T06

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<u>Problem 6.2:</u>

We have the travelling Gaussian wave function

$$\psi(x,0) = \frac{1}{\pi^{1/4}\, l_{ho}^{1/2}} e^{-x^2/2l_{ho}^2} e^{ik_0x}$$

where k_0 is a real constant

a. By Eq 2.104 in the text,

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,0) e^{-ikx}\, dx$$

Substituting in $\psi(x,0)$:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\pi^{1/4} l_{ho}^{1/2}} e^{-x^2/2l_{ho}^2} e^{ik_0x} e^{-ikx}\, dx$$

$$= \frac{1}{\sqrt{2\pi l_{ho}\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-x^2/2l_{ho}^2 - ix(k-k_0)}\, dx$$

By Eq (13) in the formula sheet,

$$\int_{-\infty}^{\infty} e^{-iax} e^{-\frac{x^2}{b^2}}\, dx = b\sqrt{\pi}\, e^{-\frac{1}{4}a^2b^2}$$

which is of the form of the exponential integral above, with

$a = (k-k_0)$ and $b = \sqrt{2}\, l_{ho}$

So, the equation is

$$\phi(k) = \frac{1}{\sqrt{2\pi l_{ho}\sqrt{\pi}}} \sqrt{2\pi}\, l_{ho}\, e^{-\frac{1}{2}(k-k_0) l_{ho}^2}$$

$$= \frac{2\pi\sqrt{l_{ho}\sqrt{\pi}}}{2\pi\, l_{ho}\sqrt{\pi}}\, l_{ho}\, e^{-\frac{1}{2}(k-k_0)l_{ho}^2}$$

$$= \sqrt{\frac{l_{ho}}{\sqrt{\pi}}}\, e^{-\frac{1}{2}(k-k_0)l_{ho}^2}$$

Using this, the wavefunction in terms of t can be found by

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk$$

Substituting in $\phi(k)$,

$$\psi(x,t) = \sqrt{\frac{l_{ho}}{2\pi\sqrt{\pi}}} \int_{-\infty}^{\infty} e^{-\frac{1}{2}(k-k_0)l_{ho}^2 + i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk$$

Looking at the exponent only:

$$-\frac{1}{2}(k-k_0)l_{ho}^2 + ikx - k^2\frac{i\hbar}{2m}t = \frac{1}{2}k_0 l_{ho}^2 - ik\left(-x - \frac{1}{2}i l_{ho}^2\right)$$

$$- k^2\left(\sqrt{2m}\right)^{-2}$$

$$-\frac{1}{2}(k-k_0)l_{ho}^2 + ikx - k^2\frac{i\hbar}{2m}t = \frac{1}{2}k_0 l_{ho}^2 - ik\left(-x-\frac{1}{2}il_{ho}^2\right) - k^2\left(\sqrt{\frac{2m}{i\hbar t}}\right)^{-2}$$

Therefore the exponential integral is

$$e^{\frac{1}{2}k_0 l_{ho}^2}\int_{-\infty}^{\infty} e^{-ik(-x-\frac{1}{2}il_{ho}^2)} e^{-\frac{k^2}{(\sqrt{\frac{2m}{i\hbar t}})^2}}\,dk$$

(which is of the same form as Eq (13) from the tutorial sheet, with solution)

$$\int_{-\infty}^{\infty} e^{-ik(-x-\frac{1}{2}il_{ho}^2)} e^{-\frac{k^2}{(\sqrt{\frac{2m}{i\hbar t}})^2}}\,dk = \sqrt{\frac{2m}{i\hbar t}}\sqrt{\pi}\, e^{-\frac{1}{4}(-x-\frac{1}{2}il_{ho}^2)^2\times\frac{2m}{i\hbar t}}$$

$$= \sqrt{\frac{2m\pi}{i\hbar t}}\exp\left(-\frac{m(x^2+xil_{ho}^2-\frac{1}{4}l_{ho}^4)}{2i\hbar t}\right)$$

Therefore the wavefunction, $\Psi(x,t)$, becomes

$$\Psi(x,t) = \sqrt{\frac{l_{ho}}{2\pi\sqrt{\pi}}}\, e^{l_{ho}^2\left(\frac{1}{2}k_0+\frac{m l_{ho}^2}{8i\hbar t}\right)}\sqrt{\frac{2m\pi}{i\hbar t}}\, e^{-\frac{m(x^2+ixl_{ho}^2)}{2i\hbar t}}$$

$$\Psi(x,t) = \sqrt{\frac{l_{ho}m}{i\sqrt{\pi}\hbar t}}\, e^{l_{ho}^2\left(\frac{1}{2}k_0+\frac{m l_{ho}^2}{8i\hbar t}\right)} e^{\frac{-m(x^2+ixl_{ho}^2)}{2i\hbar t}}$$

Define $a \equiv \frac{1}{2}l_{ho}^2$ and $\theta \equiv \frac{2\hbar a t}{m} = \frac{\hbar l_{ho}^2 t}{m}$

as well as $w \equiv \sqrt{\frac{a}{1+\theta^2}}$

- I don't have the time to finish Problem 6.2. I know that it's good practice but I've already put too much time into this assignment for only 4%.

Problem 6.5:

- The step potential is given by:

$$V(x) = \begin{cases} 0 & x \leq 0 \\ V_0 & x > 0 \end{cases}$$

a. The wavefunction in this case consists of a superposition of a forward and backward travelling wave, for both regions of the potential.

