PHYS 4380 Quantum Mechanics I

Homework Assignment 11

Due date: November 29, 2018

Instructor: Dr. Daniel Erenso Name: ____________________

Mandatory problems: 2 & 5

Student signature:____

Student Comment:_____________________________________
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Problem #	1	2	3	4	5	Score
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1. *This is example we partially did in class. You need to work out only part (e), (f), (g) (h), and (i) Particle in a one-dimensional box:* Consider a particle of mass m in a potential defined by

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

(a) Find the energy eigenvalues and eigen functions.

(b) Verify that if the energy eigen functions are orthogonal.

(c) Are the energy eigen functions orthonormal. If not normalize it.

(d) For the ground state find the energy, the expectation value for $\langle p_x \rangle, \langle p_x^2 \rangle$, and the uncertainty Δp_x.

(e) Suppose the width of the box is $1mm$, roughly, what value of n corresponds to the state of $0.01ev$ if the particle is an electron. How cold the electron must be to be in this state (i.e. find T)

(f) Calculate the density of states in the vicinity of $0.01eV$. What is the number of states within the interval of $0.0001eV$ about the energy of $0.01eV$. Hint: Density of state is given by dn/dE.

(g) By plotting the energy eigen functions for the ground state and the first few excited state and observing the symmetry determine the eigen function for a particle of mass m in a potential $V(x)$ defined by

$$V(x) = \begin{cases} \infty & x < -a/2 \\ 0 & -a/2 < x < a/2 \\ \infty & a/2 < x \end{cases}$$

(h) For the ground state find the expectation value for $\langle x \rangle, \langle x^2 \rangle$, and the uncertainty Δx.

(i) Using the results in part (d) and (h) show that $\Delta x \Delta p_x > \frac{\hbar}{2}$.

Solution:

(a) The energy eigenvalue equation in the region, $0 < x < a$, can be expressed as

$$-\frac{\hbar^2}{2m}\frac{d^2 u(x)}{dx^2} = Eu(x), \tag{1}$$

which can be expressed as

$$\frac{d^2 u(x)}{dx^2} + q^2 u(x) = 0, \tag{2}$$

where

$$q^2 = \frac{2mE}{\hbar^2}. \tag{3}$$

The solution to Eq. (3) is given by

$$u(x) = A\cos(qx) + B\sin(qx). \tag{4}$$

Since the particle can not exist outside the box the eigen function must vanish at the boundaries,

$$u(0) = 0 \Rightarrow A = 0, u(a) = 0 \Rightarrow B\sin(qa) = 0 \Rightarrow q = \frac{n\pi}{a}, n = 1, 2, 3... \tag{5}$$

Therefore the eigen function and the corresponding eigen values are discrete and are given by

$$u_n(x) = B_n \sin\left(\frac{n\pi}{a}x\right), E_n = \frac{\pi^2\hbar^2 n^2}{2ma^2}. \tag{6}$$

(b) If the energy eigen functions are orthogonal it must satisfy the condition (*From Theoretical Physics 1*)

$$\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \begin{cases} const & n = m \\ 0 & n \neq m \end{cases} \tag{7}$$

Using the eigen function in part (a) we have

$$\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = B_n^2 \int_0^a \sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{a}x\right) dx \tag{8}$$

and using

$$\sin\left(\frac{n\pi}{a}x\right) \sin\left(\frac{m\pi}{a}x\right) = \frac{1}{2}\left[\cos\left(\frac{(n-m)\pi}{a}x\right) - \cos\left(\frac{(n+m)\pi}{a}x\right)\right] \tag{9}$$

we find

$$\begin{aligned} \int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx &= \frac{B_n^2}{2} \int_0^a \left[\cos\left(\frac{(n-m)\pi}{a}x\right) - \cos\left(\frac{(n+m)\pi}{a}x\right)\right] dx \\ &= \frac{B_n^2}{2} \int_0^a \cos\left(\frac{(n-m)\pi}{a}x\right) dx = \frac{B_n^2}{2} \begin{cases} \int_0^a dx & n = m \\ 0 & n \neq m \end{cases} \end{aligned} \tag{10}$$

$$\Rightarrow \int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \begin{cases} \frac{aB_n^2}{2} & n = m \\ 0 & n \neq m \end{cases} \tag{11}$$

Therefore the eigen functions are orthonormal

(c) Although the eigen functions are orthogonal we can not say it is orthonormal. For the functions to be orthonormal the orthonormality condition

$$\int_{-\infty}^{\infty} u_n^*(x)\, u_m(x)\, dx = \delta_{nm} \tag{12}$$

must be satisfied. Using the result in part (b), the orthonormalized eigen functions can be written as

$$u_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right). \tag{13}$$

(d) The ground state energy is the minimum energy which is given by the minimum quantum number, $n = 1$

