E&R - Ch. 6, Problem 2

In this problem, we have a particle traveling in the $-x$ direction and incident on a step located at $x = 0$. The particle is initially in the region of $x > 0$ where the potential $V(x) = V_o$ and the step represents a potential drop to $V(x) = 0$ for $x < 0$.

We can keep the coefficients of the wave equations in each region to be consistent with what we have previously defined. The equation for the region where $x > 0$ is:

$$\psi_{II}(x) = A\exp(-ik_{II}x) + B\exp(ik_{II}x) \quad \text{where} \quad k_{II} = \sqrt{\frac{2m(E - V_o)}{\hbar^2}}$$

where A is the coefficient for the wave traveling towards $-x$ and B is the reflected wave in the $+x$ direction. The equation for the region where $x < 0$ is:

$$\psi_I(x) = C\exp(-ik_Ix) \quad \text{where} \quad k_{II} = \sqrt{\frac{2mE}{\hbar^2}}$$

where C is the coefficient for the transmitted wave at the potential step. We can eliminate D since the particle can not be transmitted across the step from $-x$ to $+x$.

Utilizing boundary conditions for the continuity of $d\psi(x)/dx$ and $\psi(x)$ across the step at $x = 0$, we obtain:

$$A + B = C$$
$$-k_{II}A + k_{II}B = -k_IC$$

Since the objective is to obtain reflection (R) and transmission (T) coefficients, we can rearrange the two boundary condition equations to find B/A and C/A. These are:

$$\left(\frac{B}{A}\right) = \frac{k_{II} - k_I}{k_{II} + k_I} \tag{1}$$
$$\left(\frac{C}{A}\right) = \frac{2k_{II}}{k_{II} + k_I} \tag{2}$$

From Section 6-4, we know that R and T can be expressed as:

$$R = \frac{B^*B}{A^*A}$$
$$T = \frac{v_IC^*C}{v_{II}A^*A}$$

where v_I and v_{II} have been inverted from Eq 6-41 due to the change in particle direction. Plugging in our values from Equations 1 and 2 and letting $v_i = \hbar k_i/m$, R and T can be written as:

$$\begin{aligned} R &= \frac{B^2}{A^2} = \left(\frac{k_{II} - k_I}{k_{II} + k_I}\right)^2 \\ &= \left(\frac{k_I - k_{II}}{k_I + k_{II}}\right)^2 \\ T &= \left(\frac{\hbar k_I/m}{\hbar k_{II}/m}\right)\left(\frac{2k_{II}}{k_{II} + k_I}\right)^2 \\ &= \frac{4k_I k_{II}^2}{k_{II}(k_{II} + k_I)^2} \\ &= \frac{4k_I k_{II}}{(k_I + k_{II})^2} \end{aligned}$$

The equations for R and T are identical to those found in Equations 6-40 and 6-42. ■

E&R - Ch. 6, Problem 7

Since this problem is a modification of Problem 5 ($E > V_o$ compared to $E < V_o$), the algebra that results in the tunneling equation did not have to be shown. This was not clear, and the work is shown below for those who are interested.

Part A The potential for this problem is:

$$V(x) = \begin{cases} 0 & \text{for} \quad x < 0 \\ V_o & \text{for} \quad 0 < x < a \\ 0 & \text{for} \quad x > a \end{cases}$$

For the general solution, regions I, II, and III correspond to $x < 0$, $0 < x < a$, and $x > a$ respectively. The particle is also assumed to be traveling in the $+x$ direction with $E > V_o$. The general solution is then:

$$\begin{aligned} \psi_I(x) &= A\exp(ik_I x) + B\exp(-ik_I x) \\ \psi_{II}(x) &= F\exp(ik_{III} x) + G\exp(-ik_{III} x) \\ \psi_{III}(x) &= C\exp(ik_I x) \end{aligned}$$

where

$$\begin{aligned} k_I &= \sqrt{\frac{2mE}{\hbar^2}} \\ k_{III} &= \sqrt{\frac{2m(E - V_o)}{\hbar^2}} \end{aligned}$$

and $D = 0$ since the particle can not travel from $+x$ to $-x$ across the step at $x = a$. Utilizing boundary conditions for the continuity of $\psi(x)$ across the step at $x = 0$ and $x = a$, we obtain:

$$\begin{aligned} A + B &= F + G \\ F\exp(ik_{III} a) + G\exp(-ik_{III} a) &= C\exp(ik_I a) \end{aligned}$$