For the region $x \leq 0$ (i.e for the free particle)

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

(Solution to Schrodinger Eq of $\frac{\partial^2\psi}{\partial x^2} = -k_1^2\psi$)

where $k_1 = \frac{\sqrt{2mE}}{\hbar}$

In terms of trigonometric functions,

$$\psi_1(x) = (A+B)\cos(k_1x) + i(A-B)\sin(k_1x)$$

The case for $x > 0$ is analogous, albeit with different coefficients and energies

(Solution to Schrodinger Eq of)

The case for $x>0$ is analogous, albeit with different coefficients and energies

$$\psi_2(x) = Ce^{-k_2 x} + De^{k_2 x}$$ (Solution to Schrodinger Eq of $\frac{\partial^2 \psi}{\partial x^2} = k_2^2 \psi$)

where $k_2 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

Since the particle is free for $x \le 0$, $E > 0$.
The coefficient A is the incident amplitude, B the reflected amplitude, C is the transmitted amplitude, and $D=0$ (since particle coming from left).

Therefore the wavefunction in terms of x is

$$\psi(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x \le 0 \\ Ce^{-k_2 x} & x > 0 \end{cases}$$

There are two boundary conditions at $x=0$:

$$\psi_1(0) = \psi_2(0) \quad (1)$$

and $$\frac{\partial}{\partial x}\psi_1(0) = \frac{\partial}{\partial x}\psi_2(0) \quad (2)$$

Evaluating the first boundary condition gives

$$\psi_1(0) = \psi_2(0)$$

$$\Rightarrow Ae^0 + Be^0 = Ce^0$$

$$\Rightarrow A+B = C \quad (*)$$

Evaluating the second boundary condition gives

$$-ik_1(A-B) = -k_2 C$$

$$\Rightarrow k_1(A-B) = ik_2 C \quad (**)$$

We want the reflection coefficient

$$R = \frac{|B|^2}{|A|^2}$$

So divide $(*)$ by $(**)$ and rearrange:

$$\frac{A+B}{k_1(A-B)} = \frac{C}{ik_2 C}$$

$$\Rightarrow A+B = \frac{k_1}{ik_2}(A-B)$$

$$1 + \frac{B}{A} = \frac{k_1}{ik_2}\left(1 - \frac{B}{A}\right)$$

$$\Rightarrow 1 + \frac{B}{A} = -\frac{k_1}{ik_2}\frac{B}{A} + \frac{k_1}{ik_2}$$

$$\Rightarrow \frac{B}{A} + \frac{k_1}{ik_2}\frac{B}{A} = \frac{k_1}{ik_2} - 1$$

$$\Rightarrow \frac{B}{A}\left(1 + \frac{k_1}{ik_2}\right) = \frac{k_1}{ik_2} - 1$$

$$\frac{B}{A} = \frac{\left(\frac{k_1}{ik_2} - 1\right)}{\left(1 + \frac{k_1}{ik_2}\right)}$$

$$\Rightarrow \left(\frac{B}{A}\right)^2 = \frac{|B|^2}{|A|^2} = \frac{\left|\frac{k_1}{ik_2} - 1\right|^2}{\left|\frac{k_1}{ik_2} + 1\right|^2} = \frac{\left|-\frac{k_1}{k_2}i - 1\right|^2}{\left|1 - \frac{k_1}{k_2}i\right|^2} \quad (\Delta)$$

Since both k_1 and k_2 are real ($E>0$, $m>0$, $V_0>E$

Since both k_1 and k_2 are real ($E>0$, $m>0$, $V_0>E \Rightarrow V_0-E>0$),
wolfram alpha gives $(\Delta)=1$

Therefore $R=1$

Intuitively, this makes sense. The particle does not have enough energy to overcome the potential ($E<V_0$) and so it will always be reflected.

b. This case is (mostly) analogous to the first part, albeit with a different solution to ψ_2

$$\Rightarrow \quad \frac{\partial \psi^2}{\partial x^2} = -\left(\frac{2m(E-V_0)}{\hbar^2}\right)\psi = -k_3^2\psi$$

$$\Rightarrow \quad \psi_2(x) = Ce^{-ik_3x} \qquad \text{where } k_3 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

Easy to see (from **) that the i can be omitted, and $k_2 \rightarrow k_3$. (**) becomes

$$k_1(A-B) = k_3C$$

$$\Rightarrow \quad A-B = \frac{k_3}{k_1}(A+B)$$

$$\Rightarrow \quad 1-\frac{B}{A} = \frac{k_3}{k_1}\left(1+\frac{B}{A}\right)$$

$$\frac{B}{A}\left(1+\frac{k_3}{k_1}\right) = 1-\frac{k_3}{k_1}$$

$$\Rightarrow \quad \frac{B}{A} = \frac{1-\frac{k_3}{k_1}}{1+\frac{k_3}{k_1}} = \frac{k_1-k_3}{k_1+k_3}$$

To help simplify this later, multiply by $\frac{(k_1-k_3)^2}{(k_1-k_3)^2}$

$$\Rightarrow \quad \frac{B^2}{A^2} = \frac{(k_1-k_3)^2}{(k_1+k_3)^2}\frac{(k_1-k_3)^2}{(k_1-k_3)^2} = \frac{(k_1-k_3)^4}{(k_1^2-k_3^2)^2}$$

With these powers, $\frac{2m}{\hbar}$ cancels out of k_1 and k_3, leaving

$$\frac{B^2}{A^2} = \frac{(\sqrt{E}-\sqrt{E-V_0})^4}{(E-E+V_0)^2}$$

$$= \frac{(\sqrt{E}-\sqrt{E-V_0})^4}{V_0^2}$$

Easy to see that both numerator and denominator are positive and real (since $E>V_0$)

$$\Rightarrow \quad \frac{B^2}{A^2} = \frac{|B|^2}{|A|^2} = R = \frac{(\sqrt{E}-\sqrt{E-V_0})^4}{V_0^2}$$