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2}. \tag{14}$$

The expectation values for $\langle p_x \rangle$ which is given by

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t) \left(-i\hbar\frac{\partial}{\partial x}\right) \psi(x,t)\, dx, \tag{15}$$

can be expressed for the ground state as in terms of the energy eigen functions as

$$\begin{aligned} \langle p_x \rangle &= \int_{-\infty}^{\infty} u_1^*(x) \left(-i\hbar\frac{\partial}{\partial x}\right) u_1(x)\, dx = -\frac{2i\hbar}{a} \int_0^a \sin\left(\frac{\pi}{a}x\right) \left(\frac{\partial \sin\left(\frac{\pi}{a}x\right)}{\partial x}\right) dx \\ &= -\frac{2i\hbar}{a}\frac{\pi}{a} \int_0^a \sin\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}x\right) dx \Rightarrow \langle p_x \rangle = 0. \end{aligned} \tag{16}$$

For $\left\langle p_x^2 \right\rangle$, we can use the energy eigenvalue. We know that in the region $0 < x < a$, since $V(x) = 0$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} \Rightarrow \left\langle \hat{H} \right\rangle = \left\langle \frac{\hat{p}_x^2}{2m} \right\rangle = E_n \Rightarrow \frac{\left\langle \hat{p}_x^2 \right\rangle}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \Rightarrow \left\langle \hat{p}_x^2 \right\rangle = \frac{\pi^2\hbar^2}{a^2}. \tag{17}$$

Then the uncertainties in momentum

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} \Rightarrow \Delta p = \frac{\pi\hbar}{a} \tag{18}$$

(e) For a width

$$a = 10^{-2}m \tag{19}$$

and energy

$$E = 0.01ev = 0.01 \times 1.6 \times 10^{-19}J \tag{20}$$

solving for n from Eq. (6), we find

$$n = \sqrt{\frac{2ma^2E_n}{\pi^2\hbar^2}} = 1.63 \times 10^4.$$

For a free particle in one dimensional box, the thermal energy equal to the kinetic energy (total energy) is given by

$$E = \frac{1}{2}KT, \tag{21}$$

where $K = 8.62 \times 10^{-5}ev/K$ is the Boltzman constant. Then temperature becomes

$$T = \frac{2E}{K} = \frac{2 \times 0.01ev}{8.62 \times 10^{-5}ev/K} = 232K. \tag{22}$$

(f) The density of state is given by $\frac{dn}{dE}$. Using the energy

$$E(n) = \frac{\pi^2\hbar^2}{2ma^2}n^2, \tag{23}$$

we may write

$$dE = \frac{\pi^2\hbar^2 n}{ma^2}dn \Rightarrow \frac{dn}{dE} = \frac{ma^2}{\pi^2\hbar^2 n} = \frac{n}{2\left(\frac{\pi^2\hbar^2n^2}{2ma^2}\right)} = \frac{n}{2E}. \tag{24}$$

Numerically

$$\frac{dn}{dE} = \frac{n}{2E} = \frac{1.63 \times 10^4}{2 \times 10^{-2}ev} = 0.82 \times 10^6 \frac{1}{ev}. \tag{25}$$

Therefore, the number of states, Δn in an energy interval $\Delta E = 0.0001eV$ is

$$\Delta n = \int_E^{E+\Delta E} \frac{dn}{dE}dE = 0.82 \times 10^6 \frac{1}{ev}\Delta E = 82 \tag{26}$$

states.

(g) The plots for the eigen functions are given belowFor a particle in a one dimensional box with boundaries at $x = -a/2$ and $x = a/2$

$$V(x) = \begin{cases} \infty & x < -a/2 \\ 0 & -a/2 < x < a/2 \\ \infty & a/2 < x \end{cases} \tag{27}$$

the eigen functions can be determined by shifting the graphs to the left by 0.5a. That leads to

$$\begin{aligned} u_n(x) &= B_n \sin\left(\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right) \\ &= B_n\left[\sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{a}\right)\sin\left(\frac{n\pi}{2}\right)\right] \end{aligned} \tag{28}$$

$$\Rightarrow u_n(x) = \begin{cases} B_n \sin\left(\frac{n\pi x}{a}\right) & n = even \\ B_n \cos\left(\frac{n\pi x}{a}\right) & n = odd \end{cases} \tag{29}$$

where we have included the negative signs into the normalization constant.

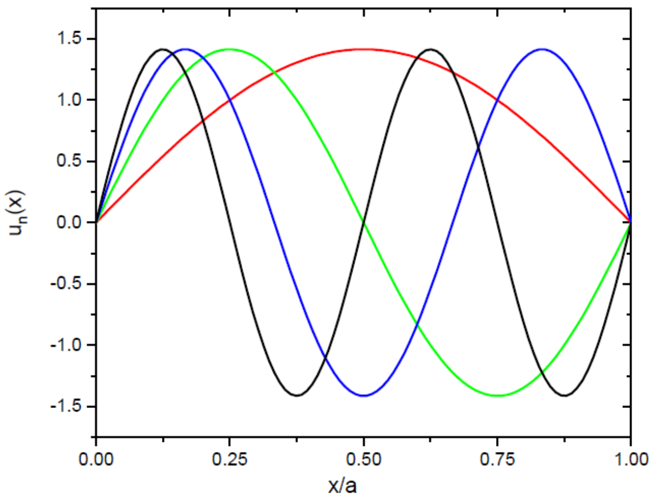


Figure 1: The energy eigen functions: $n = 1$ (Red), $n = 2$ (green), $n = 3$ (blue), and $n = 4$ (black).

