LECTURE 14: More on Probability Current, Expectation Values and Operators

Goals of the lecture: Complete the background knowledge necessary to solve 1-D problems

What I expect you to learn:

- What is a Hermitian Operator
- What is a commutator
- What is Ehrenfest's theorem (link between QM and classical mech.)

(Roughly corresponds to sections 3.1 to 3.4 of textbook)

PROBABILITY CURRENT DENSITY

RECALL :

$$\frac{\partial}{\partial T}\int_V \rho(\vec{r},t)\, dT\, d\vec{r} = -\int_V \vec{\nabla}\cdot\vec{J}\, d\vec{r} = -\int_S \vec{J}\cdot d\vec{S}$$

Gauss Theorem

in english : THE RATE OF CHANGE OF THE PROBABILITY OF FINDING THE PARTICLE IN VOLUME V IS EQUAL TO THE PROBABILITY FLUX PASSING THROUGH THE SURFACE S BOUNDING V.

$$\vec{J}(\vec{r},t) = \frac{\hbar}{2mi}\left[\psi^*(\vec{\nabla}\psi) - (\nabla\psi^*)\psi\right]$$

$\vec{J}$ → probability current density

ψ^* → prob. density , $\frac{\nabla\psi}{m}$ → velocity

PROBABILITY CURRENT

$\boxed{\text{Example}}$ (will be useful for some 1-d problems) *

What is the probability current for:

a) $\psi(x) = Ae^{ikx} + Be^{-ikx}$, b) $\psi(x) = Ae^{-\alpha x}$
α is real

a: $\frac{\hbar}{2im}\left(\psi^* \frac{d\psi}{dx} - \frac{d\psi^*}{dx}\psi\right)$

$$= \frac{\hbar}{2im}\Big[(A^* e^{-ikx} + B^* e^{ikx})\, ik(Ae^{ikx} - Be^{-ikx}) - ik(A^* e^{-ikx} - B^* e^{ikx})(Ae^{ikx} + Be^{-ikx})\Big]$$

$$= \frac{\hbar k}{2m}\Big[A^*A - B^*B - A^*Be^{-2ikx} + B^*Ae^{2ikx} + A^*A - B^*B + A^*Be^{-2ikx} - B^*Ae^{2ikx}\Big]$$

$$\boxed{= \frac{\hbar k}{m}\left(|A|^2 - |B|^2\right)}$$

b: $\psi^* = \psi$, $\frac{d\psi^*}{dx} = \frac{d\psi}{dx} \Rightarrow \vec{j} = 0$

PROBABILITY CONSERVATION (CONT)

RECALL : $H = T + V = -\frac{\hbar^2}{2m}\nabla^2 + V$

↪ Hamiltonian

$$\Rightarrow i\hbar \frac{\partial}{\partial t}\psi(r,t) = H\psi(r,t)$$

→ complex conjugate $= -i\hbar \frac{d\psi^*}{dt} = (H\psi)^*$

we have:

$$\frac{\partial}{\partial t}\int P(r,t)\,dr = \frac{\partial}{\partial t}\int |\psi(r,t)|^2\,dr$$

$$= \int \left[\psi^*\left(\frac{\partial\psi}{\partial t}\right) + \left(\frac{\partial\psi^*}{\partial t}\right)\psi\right] dr$$

$$= \int \left[\psi^* \frac{H}{i\hbar}\psi + \frac{1}{-i\hbar}(H\psi)^*\psi\right] dr$$

$$= \frac{1}{i\hbar}\int \left[\psi^* H\psi - (H\psi)^*\psi\right] dr = 0$$

$$\Rightarrow \int \psi^*(H\psi)\,dr = \int (H\psi)^*\psi\,dr$$

Operators with this property are Hermitian operators

HERMITIAN OPERATORS

WE JUST SAW THAT PROBABILITY CONSERVATION IMPLIED THAT H WAS A HERMITIAN OPERATOR.

WHAT ABOUT THE POSITION OPERATOR "x" i.e.

$$\langle x \rangle = \int \psi^* x \psi \, dx$$

→ x gives real values for the position ⇒ HERMITIAN

$$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \, dx$$

→ what about momentum operator?

$$\langle p \rangle = \int \varphi(p)^* \, p \, \varphi(p) \, dp$$ → p is HERMITIAN

NOTE:

- THE AVERAGE OF OBSERVABLES HAVE TO BE REAL
- THE EIGENVALUES OF HERMITIAN OPERATORS ARE REAL

HERMITIAN OPERATORS (CONT.)

