PH 112: Quantum Physics and Applications

S. Shankaranarayanan
shanki@iitb.ac.in

Week 04 Lecture 1: Implications of Born interpretation

D3, Spring 2023

Schrodinger Equation: Recap

Time-dependent Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$

Time-independent Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi=E\psi$$

Born interpretation

$$\int_a^b |\Psi(x,t)|^2 dx = \left\{ \begin{array}{c} \text{Probability of finding the particle} \\ \text{between } a \text{ and } b \text{, at time } t. \end{array} \right\}$$

Normalization of Wave-function

$$\int_{-\infty}^{\infty} P(x)dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

Comparison of Classical and Quantum Mechanics

- Newton's second law and Schrodinger's wave equation are both differential equations.
- Newton's second law can be derived from the Schrödinger wave equation, so Schrodinger equation is more fundamental. (Ehrenfest theorem)
- Classical mechanics only appears to be more precise because it deals with macroscopic phenomena. The underlying uncertainties in macroscopic measurements are just too small to be significant.

Properties of the wave function $\Psi(x, t)$

- Should be defined everywhere and finite every-where in space and at all times.

- Should be single-valued.

- Ψ and its first derivative should be continuous.

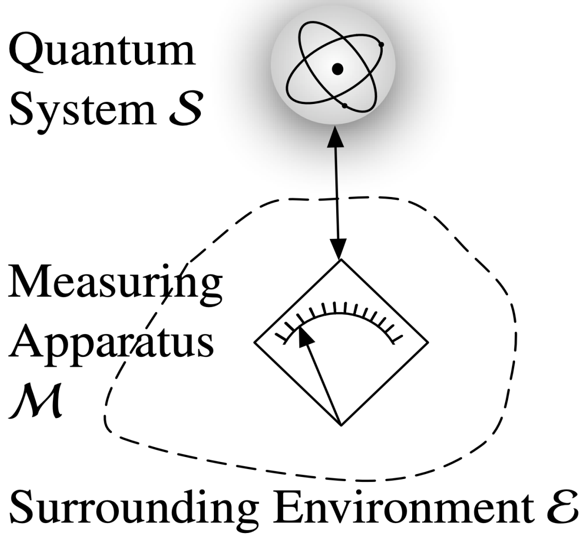
- If Ψ is a solution of Schrodinger equation then so is $c\Psi$ where c is constant.

- $\Psi \rightarrow 0$ as $x \rightarrow \pm\infty$ so that Ψ can be normalized

$$\int_{-\infty}^{\infty} P(x)dx = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 dx = 1$$

Implications of Born’s interpretation

Consequence of Probability



- So, what are we measuring with statistical interpretation?

  We aren't measuring anything. We give predictions for what we expect from a measurement.

- Probabilistic outcomes feature in classical physics (like tossing a coin). Probability enters because there is insufficient information to make a definite prediction.

- According to classical physics, in principle, that missing information can be found.

Heisenberg Uncertainty principle states that accessing such states simultaneously is impossible.

Expectation Values: Discrete case

Example: Let 14 people be in a room. Let N(j) represent the number of people of age j.

N(14)=1, N(15)=1, N(16)=3, N(22)=2, N(24)=2, N(25)=5

- The total number of people in the room is

$$N = \sum_{j=0}^{\infty} N(j)$$

- What is the probability that a randomly selected person in the group is 15?

$$P(j) = N(j)/N \qquad \sum_{j=0}^{\infty} P(j) = 1$$

- What is the average age?

$$\langle j \rangle = \frac{\sum jN(j)}{N} = \sum_{j=0}^{\infty} jP(j) = 21$$

Value is not necessarily we can expect with a single measurement (like 21 in the example)

Expectation Values: Discrete case

Example: Let 14 people be in a room. Let N(j) represent the number of people of age j.

