Physics 606

Quantum Mechanics I

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Homework #4

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1 Problem #1

For a step potential given by

$$U(x) = \begin{cases} 0 & x < 0 \\ U_0 & x > 0 \end{cases}$$

with an energy, E, in the range: $0 < E < U_0$. We see that we have two regions, region I is $x < 0$ and region II is given by $x > 0$. In the region I we have a free particle with a wave-function

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx}$$

where the positive exponent is related to the right moving incident wave and the negative exponent is the left moving reflection wave. We note that k is given by

$$k = \frac{\sqrt{2\mu E}}{\hbar}.$$

Then for region II we note that $U_0 > E$ which yields an exponential decay given by

$$\psi_{II}(x) = Ce^{-\kappa x}$$

where κ is a real positive constant given by

$$\kappa = \frac{\sqrt{2\mu(U_0 - E)}}{\hbar}.$$

We need to use the continuity of the wave-function and it's derivative to find the coefficients A, B, and C. First we see that the wave-function at $x = 0$

$$\begin{gathered} \psi_I(x=0) = \psi_{II}(x=0) \\ \Downarrow \\ Ae^{ik0} + Be^{-ik0} = Ce^{-\kappa 0} \\ A + B = C \end{gathered}$$

then we take the first spacial derivative of the wave-function at $x = 0$ as

$$\begin{gathered} \psi_I'(x=0) = \psi_{II}'(x=0) \\ \Downarrow \\ A(ik)e^{ik0} + B(-ik)e^{-ik0} = C(-\kappa)e^{-\kappa 0} \\ ik(A - B) = -\kappa C \end{gathered}$$

Using these two continuity conditions we can calculate the reflection by noting that $|B|^2$ is the magnitude of the reflected wave which implies that

$$\text{Reflection Coefficient} \rightarrow R \equiv \left|\frac{B}{A}\right|^2$$

So we can solve for the ratio by

$$
\begin{aligned}
ik(A-B) &= -\kappa C \\
ik(A-B) &= -\kappa(A+B) \\
\frac{ik}{\kappa}A - \frac{ik}{\kappa}B &= -A - B \\
\frac{ik}{\kappa}A + A &= \frac{ik}{\kappa}B - B \\
\left(\frac{ik}{\kappa}+1\right)A &= \left(\frac{ik}{\kappa}-1\right)B
\end{aligned}
$$

$$\Downarrow$$

$$\frac{B}{A} = \frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}$$

So we can calculate the magnitude squared by

$$
\begin{aligned}
R = \left|\frac{B}{A}\right|^2 &= \left(\frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}\right)\left(\frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}\right)^* \\
&= \left(\frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}\right)\left(\frac{-\frac{ik}{\kappa}+1}{-\frac{ik}{\kappa}-1}\right) \\
&= \frac{\frac{k^2}{\kappa^2}+1}{\frac{k^2}{\kappa^2}+1} = 1
\end{aligned}
$$

We note that for an infinitely deep potential barrier where we have an energy less that the barrier potential we have complete reflection. We can also think about limiting cases the first being when $E \to \infty$ we see that in this limit we have $E >> U_0$ which makes

$$\lim_{E\to\infty} \kappa = \lim_{E\to\infty} \sqrt{2\mu(U_0-E)}/\hbar = i\sqrt{2\mu E}/\hbar = ik$$

so we see that in the limit

$$
\begin{aligned}
\lim_{E\to\infty} R = \lim_{E\to\infty}\left|\frac{B}{A}\right|^2 &= \lim_{E\to\infty}\left(\frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}\right)\left(\frac{\frac{ik}{\kappa}+1}{\frac{ik}{\kappa}-1}\right)^* \\
&= \left(\frac{\frac{ik}{ik}+1}{\frac{ik}{ik}-1}\right)\left(\frac{\frac{ik}{ik}+1}{\frac{ik}{ik}-1}\right)^* \\
&= \left(\frac{2}{1-1}\right)\left(\frac{2}{1-1}\right)^* = 0
\end{aligned}
$$