Similarly, boundary conditions for the continuity of $d\psi(x)/dx$ across the step at $x = 0$ and $x = a$ results in:

$$k_I A - k_I B = k_{III} F - k_{III} G$$
$$k_{III} F \exp(ik_{III} a) - k_{III} G \exp(-ik_{III} a) = k_I C \exp(ik_I a)$$

We can now start isolating variables to make these equations a little easier to work with. From the first boundary condition equations, we can write:

$$A + B - G = F$$

and

$$(A + B - G)\exp(ik_{III} a) + G\exp(-ik_{III} a) = C\exp(ik_I a) \quad (3)$$
$$\hookrightarrow A\exp(ik_{III} a) + B\exp(ik_{III} a) - G\left[\exp(ik_{III} a) - \exp(-ik_{III} a)\right] = C\exp(ik_I a) \quad (4)$$

Performing the same substitution with the second set of boundary conditions results in:

$$k_I A - k_I B = k_{III}(A + B - G) - k_{III} G \quad (5)$$
$$\hookrightarrow A(k_I - k_{III}) - B(k_I + k_{III}) = -2k_{III} G \quad (6)$$

and

$$k_{III}(A + B - G)\exp(ik_{III} a) - k_{III} G\exp(-ik_{III} a) = k_I C\exp(ik_I a) \quad (7)$$
$$\hookrightarrow k_{III} A\exp(ik_{III} a) + k_{III} B\exp(ik_{III} a) - k_{III} G\left[\exp(-ik_{III} a) + \exp(ik_{III} a)\right] = k_I C\exp(ik_I a) \quad (8)$$

From Equation 6, we can write:

$$G = -\frac{1}{2k_{III}}\left[A(ik_I - ik_{III}) - B(ik_I + ik_{III})\right]$$

We can then substitute this expression into Equation 4:

$$A\exp(ik_{III} a) + B\exp(ik_{III} a) + \frac{1}{2k_{III}}\left[A(ik_I - ik_{III}) - B(ik_I + ik_{III})\right] ... \quad (9)$$
$$\left[\exp(-ik_{III} a) - \exp(ik_{III} a)\right] = C\exp(ik_I a) \quad (10)$$
$$\hookrightarrow A\left[\left(\frac{1}{2} - \frac{k_I}{2k_{III}}\right)\exp(-ik_{III} a) + \left(\frac{1}{2} + \frac{k_I}{2k_{III}}\right)\exp(ik_{III} a)\right] + ... \quad (11)$$
$$B\left[\left(\frac{1}{2} + \frac{k_I}{2k_{III}}\right)\exp(-ik_{III} a) + \left(\frac{1}{2} - \frac{k_I}{2k_{III}}\right)\exp(ik_{III} a)\right] = C\exp(ik_I a) \quad (12)$$

Similarly, substituting the expression for G into Equation 8 gives:

$$k_{III} A\exp(ik_{III} a) + k_{III} B\exp(ik_{III} a) + \frac{1}{2}\left[A(ik_I - ik_{III}) - B(ik_I + ik_{III})\right] ... \quad (13)$$
$$\left[\exp(-ik_{III} a) + \exp(ik_{III} a)\right] = k_I C\exp(ik_I a) \quad (14)$$
$$\hookrightarrow A\left[\left(\frac{1}{2} - \frac{k_I}{2k_{III}}\right)\exp(-ik_{III} a) - \left(\frac{1}{2} + \frac{k_I}{2k_{III}}\right)\exp(ik_{III} a)\right] + ... \quad (15)$$
$$B\left[\left(\frac{1}{2} + \frac{k_I}{2k_{III}}\right)\exp(-ik_{III} a) - \left(\frac{1}{2} - \frac{k_I}{2k_{III}}\right)\exp(ik_{III} a)\right] = C\frac{k_I}{k_{III}}\exp(ik_I a) \quad (16)$$