N(14)=1, N(15)=1, N(16)=3, N(22)=2, N(24)=2, N(25)=5

- What is the average of the squares of the ages?

$$\langle j^2 \rangle = \sum_{j=0}^{\infty} j^2 P(j)$$

- Note that for any distribution $\langle j^2 \rangle \neq \langle j \rangle^2$

- Standard deviation of the distribution

$$\sigma = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}$$

- In general, the average value of function *f(j)* is

$$\langle f(j) \rangle = \sum_{j=0}^{\infty} f(j) P(j)$$

Expectation values for continuous distributions

- We can change from discrete to continuous variables by using the probability *P*(*x*) of observing the particle at a particular *x* *at time t*

$$\overline{x} = \frac{\int_{-\infty}^{\infty} xP(x)\,dx}{\int_{-\infty}^{\infty} P(x)\,dx}$$

- Using the wave function, the expectation value is:

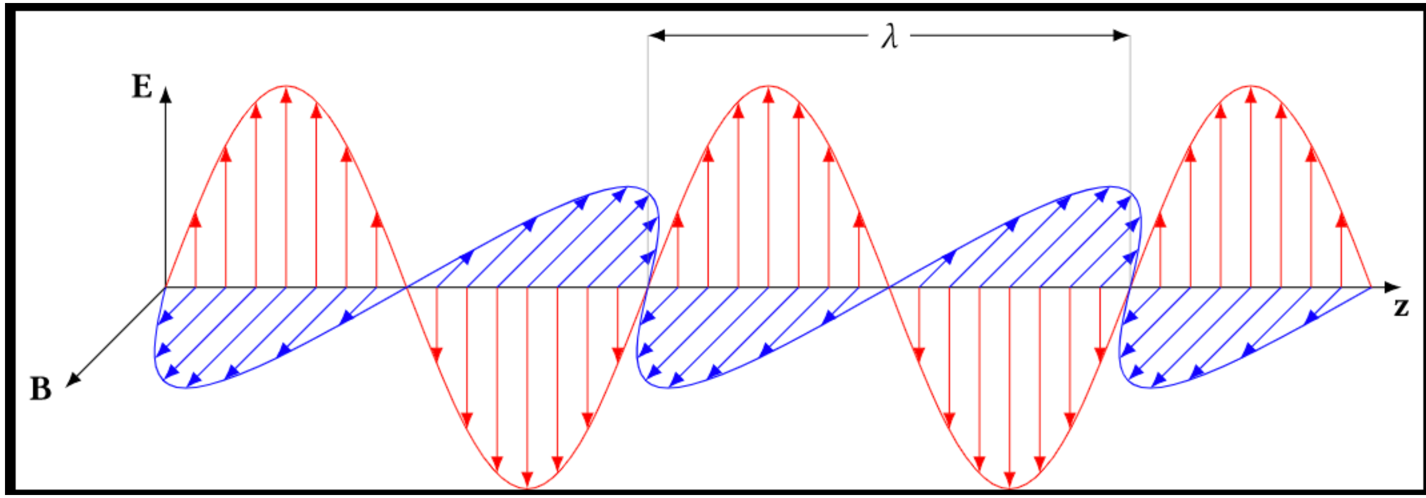
$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x\Psi^*(x,t)\Psi(x,t)\,dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)\,dx}$$

- The expectation value of any function *g*(*x*) for a normalized wave function:

$$\langle g(x) \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)g(x)\Psi(x,t)\,dx$$

To measure anything, we need to make a measurement or operation!