(h) For the ground state the expectation value for $\langle x \rangle$ and $\langle x^2 \rangle$ can be expressed as

$$\langle x \rangle = \int_{-\infty}^{\infty} u_1^*(x)\, x u_1(x)\, dx = \frac{2}{a}\int_0^a x \sin^2\left(\frac{\pi}{a}x\right) dx,$$

and

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} u_1^*(x)\, x^2 u_1(x)\, dx = \frac{2}{a}\int_0^a x^2 \sin^2\left(\frac{\pi}{a}x\right) dx = \frac{2}{a}\int_0^a x^2 \left[1 - \cos^2\left(\frac{\pi}{a}x\right)\right] dx$$

Using the relation

$$\sin^2\left(\frac{\pi}{a}x\right) = \frac{1}{2}\left[1 + \cos\left(\frac{2\pi}{a}x\right)\right]$$

one can rewrite the above expressions as

$$\langle x \rangle = \frac{1}{a}\int_0^a x\left[1 + \cos\left(\frac{2\pi}{a}x\right)\right] dx = \frac{a}{2} - \frac{1}{a}\int_0^a x \cos\left(\frac{2\pi}{a}x\right) dx,$$

and

$$\langle x^2 \rangle = \frac{1}{a}\int_0^a x^2\left[1 + \cos\left(\frac{2\pi}{a}x\right)\right] dx = \frac{a^2}{3} - \frac{1}{a}\int_0^a x^2 \cos\left(\frac{2\pi}{a}x\right) dx$$

Using integration by parts or (Mathematica), one can write

$$\begin{aligned}
\int_0^a x \cos\left(\frac{2\pi}{a}x\right) dx &= \frac{a}{2\pi}\left[\left.\frac{x \sin\left(\frac{2\pi}{a}x\right)}{\frac{2\pi}{a}}\right|_0^a - \frac{a}{2\pi}\int_0^a \sin\left(\frac{2\pi}{a}x\right) dx\right] = \left.\left(\frac{a}{2\pi}\right)^2 \cos\left(\frac{2\pi}{a}x\right)\right|_0^a \\
&\Rightarrow \int_0^a x \cos\left(\frac{2\pi}{a}x\right) dx = 0
\end{aligned}$$

and

$$\begin{aligned}
\int_0^a x^2 \cos\left(\frac{2\pi}{a}x\right) dx &= \left.\frac{x^2 \sin\left(\frac{2\pi}{a}x\right)}{\frac{2\pi}{a}}\right|_0^a - \frac{a}{\pi}\int_0^a x \sin\left(\frac{2\pi}{a}x\right) dx = -\frac{a}{\pi}\int_0^a x \sin\left(\frac{2\pi}{a}x\right) dx \\
&= \left.\frac{a}{\pi}\frac{x \cos\left(\frac{2\pi}{a}x\right)}{\frac{2\pi}{a}}\right|_0^a - \frac{a^2}{2\pi^2}\int_0^a \cos\left(\frac{2\pi}{a}x\right) dx = \frac{a^3}{2\pi^2}
\end{aligned}$$

and the expectation values become

$$\langle x \rangle = \frac{a}{2}, \langle x^2 \rangle = \frac{a^2}{3} - \frac{a^2}{2\pi^2}$$

(i) Using the results in part (d) and (h), one finds for the uncertainties

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{a^2}{3} - \frac{a^2}{2\pi^2} - \frac{a^2}{4}} = \sqrt{\frac{\pi^2-6}{12}}\frac{a}{\pi}, \Delta p_x = \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2} = \sqrt{\frac{\pi^2\hbar^2}{a^2}} = \frac{\pi\hbar}{a}$$

$$\Rightarrow \quad \Delta x \Delta p_x = \sqrt{\frac{\pi^2-6}{3}}\frac{\hbar}{2} \simeq 1.3\frac{\hbar}{2} > \frac{\hbar}{2}$$

2. Suppose the particle in the one-dimensional box considered in the example above has a wave function given by

$$\psi(x) = \begin{cases} A(x/a) & 0 < x < a/2 \\ A(1-x/a) & a/2 < x < a \end{cases} \tag{30}$$

where $A = \sqrt{12/a}$ is the normalization constant. Calculate the probability that a measurement of the energy for this particle yields the value, E_n.