So we see that as we go to infinite energy the barrier becomes infinitely small. This implies that the reflection coefficient becomes zero or we have no reflected wave. In the other limit where $E \to U_0$ we see that the wave-function in region II becomes constant because

$$\kappa = \frac{\sqrt{2\mu(U_0-U_0)}}{\hbar} = 0$$

so ψ_{II} becomes

$$\psi_{II} = Ce^{0x} = C$$

So the continuity conditions become

$$A + B = C$$
$$A - B = 0$$

So we see that $A = B$ which implies that for $E \to U_0$ we have a reflection coefficient, R, is still unity. So for up to $E = U_0$ we have full reflection if our step potential is infinitely deep.

2 Problem #2

For a two-dimensional potential well with absolutely impermeable walls we have a potential given by

$$U(x,y) = \begin{cases} 0 & 0 < x < a \\ \infty & x > a \text{ and } x < 0 \\ 0 & 0 < y < b \\ \infty & y > b \text{ and } y < 0 \end{cases}$$

We can take the overall wave function as the product of the two individual solutions as

$$\Psi(x,y) = \psi_n(x)\psi_m(y)$$

where ψ_n are the normalized eigenfunction of the one-dimensional infinite square well given by

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$
$$\psi_m(y) = \sqrt{\frac{2}{b}} \sin\left(\frac{m\pi}{b}y\right)$$

So we can write the overall wave function as

$$\Psi(x,y) = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right)$$

in the domain where $0 < x < a$ and $0 < y < b$. We note that $\Psi(x,y) = 0$ everywhere else. This allows us to find the probability of finding a particle in the region $a/3 \le x \le 2a/3, b/3 \le y \le 2b/3$ by integrating the probability density function given by $\Psi^*(x,y)\Psi(x,y)$ over this domain

$$\begin{aligned}
\int_{a/3}^{2a/3}\int_{b/3}^{2b/3} \Psi^*(x,y)\Psi(x,y)dydx &= \int_{a/3}^{2a/3}\int_{b/3}^{2b/3} \left(\sqrt{\frac{2}{a}}\sqrt{\frac{2}{b}} \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{b}y\right)\right)^2 dydx \\
&= \frac{4}{ab}\int_{a/3}^{2a/3} \sin^2\left(\frac{n\pi}{a}x\right)dx \int_{b/3}^{2b/3} \sin^2\left(\frac{m\pi}{b}y\right)dy \\
&= \frac{4}{ab}\int_{a/3}^{2a/3} \frac{1}{2}\left(1-\cos\left(2\frac{n\pi}{a}x\right)\right)dx \int_{b/3}^{2b/3} \frac{1}{2}\left(1-\cos\left(2\frac{m\pi}{b}y\right)\right)dy \\
&= \frac{1}{ab}\left(x - \frac{a}{2n\pi}\sin\left(2\frac{n\pi}{a}x\right)\right|_{a/3}^{2a/3}\left(y - \frac{2m\pi}{b}\sin\left(2\frac{m\pi}{b}y\right)\right|_{b/3}^{2b/3} \\
&= \frac{1}{ab}\left(\frac{2a}{3} - \frac{a}{2n\pi}\sin\left(2\frac{n\pi}{a}\frac{2a}{3}\right) - \frac{a}{3} + \frac{a}{2n\pi}\sin\left(2\frac{n\pi}{a}\frac{a}{3}\right)\right) \\
&\quad \times \left(\frac{2b}{3} - \frac{b}{2m\pi}\sin\left(2\frac{m\pi}{b}\frac{2b}{3}\right) - \frac{b}{3} + \frac{b}{2m\pi}\sin\left(2\frac{m\pi}{b}\frac{b}{3}\right)\right) \\
&= \left(\frac{1}{3} - \frac{1}{2n\pi}\sin\left(\frac{4n\pi}{3}\right) + \frac{1}{2n\pi}\sin\left(\frac{2n\pi}{3}\right)\right) \\
&\quad \times \left(\frac{1}{3} - \frac{1}{2m\pi}\sin\left(\frac{4m\pi}{3}\right) + \frac{1}{2m\pi}\sin\left(\frac{2m\pi}{3}\right)\right)
\end{aligned}$$