Now that we have two equations with three unknowns, we can solve for coefficients and make substitutions to find the tunneling coefficient. If we rewrite Equation 12 in terms of B and define two terms (p and q) to aid in the algebra, we have:

$$
\begin{aligned}
p &= 1 + \frac{k_I}{k_{III}} \\
q &= 1 - \frac{k_I}{k_{III}} \\
\therefore B &= \frac{C \exp(ik_I a) - \frac{A}{2}\left[q \exp(-ik_{III}a) + p \exp(ik_{III}a)\right]}{p \exp(-ik_{III}a) + q \exp(ik_{III}a)}
\end{aligned}
$$

Substituting B into Equation 16 and rearranging to express A in terms of C results in:

$$
\begin{aligned}
&\left(\frac{p \exp(-ik_{III}a) - q \exp(ik_{III}a)}{p \exp(-ik_{III}a) + q \exp(ik_{III}a)}\right)\left(C \exp(ik_I a) - \frac{A}{2}\left[q \exp(-ik_{III}a) + p \exp(ik_{III}a)\right]\right) + ... \\
&\quad \frac{A}{2}\left[q \exp(-ik_{III}a) - p \exp(ik_{III}a)\right] = C\frac{k_I}{k_{III}} \exp(ik_I a) \\
&\hookrightarrow \frac{A}{2}\left(q \exp(-ik_{III}a) - p \exp(ik_{III}a)\right) - \frac{A}{2}\frac{p \exp(-ik_{III}a) - q \exp(ik_{III}a)}{p \exp(-ik_{III}a) + q \exp(ik_{III}a)} \times ... \\
&\quad \left(q \exp(-ik_{III}a) + p \exp(ik_{III}a)\right) = C\left(\frac{k_I}{k_{III}} - \frac{p \exp(-ik_{III}a) - q \exp(ik_{III}a)}{p \exp(-ik_{III}a) + q \exp(ik_{III}a)}\right) \exp(ik_I a)
\end{aligned}
$$

We can simplify this expression even more by multiplying out terms:

$$
\begin{aligned}
&A\left(\frac{q^2 - p^2}{p \exp(-ik_{III}a) + q \exp(ik_{III}a)}\right) = \\
&\quad C\left(\frac{p \exp(-ik_{III}a)\left[k_I - k_{III}\right] + q \exp(ik_{III}a)\left[k_I + k_{III}\right]}{k_{III}\left[p \exp(-ik_{III}a) + q \exp(ik_{III}a)\right]}\right) \exp(ik_I a) \\
&\left(\frac{C}{A}\right) = \frac{k_{III} \exp(-ik_I a)\left(q^2 - p^2\right)}{-\frac{p}{k_{III}} \exp(-ik_{III}a)\left[1 - \frac{k_I}{k_{III}}\right] + \frac{q}{k_{III}} \exp(ik_{III}a)\left[1 + \frac{k_I}{k_{III}}\right]} \\
&\left(\frac{C}{A}\right) = \frac{\exp(-ik_I a)\left(q^2 - p^2\right)}{-p^2 \exp(-ik_{III}a) + q^2 \exp(ik_{III}a)}
\end{aligned}
$$

With $q^2 - p^2 = -4k_I/k_{III}$, we have:

$$
\left(\frac{C}{A}\right) = \frac{4\frac{k_I}{k_{III}} \exp(-ik_I a)}{p^2 \exp(-ik_{III}a) - q^2 \exp(ik_{III}a)} \tag{17}
$$