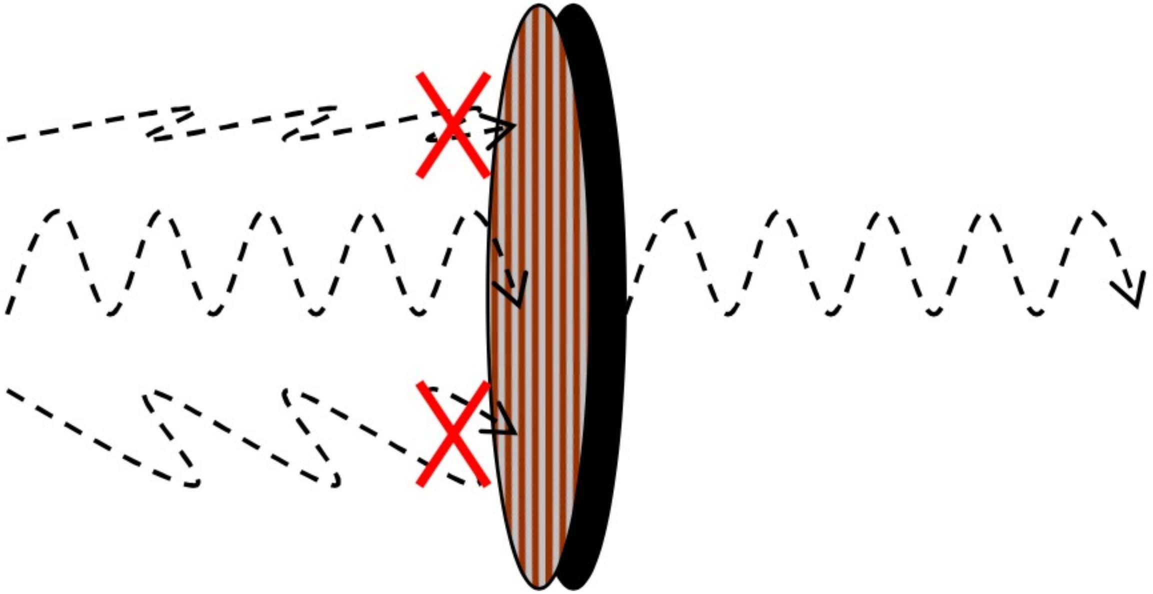
Photons and Operators



- EM waves are transverse waves.
- Plane EM waves can have Electric along x-direction or y-direction.
- Usually, light from sun, tubelight have Electric fields in randon direction!
- If you pass light though a polarization filter, like polarized lens, some of the light passes though, and some does not. Hence, the image appears darker!

Photons and Operators

Let us do a series of experiments with polarizers.

