r > R, \end{cases}$$

where

$$\frac{\hbar^2 k^2}{2m} = V_0 - \frac{\hbar^2\kappa^2}{2m} = E.$$

A finite D would result in a divergence at infinity and so is forbidden for bounded states, $D = 0$. A finite B implies that $\varphi(r) \sim r^{-1}$ diverges for small r. Although this divergence is integrable in the sense that the volume integral $\int_0^\infty \mathrm{d}r\, r^2\, |\varphi(r)|^2$ still converges so φ can still be normalized, this divergence would mean that $\psi(\boldsymbol{r})$ is strongly discontinuous at $\boldsymbol{r} = \boldsymbol{0}$ with an infinite kinetic energy. Hence $B = 0$ too. The bounded state are thus given by

$$r\varphi(r) = A\begin{cases} \sin(kr), & \text{for } r \le R, \\ \sin(kR)\mathrm{e}^{-\kappa(r-R)}, & \text{for } r > R. \end{cases}$$

$\varphi(r)$ also needs to be continuous at $r = R$ (there is no Dirac delta potential there), which gives the condition:

$$k\cos(kR) = -\kappa\sin(kR).$$

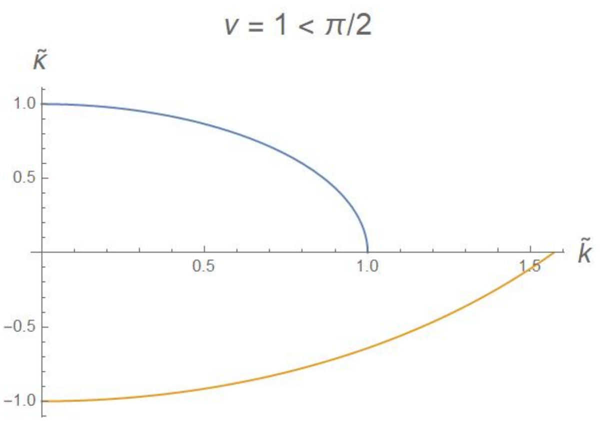
In terms of the dimensionless

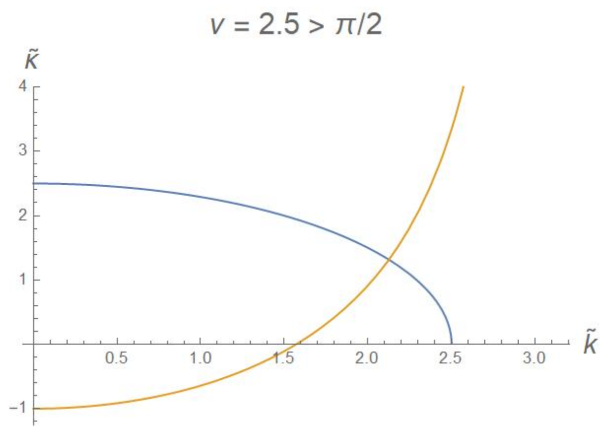
$$\tilde{k} \equiv kR, \qquad\qquad \tilde{\kappa} \equiv \kappa R$$

we thus have the transcendental set of equations

$$\tilde{k}^2 + \tilde{\kappa}^2 = \frac{2mV_0R^2}{\hbar^2} \equiv \nu^2,$$
$$\tilde{\kappa} = -\tilde{k}\cot\tilde{k}.$$

The first defines a circle and the second a curve which may or may not cross the circle. For instance:





Notice that changing the sign of $\tilde{k} \to -\tilde{k}$ only changes $\varphi(r)$ by an absolute sign. Without loss of generality, we may thus consider $\tilde{k} > 0$.

4. $\tilde{\kappa}$ must be positive for the solution to be bounded. On the other hand, $\tilde{k}$ is necessarily smaller than ν. The function $-\tilde{k}\cot\tilde{k}$ becomes positive only for $\tilde{k} > \pi/2$. Hence ν has to be larger than $\pi/2$ for a bounded state to exist; see above. This corresponds to the condition

$$V_0 > \frac{\pi^2\hbar^2}{8mR^2}.$$