Now that we have an expression for C/A, we need to substitute Equation 17 into the transmission coefficient equation[1] and replace p and q with their respective values:

$$\begin{aligned}
T &= \frac{v_I C^* C}{v_I A^* A} \\
&= \left(\frac{4\frac{k_I}{k_{III}} \exp(ik_I a)}{p^2 \exp(ik_{III}a) - q^2 \exp(-ik_{III}a)} \right) \left(\frac{4\frac{k_I}{k_{III}} \exp(-ik_I a)}{p^2 \exp(-ik_{III}a) - q^2 \exp(ik_{III}a)} \right) \\
&= \frac{16\left(\frac{k_I}{k_{III}}\right)^2}{\left(p^2 - q^2\right)^2 - p^2 q^2 \left[\exp(ik_{III}a) + \exp(-ik_{III}a)\right]^2} \\
&= \frac{16\left(\frac{k_I}{k_{III}}\right)^2}{16\left(\frac{k_I}{k_{III}}\right)^2 - p^2 q^2 \left[\exp(ik_{III}a) + \exp(-ik_{III}a)\right]^2}
\end{aligned}$$

Utilizing the p/q relationships in the denominator once more, we have:

$$T = \frac{16\left(\frac{k_I}{k_{III}}\right)^2}{16\left(\frac{k_I}{k_{III}}\right)^2 - \left(1 - \frac{k_I^2}{k_{III}^2}\right)^2 \left[\exp(ik_{III}a) + \exp(-ik_{III}a)\right]^2}$$

We can now use the relationship:

$$\left(\frac{k_I}{k_{III}}\right)^2 = \frac{E}{E - V_o}$$

to obtain a slightly modified version of Equation 6-51:

$$T = \left[1 - \frac{\left[\exp(ik_{III}a) + \exp(-ik_{III}a)\right]^2}{16\frac{E}{V_o}\left(\frac{E}{V_o} - 1\right)}\right]$$

Part B By substituting k_{II} with ik_{III} in Equation 6-49:

$$\begin{aligned}
T &= \left[1 - \frac{\left[\exp(k_{II}a) + \exp(-k_{II}a)\right]^2}{16\frac{E}{V_o}\left(\frac{E}{V_o} - 1\right)}\right] \\
&\Rightarrow \left[1 - \frac{\left[\exp(ik_{III}a) + \exp(-ik_{III}a)\right]^2}{16\frac{E}{V_o}\left(\frac{E}{V_o} - 1\right)}\right]
\end{aligned}$$

we have the same expression that was found in Part A. ■

[1] See E&R page 201 for this expression.

E&R - Ch. 6, Problem 8

The transmission coefficients from 6-49 and 6-50 are:

$$T = \left(1 + \frac{\sinh^2(k_{II}a)}{4\frac{E}{V_o}\left(1-\frac{E}{V_o}\right)}\right)^{-1} \tag{6-49}$$

$$T \approx 16\frac{E}{V_o}\left(1-\frac{E}{V_o}\right)\exp\left(-2k_{II}a\right) \tag{6-50}$$

Part A For a 2 eV electron incident on a rectangular potential barrier of height 4 eV and thickness 10^{-10} m, $k_{II}a$ is:

$$\begin{aligned}
k_{II}a &= \sqrt{\frac{2mV_oa^2}{\hbar^2}\left(1-\frac{E}{V_o}\right)} \\
&= \sqrt{\frac{2\cdot 9.1\times10^{-31}\cdot 4\cdot(10^{-10})^2\cdot 1.602\times10^{-19}}{(1.055\times10^{-34})^2}\left(1-\frac{2}{4}\right)} \\
&= 0.724
\end{aligned}$$

With this quantity, the transmission coefficient from 6-49 equals:

$$\begin{aligned}
T &= \left(1+\frac{\sinh^2(0.724)}{4\frac{2}{4}\left(1-\frac{2}{4}\right)}\right)^{-1} \\
&= 0.6164
\end{aligned}$$

and 6-50 equals:

$$\begin{aligned}
T &\approx 16\cdot\frac{2}{4}\left(1-\frac{2}{4}\right)\exp\left(-2\cdot 0.724\right) \\
&= 0.9402
\end{aligned}$$

The approximation for the transmission coefficient is not appropriate in this case since T is not very small.