Solution: We recall the wave function in terms of the energy eigen functions can be expressed as

$$\psi(x,t) = \sum_{n=0}^{\infty} a_n u_n(x) e^{\frac{-iE_n t}{\hbar}}, \tag{31}$$

where the expansion coefficients are determined using

$$a_n = \int_{-\infty}^{\infty} u_n^*(x)\psi(x)\,dx. \tag{32}$$

For a particle in a box described by the wave function above, we may write

$$a_n = \int_0^{a/2} u_n^*(x) A(x/a)dx + \int_{a/2}^{a} u_n^*(x) A(1-x/a)dx. \tag{33}$$

Using the result for the eigen function of a particle in a box confined in the region, $0 < x < a$

$$u_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right). \tag{34}$$

we find

$$a_n = \sqrt{\frac{2}{a}}A\int_0^{a/2}\sin\left(\frac{n\pi}{a}x\right)\frac{x}{a}dx + \sqrt{\frac{2}{a}}A\int_{a/2}^{a}\sin\left(\frac{n\pi}{a}x\right)(1-\frac{x}{a})dx \tag{35}$$

Introducing transformation of variable defined by

$$1 - \frac{u}{a} = \frac{x}{a} \tag{36}$$

we have

$$\begin{gathered} dx = -du, x = \frac{a}{2} \Rightarrow u = \frac{a}{2}, x = a \Rightarrow u = 0 \\ \sin\left(\frac{n\pi}{a}x\right) = \sin\left(n\pi - \frac{n\pi}{a}u\right) = -\cos(n\pi)\sin\left(\frac{n\pi}{a}u\right) = -(-1)^n\sin\left(\frac{n\pi}{a}u\right) \end{gathered} \tag{37}$$

so that one can express the integral

$$\begin{aligned} \int_{a/2}^{a}\sin\left(\frac{n\pi}{a}x\right)(1-\frac{x}{a})dx &= (-1)^n\int_{a/2}^{0}\sin\left(\frac{n\pi}{a}u\right)\frac{u}{a}du \\ &= -(-1)^n\int_0^{a/2}\sin\left(\frac{n\pi}{a}u\right)\frac{u}{a}du \\ \Rightarrow \int_{a/2}^{a}\sin\left(\frac{n\pi}{a}x\right)(1-\frac{x}{a})dx &= -(-1)^n\int_0^{a/2}\sin\left(\frac{n\pi}{a}x\right)\frac{x}{a}dx \end{aligned} \tag{38}$$

where we take into account the fact that u is a dummy variable in the last step. The substituting this into the equation for a_n, we find,

$$a_n = \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \int_0^{a/2} \sin\left(\frac{n\pi}{a}x\right) \frac{x}{a} dx. \tag{39}$$

We may put this equation in the form

$$\begin{aligned} a_n &= \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \frac{a}{n^2\pi^2} \int_0^{a/2} \sin\left(\frac{n\pi}{a}x\right) \frac{n\pi x}{a} d\left(\frac{n\pi x}{a}\right) \\ &\Rightarrow a_n = \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \frac{a}{n^2\pi^2} \int_0^{n\pi/2} \sin(v)\, v dv. \end{aligned} \tag{40}$$

Using integration by parts, one can rewrite

$$\begin{aligned} a_n &= \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \frac{a}{n^2\pi^2} \left\{ \left[-\cos(v)\, v\right]_0^{n\pi/2} + \int_0^{n\pi/2} \cos(v)\, dv \right\} \\ &= \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \frac{a}{n^2\pi^2} \left\{\sin(v) - \cos(v)\, v\right\}_0^{n\pi/2} \\ &\Rightarrow a_n = \sqrt{\frac{2}{a}} A \left(1-(-1)^n\right) \frac{a}{n^2\pi^2} \left\{\sin\left(\frac{n\pi}{2}\right) - \frac{n\pi}{2}\cos\left(\frac{n\pi}{2}\right)\right\} \end{aligned} \tag{41}$$

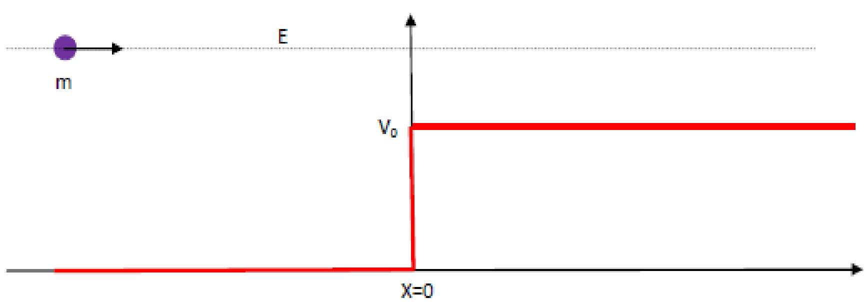
there follows that

$$a_n = \begin{cases} 0 & n = even \\ \frac{\sqrt{96}}{\pi^2 n^2} & n = 1, 5, 9... \\ -\frac{\sqrt{96}}{\pi^2 n^2} & n = 3, 7, 11.. \end{cases} \tag{42}$$

where we substituted, $A = \sqrt{12/a}$. The the probability that a measurement results in energy value E_n is given by

$$p_n = |a_n|^2 = \begin{cases} 0 & n = even \\ \frac{96}{\pi^4 n^4} & n = odd \end{cases} \tag{43}$$