We note that the probability depends on which state we are in. If we take the particle to be in the ground state which implies that $n = m = 1$ so we calculate

$$
\begin{aligned}
&= \left(\frac{1}{3} - \frac{1}{2n\pi}\sin\left(\frac{4n\pi}{3}\right) + \frac{1}{2n\pi}\sin\left(\frac{2n\pi}{3}\right)\right)\left(\frac{1}{3} - \frac{1}{2m\pi}\sin\left(\frac{4m\pi}{3}\right) + \frac{1}{2m\pi}\sin\left(\frac{2m\pi}{3}\right)\right) \\
&\Downarrow \\
&= \left(\frac{1}{3} - \frac{1}{2\pi}\sin\left(\frac{4\pi}{3}\right) + \frac{1}{2\pi}\sin\left(\frac{2\pi}{3}\right)\right)\left(\frac{1}{3} - \frac{1}{2\pi}\sin\left(\frac{4\pi}{3}\right) + \frac{1}{2\pi}\sin\left(\frac{2\pi}{3}\right)\right) \\
&= \frac{1}{9} + \frac{3}{4\pi^2} + \frac{\sqrt{3}}{3\pi} \approx 0.37
\end{aligned}
$$

3 Problem #3

For a particle of mass m_0 in a potential well given by

$$U(x) = \begin{cases} \infty, & x < 0 \\ 0, & 0 < x < a \\ U_0, & x > a \end{cases}$$

with an energy, $E < U_0$. We see that there are three distinct regions for this particle we note that for an infinite potential $\psi(x) = 0$ with a discontinuous first spacial derivative. We then see that for the zero potential we assume we have an oscillating wave-function and in the region $x > a$ we have an exponential decay. So our wave function is given by

$$\psi(x) = \begin{cases} 0, & x < 0 \\ A\sin(kx + \delta), & 0 < x < a \\ Be^{-\kappa x}, & x > a \end{cases}$$

Where k and κ are real and positive valued given by

$$\begin{aligned} k &= \frac{\sqrt{2m_0 E}}{\hbar} \\ \kappa &= \frac{\sqrt{2m_0(U_0 - E)}}{\hbar} = \sqrt{\frac{2m_0 U_0}{\hbar^2} - k^2} \end{aligned}$$

Next, we apply the continuity condition at $x = 0$ to see

$$\begin{aligned} \psi_I(x = 0) &= \psi_{II}(x = 0) \\ &\Downarrow \\ 0 &= A\sin(k0 + \delta) \\ 0 &= \sin(\delta) \qquad \Downarrow \\ \delta &= 0 \end{aligned}$$

Next we have the continuity of the wave-function and its derivative at $x = a$ to get

$$\begin{aligned} \psi_{II}(x = a) &= \psi_{III}(x = a) \\ &\Downarrow \\ A\sin(ka) &= Be^{-\kappa a} \end{aligned}$$

and

$$\begin{aligned} \psi'_{II}(x = a) &= \psi'_{III}(x = a) \\ &\Downarrow \\ Ak\cos(ka) &= -B\kappa e^{-\kappa a} \end{aligned}$$

We can divide the two continuity relations to yield

$$\begin{aligned} \frac{Ak\cos(ka)}{A\sin(ka)} &= \frac{-B\kappa e^{-\kappa a}}{Be^{-\kappa a}} \\ k\cot(ka) &= -\kappa \\ &\Downarrow \\ ka &= -\text{arccot}\left(\sqrt{\frac{2m_0 U_0}{\hbar^2 k^2} - 1}\right) \end{aligned}$$

So we note the relation between arccot(x) and arcsin(x) is

$$\operatorname{arccot}(x) = n\pi - \arcsin\left(\sqrt{\frac{1}{x^2+1}}\right)$$

which uses the periodicity of the cot function. This identity yields

$$\begin{aligned}
ka &= n\pi - \arcsin\left(\sqrt{\frac{1}{\frac{2m_0U_0}{\hbar^2k^2} - 1 + 1}}\right) \\
ka &= n\pi - \arcsin\left(\frac{\hbar k}{\sqrt{2m_0U_0}}\right)
\end{aligned}$$