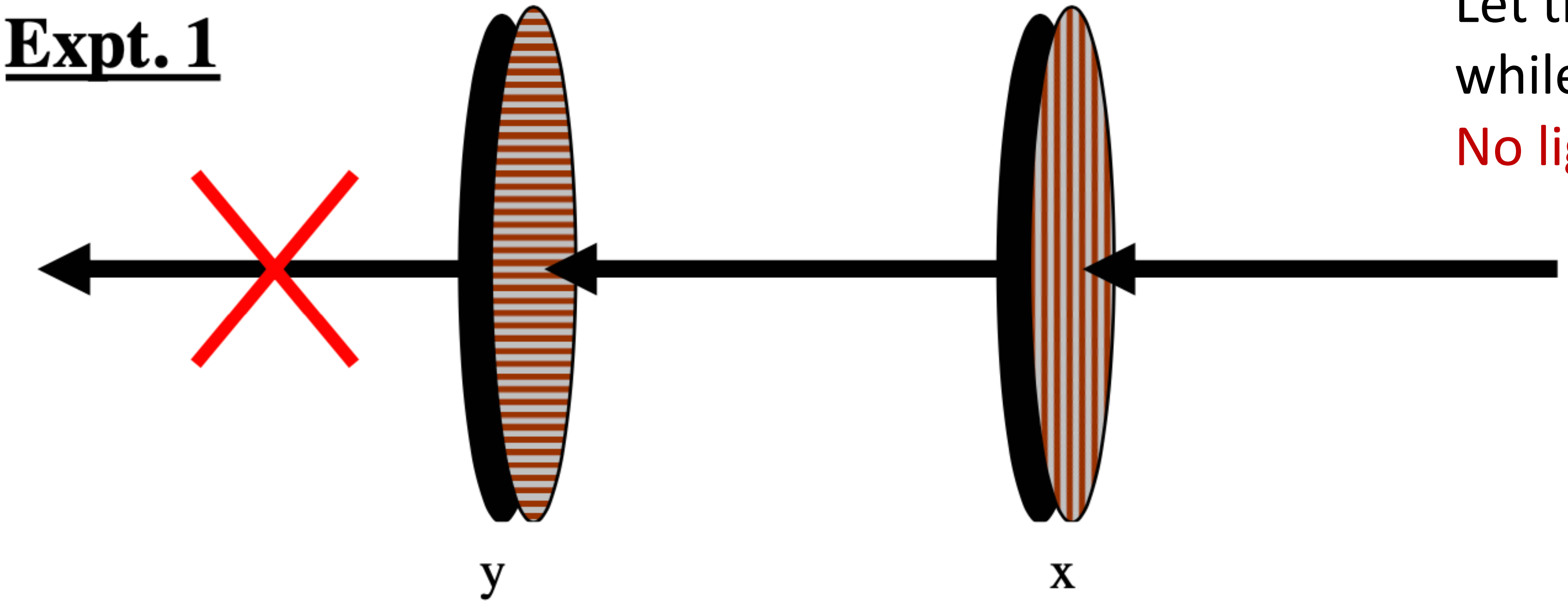


x-polarizer will only allow x-polarized light.
y-polarizer will only allow y-polarized light.

Here the round circle represents a polarization filter, and the vertical lines indicate that it is a polarization filter in the *x* direction. The polarization filter performs a simple **measurement**; it tells us how much of the light is polarized in a given direction.

Experiment 01: Two Polarization measurements

It gets interesting when we start to consider multiple polarization measurements being applied to one laser beam.