Part B

$$\begin{aligned}
k_{II}a &= \sqrt{\frac{2\cdot 9.1\times10^{-31}\cdot 4\cdot(9\times10^{-9})^2\cdot 1.602\times10^{-19}}{(1.055\times10^{-34})^2}\left(1-\frac{2}{4}\right)} \\
&= 65.144 \\
T &= \left(1+\frac{\sinh^2(65.144)}{4\frac{2}{4}\left(1-\frac{2}{4}\right)}\right)^{-1} \\
&= 1.044\times10^{-56} \\
T &\approx 16\cdot\frac{2}{4}\left(1-\frac{2}{4}\right)\exp\left(-2\cdot 65.144\right) \\
&= 1.044\times10^{-56}
\end{aligned}$$

Part C

$$k_{II}a = \sqrt{\frac{2 \cdot 9.1 \times 10^{-31} \cdot 4 \cdot \left(10^{-9}\right)^2 \cdot 1.602 \times 10^{-19}}{\left(1.055 \times 10^{-34}\right)^2}\left(1 - \frac{2}{4}\right)}$$
$$= 7.238$$
$$T = \left(1 + \frac{\sinh^2(7.238)}{4\frac{2}{4}\left(1 - \frac{2}{4}\right)}\right)^{-1}$$
$$= 2.066 \times 10^{-6}$$
$$T \approx 16 \cdot \frac{2}{4}\left(1 - \frac{2}{4}\right)\exp\left(-2 \cdot 7.238\right)$$
$$= 2.066 \times 10^{-6}$$

■

E&R - Ch. 6, Problem 19

The standing wave general solution is:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

To verify that this is a valid solution, we need to substitute it into the time-independent Schrödinger equation (TISE) and determine if an equality exists. Looking at the second spatial derivative, we have:

$$\frac{d^2\psi(x)}{dx^2} = -Ak^2\sin(kx) - Bk^2\cos(kx)$$

The TISE for the standing wave general solution is then:

$$-\frac{\hbar^2}{2m}\left(-Ak^2\sin(kx) - Bk^2\cos(kx)\right) = E\psi(x)$$
$$\frac{\hbar^2k^2}{2m}\left(A\sin(kx) + B\cos(kx)\right) = E\psi(x)$$
$$\frac{\hbar^2k^2}{2m}\psi(x) = E\psi(x)$$

Therefore, the standing wave general solution is a solution to the Schrödinger equation due to the existence of valid eigenvalues (or energy values):

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

■

Problem 5

In this problem, we consider an infinite spherical potential well with the following properties:

$$V(r) = \begin{cases} 0 & \text{for } \ 0 < r < r_o \\ \infty & \text{for } \quad r > r_o \end{cases}$$

In the lowest energy state, we know that $n = 1$ and $l, m_l = 0$. Inside the spherical well, we also have $V = 0$. With these values, the spherical form of the time-independent Schrödinger wave equation can be simplified:

$$\begin{aligned} \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu r^2}{\hbar^2}E &= \frac{m_l^2}{\sin^2(\theta)} - \frac{1}{\Theta\sin(\theta)}\frac{d}{d\theta}\left(\sin(\theta)\frac{d\Theta}{d\theta}\right) \\ \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu R}{\hbar^2}E &= l(l+1)\frac{R}{r^2} \\ \Rightarrow \frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu R}{\hbar^2}E &= 0 \end{aligned}$$

We can utilize the definitions provided in the problem, namely that the radial wave function $R(r) = \chi(r)/r$. Evaluating the derivative on the right hand side, we have:

$$\begin{aligned} \frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{d}{dr}\left(\frac{\chi(r)}{r}\right)\right] + \frac{2\mu\chi(r)}{\hbar^2 r}E &= 0 \\ \frac{1}{r^2}\frac{d}{dr}\left[r^2\left(\frac{1}{r}\frac{d\chi(r)}{dr} - \frac{\chi(r)}{r^2}\right)\right] + \frac{2\mu\chi(r)}{\hbar^2 r}E &= 0 \\ \frac{1}{r^2}\left(\frac{d^2\chi(r)}{dr^2}r + \frac{d\chi(r)}{dr} - \frac{d\chi(r)}{dr}\right) + \frac{2\mu\chi(r)}{\hbar^2 r}E &= 0 \\ \Rightarrow \frac{d^2\chi(r)}{dr^2} + \frac{2\mu}{\hbar^2}E\chi(r) &= 0 \end{aligned}$$