3. For a step potential shown in the figure below show that the probability that the particle gets reflected is given



by the ratio of the reflected flux to the incident flux

$$\frac{j_{re}}{j_{in}} = \left|\frac{q-k}{q+k}\right|^2$$

and for the probability that it gets transmitted

$$\frac{j_{tr}}{j_{in}} = \frac{4\,|kq|}{|q+k|^2}$$

where

$$k^2 = \frac{2mE}{\hbar^2}.$$

and

$$q^2 = \frac{2m\,(E-V_0)}{\hbar^2}.$$

Solution: The Shrödinger equation in the region $x<0$ can be written as

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}=Eu(x)\Rightarrow\frac{d^2u(x)}{dx^2}+\frac{2mE}{\hbar^2}u(x)=0$$
$$\Rightarrow\frac{d^2u(x)}{dx^2}+k^2u(x)=0, \tag{44}$$

where

$$k^2=\frac{2mE}{\hbar^2}. \tag{45}$$

In the region $x>0$

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V_0u(x)=Eu(x)\Rightarrow\frac{d^2u(x)}{dx^2}+\frac{2m(E-V_0)}{\hbar^2}u(x)=0$$
$$\Rightarrow\frac{d^2u(x)}{dx^2}+q^2u(x)=0, \tag{46}$$

where

$$q^2=\frac{2m(E-V_0)}{\hbar^2}. \tag{47}$$

The general solutions of Eqs. (44) and (46) are given by

$$u(x)=\begin{cases} Ae^{ikx}+Re^{-ikx}, & x<0\\ Te^{iqx}, & x>0\end{cases} \tag{48}$$

where we dropped the De^{-iqx} term in the region $x>0$ since there is nothing that causes the particle to reverse its direction. However, in the region $x<0$, that particle could get reflected because of the potential it encountered at $x=0$ and we keep the term Re^{-ikx}.Imposing the condition that the wave function and its derivative must be continuous everywhere including at, $x=0$, where the potential abruptly changes, we find

$$A+R=T, ik(A-R)=iqT\Rightarrow A+R=T, A-R=\frac{q}{k}T \tag{49}$$

In terms of the incident wave amplitude A, we may write

$$R=\left(\frac{q-k}{q+k}\right)A, T=\frac{2k}{q+k}A \tag{50}$$

The incident, reflected, and transmitted flux: We recall that the probability current density, $J(x,t)$, which is given by

$$J(x,t)=\frac{\hbar}{2mi}\left[\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t)-\psi(x,t)\frac{\partial}{\partial x}\psi^*(x,t)\right], \tag{51}$$

tells us the flux of particles incident, reflected or transmitted at a given position, x and at time, t. Using this relation and the results obtained above we may write the net flux of particle incident at $x=0$ as

$$J_{net\ in}(0,t)=\frac{\hbar}{2mi}\left[u^*(x)\frac{\partial}{\partial x}u(x)-u(x)\frac{\partial}{\partial x}u^*(x)\right]_{x=0}, \tag{52}$$

using the wave function for $x<0$, we have

$$u^*(x)\frac{\partial}{\partial x}u(x)=ik\left(Ae^{-ikx}+Re^{ikx}\right)\left(Ae^{ikx}-Re^{-ikx}\right)$$
$$\Rightarrow\left[u^*(x)\frac{\partial}{\partial x}u(x)\right]_{x=0}=ik(A^*+R^*)(A-R)=ik\left(|A|^2-|R|^2\right) \tag{53}$$

and

$$u(x)\frac{\partial}{\partial x}u^*(x)=-ik\left(Ae^{ikx}+Re^{-ikx}\right)\left(A^*e^{-ikx}-R^*e^{ikx}\right)$$
$$\Rightarrow\left[u(x)\frac{\partial}{\partial x}u^*(x)\right]_{x=0}=-ik\left(|A|^2-|R|^2\right) \tag{54}$$

so that

$$J_{net\ in}(0,t) = \frac{\hbar}{2mi}\left[ik\left(|A|^2 - |R|^2\right) + ik\left(|A|^2 - |R|^2\right)\right], \tag{55}$$

$$\Rightarrow \quad J_{net\ in}(0,t) = \frac{\hbar k}{m}\left(|A|^2 - |R|^2\right). \tag{56}$$

The net flux of particle transmitted into the region, $x > 0$

$$J_{net\ tr}(0,t) = \frac{\hbar}{2mi}\left[u^*(x)\frac{\partial}{\partial x}u(x) - u(x)\frac{\partial}{\partial x}u^*(x)\right]_{x=0},$$

using the wave function in the region $x > 0$, we have

$$u^*(x)\frac{\partial}{\partial x}u(x) = iqT^*e^{-iqx}Te^{iqx} = iq|T|^2 \Rightarrow \left[u^*(x)\frac{\partial}{\partial x}u(x)\right]_{x=0} = iqT^2 \tag{57}$$

and

$$\left[u(x)\frac{\partial}{\partial x}u^*(x)\right]_{x=0} = -iqT^2 \tag{58}$$

so that

$$J_{tr}(0,t) = \frac{\hbar q}{m}T^2. \tag{59}$$

Recalling that

$$\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}J(x,t) \tag{60}$$

when the wave function does not change with time

$$-\frac{\partial}{\partial x}J(x,t) = \frac{\partial}{\partial t}P(x,t) = 0 \Rightarrow J(x,t) = \text{constant} \tag{61}$$

which gives

$$\frac{\hbar k}{m}\left(|A|^2 - |R|^2\right) = \frac{\hbar q}{m}|T|^2 \tag{62}$$