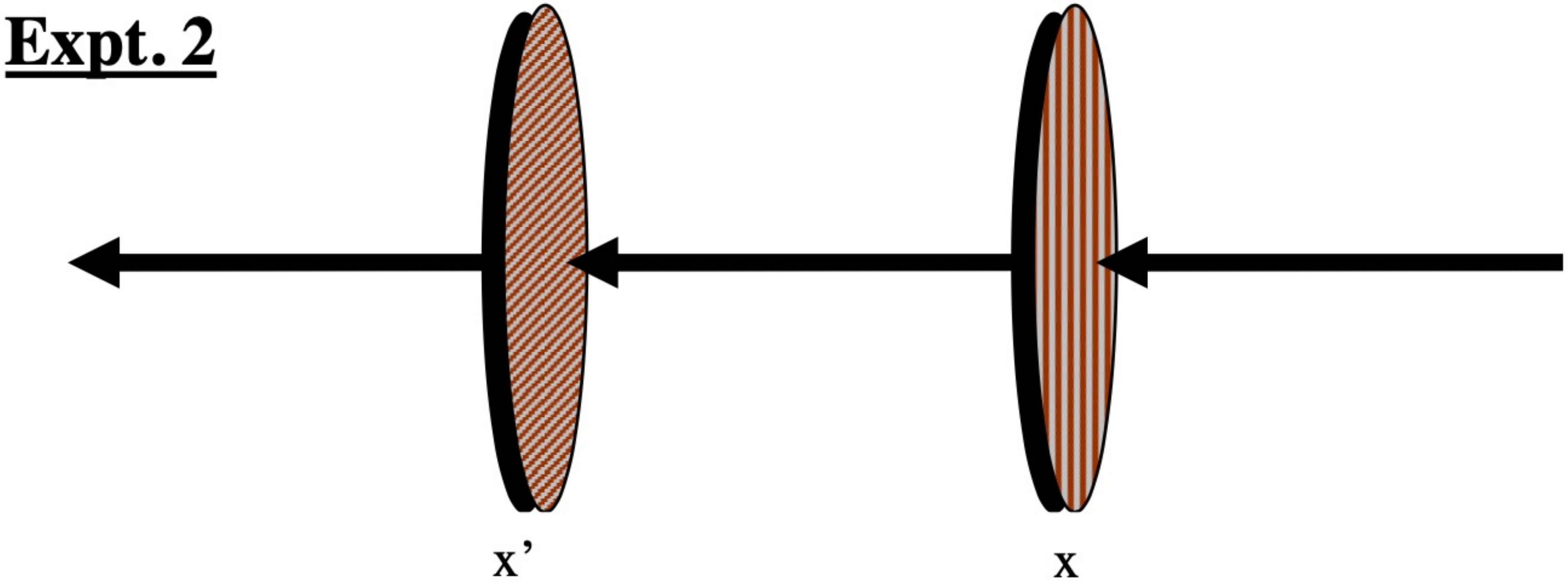


Let the first filter be *x-polarizer* while the second filter is *y-polarizer.* No light gets transmitted.

$$Output\ signal\ =\ Operation\ 2 \times Operation 1 \times Input\ signal$$

Experiment 02: Two Polarization measurements

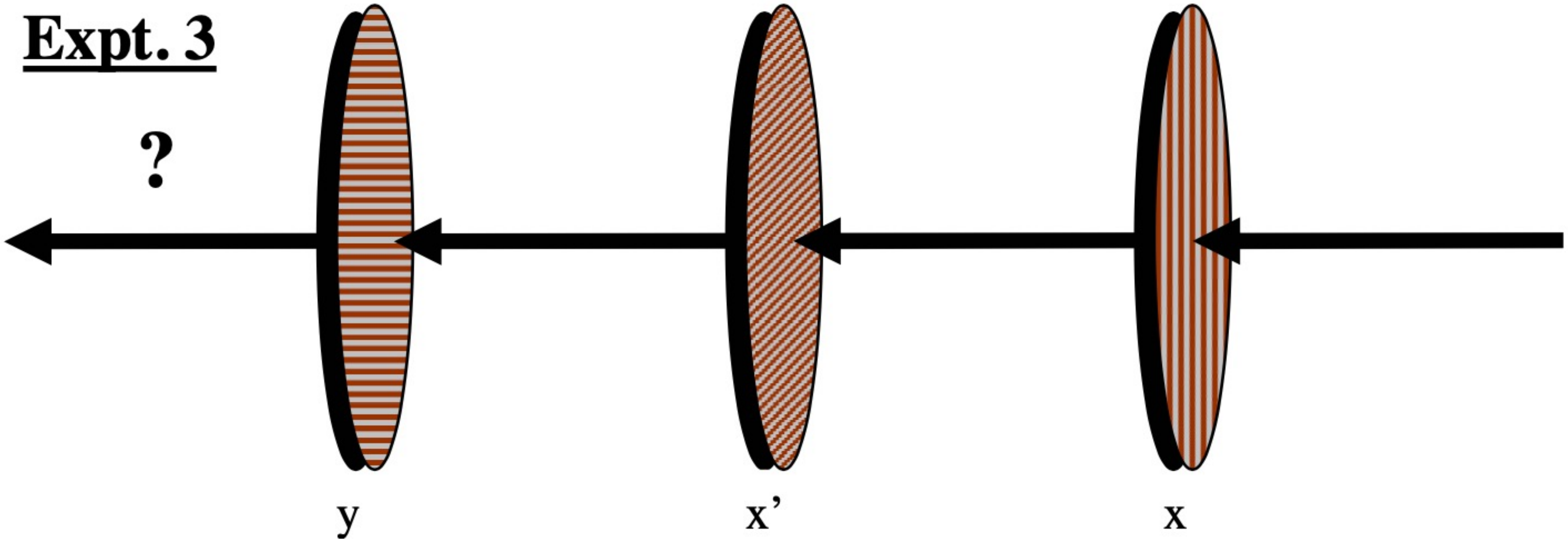
Let us perform another experiment where the first filter is *x-polarizer* while the second filter is aligned at a 45 degree angle to *x*. In this case, we do get some transmission.



