1. Consider the potential given by

\[ V(x) = \begin{cases} \infty & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > a \end{cases} \]

Consider the scattering state and assume that free particles of energy \( E \) are sent in from \(+\infty\).

(a) Write down the Schrödinger equation in regions \( 0 < x < a \) and \( x > a \), respectively.

(b) Obtain the general solution of the Schrödinger equation in regions \( 0 < x < a \) and \( x > a \), respectively.

(c) Write down all boundary conditions that must be satisfied by the wave functions and their derivatives.

(d) Apply the boundary conditions to show that the ratio of the amplitude of the reflected wave to the amplitude of the incident wave can be written in the form \( C e^{i\delta} \).

(e) Calculate \( C \) and obtain an expression from which \( \delta \) can be calculated.

**Solution:**

(a) The Schrödinger equations are

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi_1}{dx^2} - V_0 \psi_1 = E \psi_1 \quad (0 < x < a) \]  
\[ (1-1) \]

\[ -\frac{\hbar^2}{2m} \frac{d^2 \psi_2}{dx^2} = E \psi_2 \quad (x > a) \]  
\[ (1-2) \]
(b) Consider first the region \(0 < x < a\). Let

\[
k_1 = \sqrt{\frac{2m(E + V_0)}{\hbar^2}}
\]  

(1-3)

The Schrödinger equation (1-1) can be written as

\[
\frac{d^2\psi_1}{dx^2} + k_1^2\psi_1 = 0 \quad (0 < x < a)
\]

The general solution of this equation is

\[
\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}
\]  

(1-4)

Similarly in the region \(x > a\), let

\[
k_2 = \sqrt{\frac{2mE}{\hbar^2}}
\]

(1-5)

The Schrödinger equation (1-2) in this region can be written as

\[
\frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 = 0 \quad (x > a)
\]

and the general solution of this equation is

\[
\psi_2(x) = D e^{ik_2x} + F e^{-ik_2x}
\]

(1-6)

(c) The boundary conditions are:

i. Since \(V = \infty\) in the region \(x < 0\), the wave function must equal to zero at \(x = 0\), i.e.,

\[
\psi_1(0) = 0
\]

(1-7)

ii. The wave function must be continuous at \(x = a\), i.e.,

\[
\psi_1(a) = \psi_2(a)
\]

(1-8)

iii. The derivative of the wave function must be continuous at \(x = a\), i.e.,

\[
\left.\frac{d\psi_1}{dx}\right|_{x=a} = \left.\frac{d\psi_2}{dx}\right|_{x=a}
\]

(1-9)

(d) Applying the boundary conditions (1-7)-(1-9) to the wave functions (1-4) and (1-6), we get the following:

\[
A + B = 0
\]

(1-10)

\[
A e^{ik_1a} + B e^{-ik_1a} = D e^{ik_2a} + F e^{-ik_2a}
\]

(1-11)

\[
ik_1(A e^{ik_1a} - B e^{-ik_1a}) = ik_2(D e^{ik_2a} - F e^{-ik_2a})
\]

(1-12)
Since this is a scattering problem, we assume that the energy of the particle $E$ (thus $k_1$ and $k_2$) and the amplitude of the incoming wave $F$ are known. $F$ is related to the probability current (or flux) of the incoming particles. We try to solve for the amplitude of the outgoing wave from the above equations by eliminating $A$ and $B$.

Express $B$ in terms of $A$ using Eq. (1-10) and substitute it into Eqs. (1-11) and (1-12), we get
\[
A(e^{ik_1a} - e^{-ik_1a}) = De^{ik_2a} + Fe^{-ik_2a}
\]
\[
k_1A(e^{ik_1a} + e^{-ik_1a}) = k_2(De^{ik_2a} - Fe^{-ik_2a})
\]
Dividing the two equations, we get
\[
k_1(e^{ik_1a} + e^{-ik_1a}) = k_1\cos(k_1a) = k_2 D e^{ik_2a} - Fe^{-ik_2a}
\]
\[
k_1(e^{ik_1a} - e^{-ik_1a}) = k_1\sin(k_1a) = k_2 D e^{ik_2a} + Fe^{-ik_2a}
\]
We can solve for $D$ in terms of $F$ from this equation. First
\[
[k_1\cos(k_1a)e^{ik_2a} - ik_2\sin(k_1a)e^{ik_2a}] D = -[k_1\cos(k_1a)e^{-ik_2a} + ik_2\sin(k_1a)e^{-ik_2a}] F
\]
Thus
\[
\frac{D}{F} = \frac{k_1\cos(k_1a) + ik_2\sin(k_1a)}{k_1\cos(k_1a) - ik_2\sin(k_1a)} e^{-2ik_2a} = \frac{k_1\cos(k_1a) + ik_2\sin(k_1a)}{k_1\cos(k_1a) - ik_2\sin(k_1a)} e^{-2ik_2a+i\pi}
\]
since $-1 = e^{i\pi}$.