We next note that for a discrete spectrum to have a condition on k such that

$$k < \sqrt{\frac{2m_0U_0}{\hbar}}.$$

Therefore, we can see in the limiting case where $k = \sqrt{2m_0U_0}/\hbar$ we can find the total number of discrete states n by

$$\begin{aligned}
a\frac{\sqrt{2m_0U_0}}{\hbar} &= n\pi - \arcsin\left(\frac{\hbar k}{\sqrt{2m_0U_0}}\frac{\sqrt{2m_0U_0}}{\hbar}\right) \\
a\frac{\sqrt{2m_0U_0}}{\hbar} &= n\pi - \arcsin(1) \\
a\frac{\sqrt{2m_0U_0}}{\hbar} &= n\pi - \frac{\pi}{2} \\
&\Downarrow \\
n &= \frac{\sqrt{2m_0a^2U_0}}{\hbar\pi}
\end{aligned}$$

And for for $a^2U_0 = 110\hbar^2/m_0$ we can find the number of states as

$$\begin{aligned}
n &= \frac{\sqrt{2m_0a^2U_0}}{\hbar\pi} \\
&\Downarrow \\
n &= \sqrt{\frac{2m_0}{\hbar^2\pi^2}\frac{110\hbar^2}{m_0}} \\
&= \frac{\sqrt{220}}{\pi} \approx 4.7
\end{aligned}$$

This implies that for the given energy there are four discrete states.

4 Problem #4

For the triangle potential barrier given by

$$U(x) = \begin{cases} 0 & x < -a \\ \frac{U_0}{a}x + U_0 & -a < x < 0 \\ -\frac{U_0}{a}x + U_0 & 0 < x < a \\ 0 & x > a \end{cases}$$

we can calculate the transmission coefficient, D, for a particle of mass m_0 by the equation given by the quasiclassical approximation.

$$D = \exp\left(-\frac{2}{\hbar}\int_{x_1}^{x_2}\sqrt{2m_0(U(x)-E)}dx\right) \tag{4.1}$$

where x_1 and x_2 are the classical turning points given when $E = U(x)$. Which we can find as

$$\begin{aligned} E &= \frac{U_0}{a}x_1 + U_0 \\ &\Downarrow \\ x_1 &= \frac{a}{U_0}(E - U_0) \\ &= a\left(\frac{E}{U_0} - 1\right) \end{aligned}$$

and

$$\begin{aligned} E &= -\frac{U_0}{a}x_2 + U_0 \\ &\Downarrow \\ x_2 &= -\frac{a}{U_0}(E - U_0) \\ &= a\left(1 - \frac{E}{U_0}\right) \end{aligned}$$

Now, we can calculate the integral in equation 4.1 by

$$\begin{aligned} \int_{x_1}^{x_2}\sqrt{2m_0(U(x)-E)}dx &= \sqrt{2m_0}\int_{x_1}^{0}\sqrt{\frac{U_0}{a}x + U_0 - E}dx + \sqrt{2m_0}\int_{0}^{x_2}\sqrt{-\frac{U_0}{a}x + U_0 - E}dx \\ &= \sqrt{2m_0}\left(\frac{2a}{3U_0}\left(\frac{U_0}{a}x + U_0 - E\right)^{3/2}\right|_{x_1}^{0} + \sqrt{2m_0}\left(-\frac{2a}{3U_0}\left(-\frac{U_0}{a}x + U_0 - E\right)^{3/2}\right|_{0}^{x_2} \\ &= \sqrt{2m_0}\frac{2a}{3U_0}\left((U_0 - E)^{3/2} + (U_0 - E)^{3/2}\right) \\ &= \frac{4a\sqrt{2m_0}}{3U_0}(U_0 - E)^{3/2} \end{aligned}$$