$$Output = \ Operation\ 3 \times Operation 1 \times Input$$

Experiment 03: Three Polarization measurements

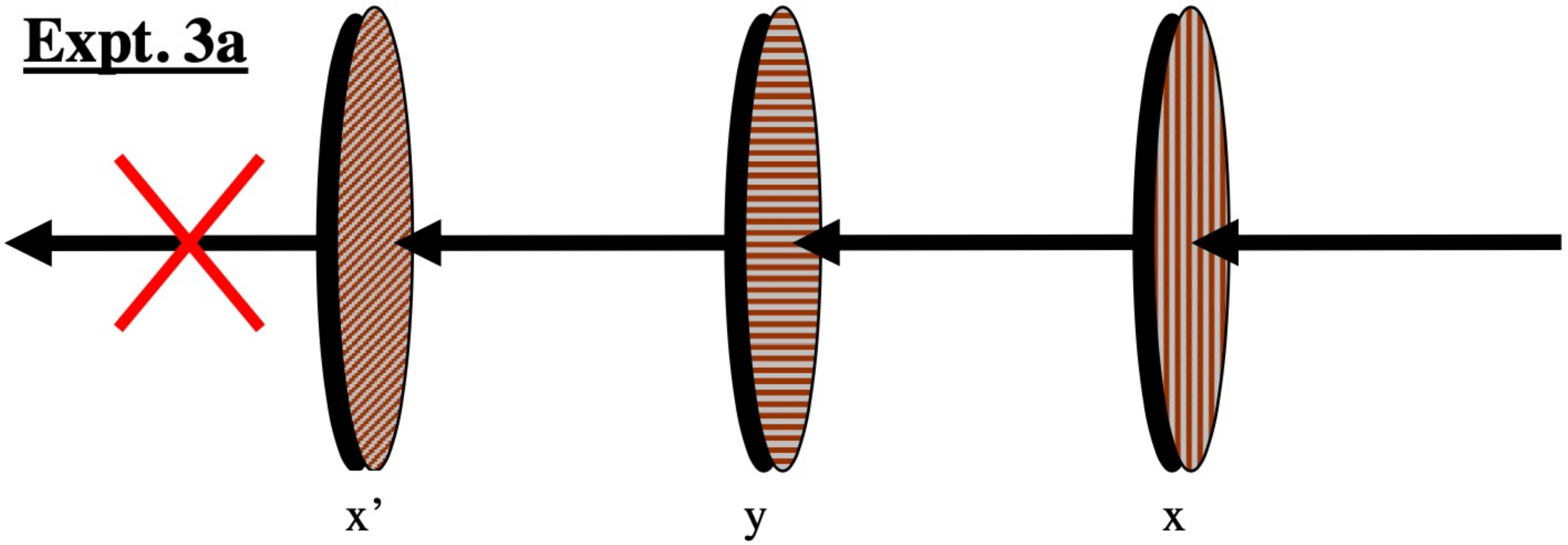
Let's take the beam of light produced in Expt. 2 and measure its polarization in the *y* direction. Will we get some light?



$$Output = \ Operation\ 2 \times Operation\ 3 \times Operation 1 \times Input$$

Experiment 03a: Three Polarization measurements

Let us swap y and x’ polarizer. Will we get any light?



$$Output = \; Operation\ 3 \times Operation\ 2 \times Operation1 \times Input$$

How do explain these results?

- This referred to as three-polarizer paradox. It was proposed by Dirac.
- He proposed to explain the importance of operations (operators) in Q.Mech.
- Experimental observations do not commute with one another.
  The action of applying the y-filter does not commute with the use of an x'-filter.
- We know the numbers commute with each other. However, matrices do not commute.
- Unlike C. Mech., operations in Q.Mech are not represented by numbers, instead by matrices!
- In Q.Mechs: All observables are associated with operators.

What is an Operator?

It is a rule that transforms a given function into another function.