WE WILL POSTULATE THE FOLLOWING (more on QM postulates in 2 weeks):

- To a physical quantity represented by a dynamical variable $A(\vec{r}, \vec{p}, t)$ we associate a linear operator:

$$A(\vec{r}, -i\hbar\vec{\nabla}, t)$$

linear: $A(c_1\psi_1 + c_2\psi_2) = c_1(A\psi_1) + c_2(A\psi_2)$

- We obtain the expectation value from A this way:

$$\langle A \rangle = \int \psi^*(\vec{r}, t)\, A(\vec{r}, -i\hbar\vec{\nabla}, t)\, \psi(\vec{r}, t)\, d\vec{r}$$

- The results of measurements of A (and therefore $\langle A \rangle$) must be real quantities so A must be Hermitian

OPERATORS AND PHYSICAL QUANTITIES

PHYSICAL QUANTITY	OPERATOR
position coordinate x, r	$x \, , \, r$
momentum $p_x \, , \, \vec{p}$	$-i\hbar \frac{\partial}{\partial x} \, , \, -i\hbar \vec{\nabla}$
Kinetic Energy $= T = \frac{p^2}{2m}$	$-\frac{\hbar^2}{2m} \nabla^2$
Potential Energy $V(\vec{r},t)$	$V(\vec{r},t)$
Total Energy $\frac{p^2}{2m} + V(\vec{r},t)$	$H = \frac{-\hbar^2}{2m} \nabla^2 + V(\vec{r},t)$
etc.	etc.

Ehrenfest Theorem: relations between CM and QM

CM (classical mech.)	QM
$\vec{v} = \frac{d\vec{r}}{dt} = \frac{\vec{p}}{m}$	$\frac{d\langle r \rangle}{dt} = \frac{\langle p \rangle}{m}$
$\vec{F} = m\vec{a} = \frac{d\vec{p}}{dt} = -\nabla V$	$\frac{d\langle p \rangle}{dt} = -\langle \nabla V \rangle$

MORE ON OPERATORS (an aside and a look forward)

We will soon represent a quantum state by a vector: $|\psi\rangle$ → Dirac notation

We will often represent operators by matrices. For instance, when we deal with angular momentum.

Let's look at an operator you can relate to:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$O(2)$ → rotations in 2D

A Hermitian matrix (representing a Hermitian op.) is equal to its conjugate transpose. Example:

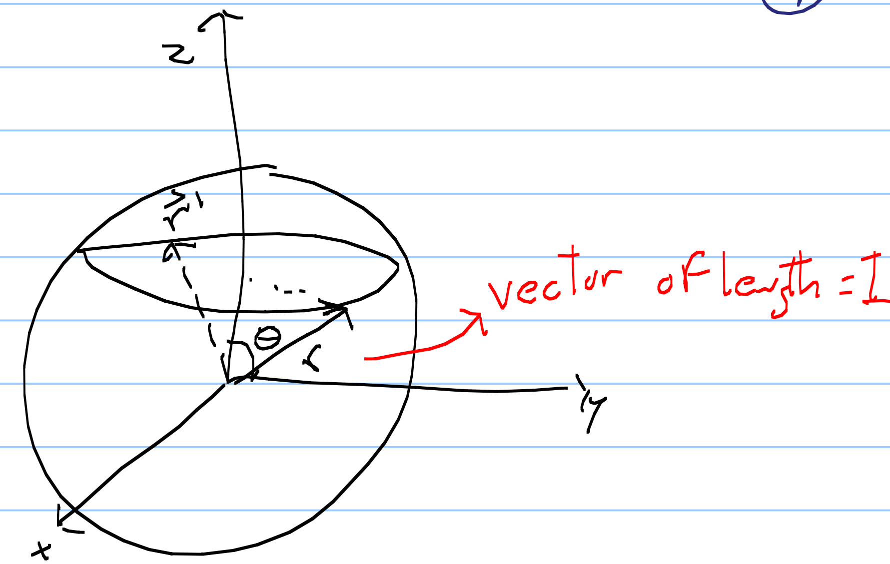
$$\begin{pmatrix} 3 & 2+i \\ 2-i & 1 \end{pmatrix} \xrightarrow{\text{Transpose}} \begin{pmatrix} 3 & 2-i \\ 2+i & 1 \end{pmatrix} \xrightarrow{\text{C.C}} \begin{pmatrix} 3 & 2+i \\ 2-i & 1 \end{pmatrix}$$