The coefficient involving $k_1$ and $k_2$ is just a complex number and we can write it as
\[
\frac{k_1\cos(k_1a) + ik_2\sin(k_1a)}{k_1\cos(k_1a) - ik_2\sin(k_1a)} = Ce^{i\delta_1}.
\]

Then
\[
\frac{D}{F} = Ce^{i(\pi - 2k_2a + \delta_1)} = Ce^{i\delta}
\]
(e) To find out $C$ and $\delta_1$, we note that
\[
k_1\cos(k_1a) + ik_2\sin(k_1a) = \sqrt{k_1^2 \cos^2(k_1a) + k_2^2 \sin^2(k_1a)} e^{i\phi}
\]
\[
k_1\cos(k_1a) - ik_2\sin(k_1a) = \sqrt{k_1^2 \cos^2(k_1a) + k_2^2 \sin^2(k_1a)} e^{-i\phi}
\]
where
\[
\tan \phi = \frac{k_2 \sin(k_1a)}{k_1 \cos(k_1a)} = \frac{k_2}{k_1} \tan(k_1a)
\]
Therefore,
\[
C = 1
\]
\[
\delta_1 = 2\phi = 2\tan^{-1}\left(\frac{k_2}{k_1} \tan(k_1a)\right)
\]
and
\[
\delta = \pi - 2k_2a + 2\tan^{-1}\left(\frac{k_2}{k_1} \tan(k_1a)\right)
\]
Note that $\delta = \pi$ if $k_1 = k_2$. 

2. The Laplacian operator $\nabla^2$ in cylindrical coordinates appears as

$$\nabla^2 \psi = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2}.$$ 

(a) What is the time-independent Schrödinger equation for an arbitrary potential $V(\rho, z, \phi)$, in cylindrical coordinates?
(b) Consider the cylindrical potential well (model for a quantum wire)

$$V(\rho) = \begin{cases} 
0, & \rho < a \\
\infty, & \rho \geq a
\end{cases}$$

and the $\phi, z$ independent wavefunctions $\psi = R(\rho)$. Show that $\psi$ obeys the Bessel’s equation (of zero order)

$$\rho \frac{d}{d\rho} \left( \rho \frac{dR}{d\rho} \right) + k^2 \rho^2 R = 0, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

(c) The class of solutions of the Bessel’s equation which are finite at the origin are the zeroth-order Bessel functions, $J_0(x)$ (set $x = k\rho$). The values of $x$ where $J_0(x)$ vanishes are called the zeros of $J_0$. Given that the three lowest values of these zeros are $x_1 = 2.41$, $x_2 = 5.52$, and $x_3 = 8.65$, what are the three lowest eigenenergies and eigenfunctions (as a function of $\rho$) for the potential given in part (b)?

**Solution:**

(a) The time-independent Schrödinger equation is given by

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\psi = E\psi$$

In cylindrical coordinates, this can be written as

$$-\frac{\hbar^2}{2m} \left( \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} + \frac{\partial^2 \psi}{\partial z^2} \right) + V(\rho, z, \phi)\psi = E\psi$$

(b) For the given potential and the $\phi, z$ independent wavefunctions $\psi = R(\rho)$,

$$\frac{\partial^2 \phi}{\partial \phi^2} = 0, \quad \frac{\partial^2 \phi}{\partial z^2} = 0$$

The Schrödinger equation becomes

$$-\frac{\hbar^2}{2m} \frac{1}{\rho} \frac{\partial}{\partial \rho} \left( \rho \frac{\partial \psi}{\partial \rho} \right) = E\psi \quad (\rho < a) \quad (2-1)$$
The wave function must be zero for \( \rho > a \) since \( V(\rho) = \infty \).