Examples:

1. $\hat{D}$ be an operator that differentiates a function: $\hat{D} f(x) = g(x)$

$$\hat{D}(x^2 + 3) = 2\,x$$

2. Let $\hat{3}$ be an operator that multiples a function by 3.

$$\hat{3}(x^2 + 3) = 3\,x^2 + 9$$

3. If a general operator $\hat{O}$ transforms function $f(x)$ to g(x) we write

$$\hat{O} f(x) = g(x)$$

Momentum Operator (detailed derivation at the end)

$$\Psi = e^{i(kx-\omega t)}$$

$$\frac{\partial \Psi}{\partial x} = \frac{\partial}{\partial x}\left(e^{i(kx-\omega t)}\right) = ike^{i(kx-\omega t)} = ik\Psi = i\frac{p}{\hbar}\Psi$$

$$p\Psi = -i\hbar\frac{\partial \Psi}{\partial x}$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

Energy (Hamiltonian) Operator

$$\Psi = e^{i(kx-\omega t)}$$

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}\left(e^{i(kx-\omega t)}\right) = -i\omega e^{i(kx-\omega t)} = -i\omega\Psi = -i\frac{E}{\hbar}\Psi$$

$$E\Psi = i\hbar\frac{\partial \Psi}{\partial t}$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

Time independent Schrödinger equation

Separating Time and Spatial Derivatives

- We are seeking solutions (wave functions) to the 1-D Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x)\,\Psi(x,t)$$

- Since potential is time-independent, we assume $\Psi(x,t) = \psi(x)\,\phi(t)$

- Let us define $\dot{\phi}(t) \equiv \dfrac{d\phi(t)}{dt}, \psi'(x) \equiv \dfrac{d\psi(x)}{dx}$

Separating Time and Spatial Derivatives

- Substituting this in the first equation, we have:

$$i\hbar\frac{\dot{\phi}}{\phi} = -\frac{\hbar^2}{2m}\frac{\psi''}{\psi} + V(x)$$

- LHS (RHS) depends only on $t(x) \implies$ LHS and RHS must separately be equal to a constant. Let us call the constant E.

- The time-dependence of the wave function is then completely fixed:

$$i\hbar\dot{\phi} = E\phi \implies \phi = Ae^{-iEt/\hbar}$$

Time-independent probability density

- Time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x)$$

- Full solution has time-independent probability density:

$$|\Psi(x,t)|^2 = \Psi(x,t)\Psi^*(x,t) = \psi^*(x)\psi(x)$$

- The normalization becomes an issue of spatial part alone:

$$\int_{-\infty}^{\infty} \Psi(x,t)\Psi^*(x,t)dx = \int_{-\infty}^{\infty} \psi^*(x)\psi(x) = 1$$

Summary: Classical-Mechanical Observables and Their Corresponding Quantum-Mechanical Operators

Observable		Operator	
Name	Symbol	Symbol	Operation
Position	x	$\hat{X}$	Multiply by x
	$\mathbf{r}$	$\hat{\mathbf{R}}$	Multiply by $\mathbf{r}$
Momentum	p_x	$\hat{P}_x$	$-i\hbar\frac{\partial}{\partial x}$
	$\mathbf{p}$	$\hat{\mathbf{P}}$	$-i\hbar(\mathbf{i}\frac{\partial}{\partial x}+\mathbf{j}\frac{\partial}{\partial y}+\mathbf{k}\frac{\partial}{\partial z})$
Kinetic energy	T_x	$\hat{T}_x$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
	T	$\hat{T}$	$-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})$ $=-\frac{\hbar^2}{2m}\nabla^2$

Conservation of Probability: Proof

Probability is conserved

- Since the total probability has to be conserved over entire space there should be a continuity equation like one in electrodynamics due to charge conservation.
- To get this multiply the Schrödinger equation by the complex conjugate of the wave function,

$$\psi^* H\psi = \psi^* i\hbar\frac{\partial\psi}{\partial t} = \psi^*\left[\frac{-\hbar^2\nabla^2}{2m} + V\right]\psi$$