Diagonal entries are real and eigenvalues are real

OPERATORS (a look forward)

Eigenvalue example:

OPERATOR R ROTATES $\vec{r}$ ABOUT POLAR AXIS BY A DISTANCE $= \pi$ ALONG A FIXED LATITUDE



1- WHAT ARE THE EIGENVALUES?

i.e. $R\vec{r} = \lambda\vec{r}$ → length of vector does not change $\Rightarrow x'^2 + y'^2 = x^2 + y^2$, $r'^2 = r^2 = 1$

$\Rightarrow \lambda^2 = 1$, $\lambda = \pm 1$

2- FOR WHAT VALUES OF θ do we satisfy $R\vec{r} = \lambda\vec{r}$?

- $\theta = 0$ with $\lambda = -1$
- for $\lambda = 1$ we want $\pi = n(2\pi \sin\theta)$

$\sin\theta = \frac{1}{2n}$ $n = 1, 2, 3, \ldots$

All vectors (eigenvectors) with $\theta = 30°$ will satisfy

OPERATORS (a look forward cont.)

- In quantum mechanics, we associate an operator to a physical quantity (this operator is linear and Hermitian)

- The values we can observe and eigenvalues of that operator. The values are real since the operator is Hermitian

We will see that an energy measurement for the infinite well problem will yield an energy eigenvalue and will put the system in an energy eigenstate (an eigenvector of the Hamiltonian operator)

Commutators

A big difference between QM and CM comes from the fact that the QM operators associated with physical quantities do not commute

Everyday examples of non-commutation:

- At the dentist:

  novacaine, extract tooth $\neq$ extract tooth, novacaine

- rotations in 3 dimensions

Define a commutator as

$$[A, B] = AB - BA$$

if A, B are 2d rotations $\rightarrow [A, B] = 0$

if A, B are 3d rotations, $[A, B]$ can be $\neq 0$

COMMUTATORS (CONT.)

QM example with x and p $\left(p \to -i\hbar \frac{\partial}{\partial x}\right)$

$$[x, p]\psi = (xp - px)\psi$$

$$= -i\hbar\left[x\frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}(x\psi)\right]$$

$$= -i\hbar\left[x\frac{\partial \psi}{\partial x} - \psi - x\frac{\partial \psi}{\partial x}\right]$$

$$= -i\hbar\psi$$

$$[x, p] = -i\hbar$$

THIS NON-COMMUTATIVE BEHAVIOUR IS AT HEART OF QUANTUM PHYSICS. IT IS DIRECTLY RELATED TO THE HEISENBERG UNCERTAINTY PRINCIPLE

Mid-Term Exam Information

Will be on Wednesday Oct 25th at 11:00 in class

Will cover everything we have seen up until now

In the textbook, this corresponds to sections 1.0 to 3.4

The problem sets represent good examples of what could be exam questions. The examples done in the notes or on the blackboard too.

I will provide a list of formulas (integration formulas, trigonometry, complex plane relations etc.)

You are allowed an non-programmable calculator

Practice Midterm (will post solutions next week):

Q1: Describe the the experiment performed by Davisson and Germer and the results they obtained. Explain qualitatively why this demonstrated that electrons exhibited wave-like behaviour

Q2:Using the Bohr Model, calculate the energy levels of a system consisting of the bound state of two quarks (elementary particles) with the same mass and interacting via the potential V(r) = kr (k is a constant)

Q3: A wave function is given by: $\psi(x) = A e^{-\mu|x|}$

Find A and find $\phi(p)$

Q4: Using $\langle x \rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\, x\, \psi(x,t)\, dx$

show that $\langle p \rangle = -i\hbar \int_{-\infty}^{\infty} \psi^*(x,t) \frac{\partial}{\partial x} \psi(x,t)\, dx$