From Eq. (62), we note that the incident flux is

$$j_{in} = \frac{\hbar k}{m}|A|^2 \tag{63}$$

the reflected flux

$$j_{re} = \frac{\hbar k}{m}|R|^2 \tag{64}$$

and the transmitted flux

$$j_{tr} = \frac{\hbar q}{m}|T|^2 \tag{65}$$

so that

$$\begin{aligned}\frac{\hbar k}{m}\left(|A|^2 - |R|^2\right) &= \frac{\hbar q}{m}|T|^2 \Rightarrow J_{net\ in}(0,t) = J_{net\ tr}(0,t) \\ &\Rightarrow j_{in} + j_{re} = j_{tr}\end{aligned} \tag{66}$$

Using the results in Eq. (50) the reflected and transmitted flux in terms of the amplitude of the incident wave can be expressed as

$$j_{re} = \frac{\hbar k}{m}\left|\frac{q-k}{q+k}\right|^2|A|^2 \tag{67}$$

and

$$j_{tr} = \frac{\hbar q}{m}\left|\frac{2k}{q+k}\right|^2|A|^2. \tag{68}$$

The probability that the particle gets reflected is given by the ratio of the reflected flux to the incident flux

$$\frac{j_{re}}{j_{in}} = \frac{\frac{\hbar k}{m}\left|\frac{q-k}{q+k}\right|^2 |A|^2}{\frac{\hbar k}{m}|A|^2} = \left|\frac{q-k}{q+k}\right|^2 \tag{69}$$

the probability that it gets transmitted

$$\frac{j_{tr}}{j_{in}} = \frac{\frac{\hbar q}{m}\left|\frac{2k}{q+k}\right|^2 |A|^2}{\frac{\hbar k}{m}|A|^2} = \frac{4|kq|}{|q+k|^2} \tag{70}$$

which shows that $|R|^2$ and $|T|^2$ represent the reflection and transmission probability, respectively

4. Do Chapter 8 Example 5 in my note and make a mathematical and physical justification to show that for a potential well defined by the function

$$V(x) = \begin{cases} 0 & x < -a \\ -V_0 & -a < x < a \\ 0 & x > a \end{cases} \tag{71}$$

and a particle with energy $E > 0$, the probability of reflection

$$\frac{j_{re}}{j_{in}} = \frac{|R|^2}{|A|^2} = \frac{\left(q^2 - k^2\right)^2 \sin^2(2qa)}{4(qk)^2 \cos^2(2qa) + \left(q^2 + k^2\right)^2 \sin^2(2qa)},$$

and for transmission

$$\frac{j_{re}}{j_{in}} = \frac{|T|^2}{|A|^2} = \frac{4(qk)^2}{4(qk)^2 \cos^2(2qa) + \left(q^2 + k^2\right)^2 \sin^2(2qa)}$$

can be obtained from the results you derived in Example 5. That means you must provide a mathematical and physical justification to find these equations from

$$\frac{|R|^2}{|A|^2} = \frac{\left(k^2 + q^2\right)^2 \sinh^2(2qa)}{\left(k^2 + q^2\right)^2 \sinh^2(2qa) + (2kq)^2}$$

and

$$\frac{|T|^2}{|A|^2} = \frac{(2kq)^2}{\left(k^2 + q^2\right)^2 \sinh^2(2qa) + (2kq)^2}$$

respectively.

Solution: We recall for a potential barrier (See figure below) where the total energy is positive ($E < V_0$), the probability that the incident particle gets reflected at the well is given by

$$\frac{j_{re}}{j_{in}} = \frac{|R|^2}{|A|^2} = \frac{\left(k^2 + q^2\right)^2 \sinh^2(2qa)}{\left(k^2 + q^2\right)^2 \sinh^2(2qa) + (2kq)^2}, \tag{72}$$

and gets transmitted

$$\frac{j_{re}}{j_{in}} = \frac{|T|^2}{|A|^2} = \frac{(2kq)^2}{\left(k^2 + q^2\right)^2 \sinh^2(2qa) + (2kq)^2} \tag{73}$$