- Now, consider the complex conjugate of this equation.

$$\psi H\psi^* = \psi(-i\hbar\frac{\partial\psi^*}{\partial t}) = \psi\left[\frac{-\hbar^2\nabla^2}{2m} + V\right]\psi^*$$

- If we subtract the complex conjugated equation from the original

Probability current

- We obtain $$i\hbar\frac{\partial(\psi^*\psi)}{\partial t}=\psi^*\frac{1}{2m}\left[-\hbar^2\nabla^2\right]\psi-\psi\frac{1}{2m}\left[-\hbar^2\nabla^2\right]\psi^*$$

- We add and subtract $\frac{\hbar^2}{2m}\nabla\psi^*\cdot\nabla\psi$ to the right hand side, we have

$$i\hbar\frac{\partial(\psi^*\psi)}{\partial t}=\psi^*\frac{1}{2m}\left[-\hbar^2\nabla^2\right]\psi-\frac{\hbar^2}{2m}(\nabla\psi^*\cdot\nabla\psi)$$
$$-\psi\frac{1}{2m}\left[-\hbar^2\nabla^2\right]\psi^*+\frac{\hbar^2}{2m}(\nabla\psi^*\cdot\nabla\psi)$$

- Which can be written as $$i\hbar\frac{\partial(\psi^*\psi)}{\partial t}=-\frac{\hbar^2}{2m}\nabla(\psi^*\cdot\nabla\psi)+\frac{\hbar^2}{2m}\nabla(\psi\cdot\nabla\psi^*)$$

Probability is conserved!

- Define Probability density $\rho = \psi^* \psi,$

  Probability current $\vec{j} = i\frac{\hbar}{2m}(\psi \vec{\nabla} \psi^* - \psi^* \vec{\nabla} \psi)$

- Last equation in the previous slide becomes $\frac{\partial \rho}{\partial t} = -\vec{\nabla} \cdot \vec{j}$

- Like the equation of continuity for charges!
- It shows that the probability density is locally conserved, just like the charge density is.
- So if probability increases somewhere it is because probability flows in from somewhere else.

Momentum Operator

Momentum Operator

- Expectation value <x> of the position of a particle is $$\langle \mathbf{x}(t) \rangle = \int d\mathbf{x}\, \mathbf{x}\, |\Psi^2|$$
- So, how to define <p>?
- In classical mechanics, momentum is defined as $$m\dot{\mathbf{x}} = \mathbf{p}$$
- In quantum mechanics, the expectation of momentum is $$m\langle \dot{\mathbf{x}} \rangle = \langle \mathbf{p} \rangle$$
- The temporal derivative is $$\frac{d}{dt}\langle \mathbf{x}(t) \rangle = \int d\mathbf{x}\mathbf{x} \frac{\partial}{\partial t} |\Psi(\mathbf{x}, t)|^2$$ $$= -\int d\mathbf{x}\mathbf{x} \nabla \cdot \mathbf{j}(\mathbf{x}, t)$$

Momentum Operator

- In deriving the last expression, we used the continuity equation for the probability density

- Partial integration yields $$\frac{d}{dt}\langle \mathbf{x}(t)\rangle = \int d\mathbf{x}\mathbf{j}(\mathbf{x},t)$$

- Using the definition of probability current

$$\frac{d}{dt}\langle \mathbf{x}(t)\rangle = \frac{\hbar}{2mi}\int d\mathbf{x}\left[\Psi(\mathbf{x},t)^*\nabla\Psi(\mathbf{x},t) - \Psi(\mathbf{x},t)\nabla\Psi(\mathbf{x},t)^*\right]$$

- A second partial integration yields

$$\langle p(t)\rangle = m\frac{d}{dt}\langle \mathbf{x}(t)\rangle = \int d\mathbf{x}\Psi(\mathbf{x},t)^*\frac{\hbar}{i}\nabla\Psi(\mathbf{x},t)$$