The final equation is nearly identical in form to the rectangular Schrödinger equation in free space. Utilizing the boundary conditions, $\chi(r = r_o) = 0$ and $\chi(0) = 0$, we find that the problem is similar to that of a infinite 1-D potential well which has the well known eigenenergy value:

$$E_n = \frac{\hbar^2 k_n^2}{2\mu}$$

where $k_n = \frac{n\pi}{r_o}$ for the infinite spherical well. For the case of $n = 1$,

$$\boxed{E = \frac{\hbar^2\pi^2}{2\mu r_o^2} \quad \text{for the lowest energy state.}}$$

■

Problem 6

The wave equation for the ground state of the hydrogen atom ($Z = 1$) and potential is:

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2}\exp\left(\frac{-r}{a_o}\right)$$
$$V(r) = \frac{-q^2}{4\pi\epsilon_o r}$$

where a_o is the Bohr radius and equal to:

$$\frac{4\pi\epsilon_o\hbar^2}{\mu q^2}$$

Part A The expectation value for potential, $\langle V\rangle$, is:

$$\langle V\rangle = \int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\psi_{100}^*(r)V(r)\psi_{100}(r)r^2\sin(\theta)drd\theta d\phi$$

If we take out constants, the integral can be simplified to:

$$\begin{aligned}\langle V\rangle &= -\frac{q^2}{4\pi^2\epsilon_o a_o^3}\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}\exp\left(\frac{-r}{a_o}\right)\cdot\frac{1}{r}\cdot\exp\left(\frac{-r}{a_o}\right)r^2\sin(\theta)drd\theta d\phi\\ &= -\frac{q^2}{4\pi^2\epsilon_o a_o^3}\int_{r=0}^{\infty}\int_{\theta=0}^{\pi}\int_{\phi=0}^{2\pi}r\exp\left(\frac{-2r}{a_o}\right)\sin(\theta)drd\theta d\phi\end{aligned}$$

Evaluating the $d\theta$ and $d\phi$ parts of the integal, we have:

$$\langle V\rangle = -\frac{q^2}{4\pi^2\epsilon_o a_o^3}(4\pi)\int_{r=0}^{\infty}r\exp\left(\frac{-2r}{a_o}\right)dr$$

The last simplification is to do a substitution with $u = 2r/a_o$, so:

$$\begin{aligned}u &= \frac{2r}{a_o}\\ du &= \frac{2}{a_o}dr\\ \hookrightarrow dr &= \frac{a_o}{2}du\end{aligned}$$

The integral then becomes:

$$\begin{aligned}\langle V\rangle &= -\frac{q^2}{\pi\epsilon_o a_o^3}\int_{r=0}^{\infty}\frac{a_o u}{2}\exp(-u)\frac{a_o du}{2}\\ &= -\frac{q^2}{4\pi\epsilon_o a_o}\int_{r=0}^{\infty}u\exp(-u)\,du\\ &= -\frac{q^2}{4\pi\epsilon_o a_o}\end{aligned}$$

since $\int_{r=0}^{\infty}u\exp(-u)\,du = 1$. Substituting in the Bohr radius, we obtain:

$$\boxed{\langle V\rangle = -\frac{\mu q^4}{(4\pi\epsilon_o)^2\hbar^2}}$$

Part B From Equation 7-22, the energy of the hydrogen atom is:

$$E_n = -\frac{\mu q^4}{(4\pi\epsilon_o)^2 \, 2\hbar^2 n^2}$$

For $n = 1$, we see that $E_1 = \langle V \rangle / 2$.

Part C For total energy, we have $E = K + V$. Using the expectation value from before, total energy can be expressed as a sum of the expectation values for potential and kinetic energy:

$$E = \langle K \rangle + \langle V \rangle$$

But,

$$E = \frac{\langle V \rangle}{2}$$

So we have:

$$\frac{\langle V \rangle}{2} = \langle K \rangle + \langle V \rangle$$

Therefore,

$$\boxed{\langle K \rangle = -\frac{\langle V \rangle}{2}}$$

■