Let

\[
    k = \sqrt{\frac{2mE}{\hbar^2}}
\]

Equation (2-1) can be written as

\[
    \rho \frac{d}{d\rho} \left( \rho \frac{dR}{d\rho} \right) + k^2 \rho^2 R = 0
\]  

(2-3)

The partial derivative is replaced by the normal derivative since \( \psi = R(\rho) \) is a function of \( \rho \) only. Eq.(2-3) is the Bessel's equation.

(c) Given that the solution of the Bessel's equation which are finite at \( \rho = 0 \) are the zeroth-order Bessel functions

\[
    R(\rho) = J_0(k\rho)
\]

the boundary condition at \( \rho = a \) requires that

\[
    R(a) = J_0(ka) = 0
\]

The roots of the above equation, or the zeros of \( J_0(x) \) determine the energy of the particle. Assume the \( n \)th zero of \( J_0(x) \) is \( x_n \), then

\[
    ka = \sqrt{\frac{2mEa^2}{\hbar^2}} = x_n
\]

The energy of the particle is thus

\[
    E_n = \frac{x_n^2 \hbar^2}{2ma^2}
\]

The wave function of the particle becomes

\[
    R_n(\rho) = J_0 \left( \frac{x_n \rho}{a} \right)
\]

\[
    n = 1 \quad x_1 = 2.41 \quad E_1 = \frac{(2.41)^2 \hbar^2}{2ma^2} = 5.81 \left( \frac{\hbar^2}{2ma^2} \right) \quad R_1(\rho) = J_0 \left( \frac{2.41 \rho}{a} \right)
\]

\[
    n = 2 \quad x_2 = 5.52 \quad E_2 = \frac{(5.52)^2 \hbar^2}{2ma^2} = 30.47 \left( \frac{\hbar^2}{2ma^2} \right) \quad R_2(\rho) = J_0 \left( \frac{5.52 \rho}{a} \right)
\]

\[
    n = 3 \quad x_3 = 8.65 \quad E_3 = \frac{(8.65)^2 \hbar^2}{2ma^2} = 74.82 \left( \frac{\hbar^2}{2ma^2} \right) \quad R_3(\rho) = J_0 \left( \frac{8.65 \rho}{a} \right)
\]
Some Common Mistakes

Question 1:

1. Even though there can be an incident wave and a reflected wave in each region considered, the generic term “reflected wave” in a scattering problem refers to that in region far from the scattering region. That is, the wave reflected back to where the wave is coming from. In this question, the wave comes from $x = \infty$, the reflected wave should be that traveling to $x = \infty$. If the general solutions are

$$
\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad (0 < x < a)
$$

$$
\psi_2(x) = De^{ik_2x} + Fe^{-ik_2x} \quad (x > a)
$$

the reflected wave should be $D e^{ik_2x}$.

2. Whenever there is an infinite jump in the potential, the derivative of the wave function $d\psi/dx$ is not continuous there. Therefore, it is wrong to assume that $d\psi/dx$ is continuous at $x = 0$ in this problem.

3. Other trivial mistakes such as defining

$$
k = \sqrt{-\frac{2mE}{\hbar^2}}
$$

or claiming that $Be^{ikx}$ blows up at $x \to \infty$ indicate that whoever making such mistakes are quite confused and do not know what they are doing. In this problem, $E > 0$ for scattering problem and the above definition will result in an imaginary $k$.

Question 2:

1. For this problem, the most common mistake perhaps is that many attempted to solve the whole problem using the technique of separation of variables, and of course, they ended up at nowhere. They managed to separate the Schrödinger equation into a radial equation and an angular equation, and naturally assumed that each part must be a constant which is fine. However, this problem is different from that in spherical coordinates and the constant is not necessarily $l(l + 1)$. I mentioned in the lectures that for all central force problems, the angular equation is the same and has the same solution $Y_l^m$. However, this is restricted to the central force problem and you cannot generalize to a problem with a cylindrical symmetry.

2. Many failed to recognize and use the fact that $\psi = R(\rho)$ is $\phi$ and $z$ independent. Since $\psi = R(\rho)$ does not depend on $\phi$ and $z$,

$$
\frac{\partial^2 \phi}{\partial \phi^2} = 0, \quad \frac{\partial^2 \phi}{\partial z^2} = 0
$$

and there is not much to do for you to get the result of (b). (Always read the question carefully!)
3. The Bessel’s equation describes the wave function inside the cylinder. You have to elaborate on the solution outside the cylinder, and then apply the boundary condition, to conclude that the energy of the particle is determined by the equation

$$J_0(ka) = 0$$