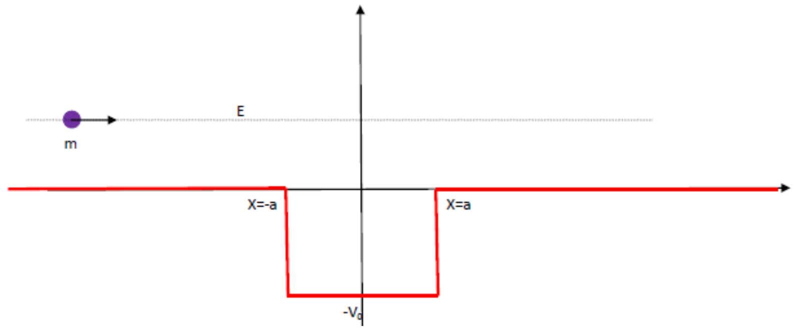
where

$$k^2 = \frac{2mE}{\hbar^2}. \tag{74}$$

and

$$q^2 = \frac{2m|E - V_0|}{\hbar^2} = \frac{2m(V_0 - E)}{\hbar^2}. \tag{75}$$

For a potential well (see the figure below) the difference is the potential V_0 is negative (i.e. $V(x) = -V_0$ in



the well) and also we are interested in the case where the total energy is is positive ($E > 0$). Under these conditions we may write the constant, q, as

$$q^2 = \frac{2m\left(-V_0 - E\right)}{\hbar^2} = -\frac{2m\left(V_0 + E\right)}{\hbar^2} \Rightarrow q = \pm iq'. \tag{76}$$

where

$$q' = \sqrt{\frac{2m\left(V_0 + E\right)}{\hbar^2}}.$$

Then using $q = \pm iq'$, one can rewrite the reflection and transmission coefficients as

$$\frac{|R|^2}{|A|^2} = \frac{\left(k^2 + (\pm iq')^2\right)^2 \sinh^2\left(\pm 2iq'a\right)}{\left(k^2 + (\pm iq')^2\right)^2 \sinh^2\left(\pm 2iq'a\right) + (\pm 2ikq')^2} = \frac{\left(k^2 - q'^2\right)^2 \sinh^2\left(\pm 2iq'a\right)}{\left(k^2 - q'^2\right)^2 \sinh^2\left(\pm 2iq'a\right) - (2kq')^2}$$

and

$$\frac{|T|^2}{|A|^2} = \frac{\left(\pm 2iq'k\right)^2}{\left(k^2 + (\pm iq')^2\right)^2 \sinh^2\left(\pm 2iq'a\right) + (\pm 2ikq')^2} = \frac{-(2kq')^2}{\left(k^2 - q'^2\right)^2 \sinh^2\left(\pm 2iq'a\right) - (2kq')^2} \tag{77}$$

Noting that

$$\begin{aligned} \sinh\left(\pm 2iq'a\right) &= i\left[\frac{e^{i\left(\pm 2q'a\right)} - e^{-i\left(\pm 2q'a\right)}}{2i}\right] = i\sin\left(\pm 2q'a\right) = \pm i\sin\left(2q'a\right) \\ &\Rightarrow \sinh^2\left(\pm 2iq'a\right) = \left[\pm i\sin\left(2q'a\right)\right]^2 = -\sin^2\left(2q'a\right) \end{aligned}$$

we find

$$\frac{|R|^2}{|A|^2} = \frac{\left(k^2 - q'^2\right)^2 \sin^2\left(2q'a\right)}{\left(k^2 - q'^2\right)^2 \sin^2\left(2q'a\right) + (2kq')^2}$$

and

$$\frac{|T|^2}{|A|^2} = \frac{(2kq')^2}{\left(k^2 - q'^2\right)^2 \sin^2\left(2q'a\right) + (2kq')^2} \tag{78}$$

Using

$$\begin{aligned} &4\left(q'k\right)^2 \cos^2\left(2q'a\right) + \left(q'^2 + k^2\right)^2 \sin^2\left(2qa\right) = 4\left(q'k\right)^2 + \left[\left(q'^2 + k^2\right)^2 - 4\left(q'k\right)^2\right] \sin^2\left(2qa\right) \\ &\Rightarrow 4\left(q'k\right)^2 \cos^2\left(2q'a\right) + \left(q'^2 + k^2\right)^2 \sin^2\left(2qa\right) = 4\left(q'k\right)^2 + \left(q'^2 - k^2\right)^2 \sin^2\left(2qa\right) \end{aligned}$$

one can rewrite

$$\frac{|R|^2}{|A|^2} = \frac{\left(k^2 - q'^2\right)^2 \sin^2\left(2q'a\right)}{4\left(q'k\right)^2 \cos^2\left(2q'a\right) + \left(q'^2 + k^2\right)^2 \sin^2\left(2qa\right)}$$

and

$$\frac{|T|^2}{|A|^2} = \frac{(2kq')^2}{4\left(q'k\right)^2 \cos^2\left(2q'a\right) + \left(q'^2 + k^2\right)^2 \sin^2\left(2qa\right)} \tag{79}$$

note that q is a dummy variable and we can rename it q as long as

$$q = q' = \sqrt{\frac{2m\left(V_0 + E\right)}{\hbar^2}}.$$

5. For a particle of mass in the 1-D potential energy well

$$V\left(x\right) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{elsewhere} \end{cases} \tag{80}$$

is at time $t = 0$ in the state

$$\psi\left(x, t = 0\right) = \begin{cases} \left(\frac{1+i}{2}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right) & 0 < x < a \\ 0 & \text{elsewhere} \end{cases} \tag{81}$$

(a) Find the wave function at a later time, $\psi\left(x, t\right)$.

(b) What is the expectation value for the energy, $\left\langle \hat{H} \right\rangle$?

(c) What is the probability that a measurement of the energy will yield the value

$$E = \frac{\pi^2 \hbar^2}{2ma^2}$$

(d) Without detailed computation, give an argument that $\langle x \rangle$ is time dependent.

Solution:

(a) We recall that

$$\psi\left(x, t\right) = \sum_{n=0}^{\infty} a_n u_n\left(x\right) e \frac{-iE_n t}{\hbar}, \tag{82}$$

and at $t = 0$,

$$\begin{aligned} \psi\left(x, t = 0\right) &= \sum_{n=0}^{\infty} a_n u_n\left(x\right) \Rightarrow \int_0^a u_m^*\left(x\right)\psi\left(x, t = 0\right)dx = \sum_{n=0}^{\infty} a_n \int_0^a u_n\left(x\right)u_m^*\left(x\right)dx. && (83) \\ &\Rightarrow \int_0^a u_m^*\left(x\right)\psi\left(x, t = 0\right)dx = \sum_{n=0}^{\infty} a_n \delta_{nm} && (84) \\ &\Rightarrow a_n = \int_0^a u_n^*\left(x\right)\psi\left(x, t = 0\right)dx. && (85) \end{aligned}$$

Then using the given wave function at the initial time

$$\psi\left(x, t = 0\right) = \left(\frac{1+i}{2}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right) + \frac{1}{\sqrt{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right) \tag{86}$$

which we may rewrite as

$$\psi\left(x, t = 0\right) = \left(\frac{1+i}{2}\right)u_1\left(x\right) + \frac{1}{\sqrt{2}}u_2\left(x\right) \tag{87}$$

we have

$$a_n = \left(\frac{1+i}{2}\right)\int_0^a u_n^*\left(x\right)u_1\left(x\right)dx + \frac{1}{\sqrt{2}}\int_0^a u_n^*\left(x\right)u_2\left(x\right)dx.$$

so that applying the orthonormality condition for the eigen fuctions

$$\int_{-\infty}^{\infty} u_n\left(x\right)u_m^*\left(x\right)dx = \delta_{nm} \tag{88}$$

one finds

$$a_n = \begin{cases} \frac{1+i}{2} & n = 1 \\ \frac{1}{\sqrt{2}} & n = 2 \\ 0 & n > 2 \end{cases}$$

Therefore, the wave functions at a later time becomes

$$\psi(x,t) = a_1 u_1(x)\, e^{\frac{-iE_1 t}{\hbar}} + a_2 u_2(x)\, e^{\frac{-iE_2 t}{\hbar}} \tag{89}$$

where

$$\begin{aligned} a_1 &= \frac{1+i}{2}, u_1(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right), E_1 = \frac{\pi^2\hbar^2}{2ma^2} \\ a_2 &= \frac{1}{\sqrt{2}}, u_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right), E_2 = \frac{2\pi^2\hbar^2}{ma^2} = 4E_1 \end{aligned}$$

(b) We have proved in class that the expectation value for the energy is independent of time and can be determined using

$$\left\langle \hat{H} \right\rangle = \sum_{n=0}^{\infty} |a_n|^2 E_n. \tag{90}$$

Using this relation and the wave function we determined, we find

$$\left\langle \hat{H} \right\rangle = |a_1|^2 E_1 + |a_2|^2 E_2 = \frac{1}{2}E_1 + \frac{1}{2}(4E_1) = \frac{5}{2}E_1 = \frac{5\pi^2\hbar^2}{4ma^2} \tag{91}$$

(c) Noting that

$$E = \frac{\pi^2\hbar^2}{2ma^2} = E_1$$

one can easily see that

$$P_1 = |a_1|^2 = \frac{1}{2}$$

(d) We recall that the expectation value for the position must be determined from

$$\langle x \rangle = \int_0^a \psi^*(x,t)\, x\psi(x,t)\, dx = \int_0^a x\, |\psi(x,t)|^2\, dx.$$

We have shown that the wave function is

$$\psi(x,t) = a_1 u_1(x)\, e^{\frac{-iE_1 t}{\hbar}} + a_2 u_2(x)\, e^{\frac{-iE_2 t}{\hbar}} \tag{92}$$

which indicates that

$$|\psi(x,t)|^2 = |a_1 u_1(x)|^2 + |a_2 u_2(x)|^2 + a_1 u_1(x)\, a_2^* u_2^*(x)\, e^{\frac{-i(E_1-E_2)t}{\hbar}} + a_1^* u_1^*(x)\, a_2 u_2(x)\, e^{\frac{i(E_1-E_2)t}{\hbar}}$$

is time dependent and therefore so does the expectation value for the position.

Another explanation can be based on the Haisenberg picture.The postion x is time dependent because it does not commute with the Hamiltonian. For the particle inside the well where the potential is zero, the Hamiltonian is given

$$\hat{H} = \frac{\hat{p}_x^2}{2m}$$

then

$$\left[\hat{x}, \hat{H}\right] = \frac{1}{2m}\left[\hat{x}, \hat{p}_x^2\right] \neq 0$$

6. Recommended problems Townsend # 6:12, 15, 17, 18, 21