## BASICS OF QUANTUM MECHANICS

Reading:<br>QM Course packet - Ch 5



Interesting things happen when electrons are confined to small regions of space (few nm). For one thing, they can behave as if they are in an artificial atom.
They emit light of particular frequencies ... we can make a solid state laser!


A Quantum Well Structure



## Particles exhibit many wave-like properties, e.g. electron diffraction.



Diffraction pattern of X-ray beam passing through Al foil


Diffraction pattern of electron beam passing through: Al foil


Electron diffraction geometry


S- G expt (spin)


Single slit (position)


In a quantum-mechanical system, the measurement we may be concerned with is "position", for which there are (infinitely) many options, not just two, as in the spin-1/2 SG system!

## Quantum Mechanics - kets and operators

The state of electron is represented by a quantity called a state vector or a ket, $|\psi\rangle$, which in general is a function of many variables, including time.

In PH425, you learned about kets that contained information about a particle' s spin state. We' ll be interested in the information contained in the ket about the particle position, momentum and energy, and how the ket develops in time.

In PH 425, you learned about the spin operators $\mathrm{S}^{2}, \mathrm{~S}_{\mathrm{z}}, \mathrm{S}_{\mathrm{x}}$ etc. We' 11 be learning about the position, momentum and energy operators.

In PH425, you represented operators as matrices (in different bases), and kets as column vectors. We will learn to represent operators as mathematical instructions (for example derivatives), and kets as functions (wavefunctions).

## Quantum Mechanics - kets and operators

You will learn to translate all the terms you learned in PH425' s matrix formulations into the wave formulation. These include
Matrix operators -> mathematical instructions
Eigenvectors -> eigenfunctions
Basis states $->$ basis functions
Eigenvalues -> Eigenvalues
Orthogonal basis states $->$ orthogonal basis functions
Projections of kets/vectors $->$ Projections of kets/functions
Measurement $->$ measurement
Superposition -> superposition of functions

The concepts from the first part of PH 424 will be relevant:
Wave equation -> Schroedinger's wave equation
Dispersion relation
Initial conditions and boundary conditions
Reflections and transmission
Fourier analysis

## Some terminology and definitions

Each of the operators has a complete set of eigenstates, and any set can be use to expand the general state.
$|x\rangle$ are the position eigenstates (states of definite position)
$\hat{x}$ is the position operator
$|p\rangle$ are the momentum eigenstates (definite momentum)
$\hat{p}$ is the momentum operator
$|\phi\rangle$ are the energy eigenstates (definite energy)
$\hat{H}$ is the energy operator
$|x\rangle$ is a ket that is the eigenstate of position

$$
\left|x_{2}\right\rangle \doteq\left(\begin{array}{c}
0 \\
1 \\
\vdots \\
0
\end{array}\right) \begin{gathered}
<-x_{1} \\
<-x_{2} \\
\vdots \\
<-x_{N}
\end{gathered}
$$

In the spins course notation, this ket represents a particle that is located precisely at position $x_{2}$.

Reminds you of a delta function, doesn't it?! Well, it should!
$|x\rangle$ is a ket that is the eigenstate of position
$\left\langle x_{1} \mid \psi\right\rangle \quad$ is a number that represents the projection of the state vector onto the ket $\left|x_{1}\right\rangle$

$\psi(x)$. We've represented the general state vector in a graphical form by projecting onto position eigenstates. This the "position representation". Careful, though ... $\psi(x)$ can be complex, so we have to plot both the real and imaginary parts for a full representation.

$$
\psi(x)=\langle x \mid \psi\rangle
$$

Then what is $\langle\psi \mid x\rangle$ ?

$$
\langle\psi \mid x\rangle=\langle x \mid \psi\rangle^{*}=\psi^{*}(x)
$$

Then we have the following identifications (not equalities)

$$
\begin{gathered}
|\psi\rangle \doteq \psi(x) \\
\langle\psi| \doteq \psi^{\prime \prime}(x)
\end{gathered}
$$

$\psi(x)$ is NOT a physically accessible quantity; we cannot measure it in the laboratory. The physically meaningful quantity is $|\psi(x)|^{2}$. This is the probability density - the probability per unit volume in 3D (or probability per unit length in 1D) of finding the particle in an infinitesimally small region located at $x$.

$$
\wp(x) \equiv \psi^{*}(x) \psi(x)=|\psi(x)|^{2}
$$

The probability of finding this particle somewhere in the universe must be 1 . This statement is represented by:

$$
\int_{-\infty}^{\infty} \wp(x) d x=\int_{-\infty}^{\infty} \psi^{*}(x) \psi(x) d x=1
$$

In bra-ket notation: $\quad\langle\psi \mid \psi\rangle=1$
This suggests that $\langle\mid\rangle \rightarrow \int_{-\infty}^{\infty} d x$

Examples .............
These 1-D wave functions are NOT properly normalized. Normalize them!
$\psi(x)=\left\{\begin{array}{cc}0 & x<0 \\ \sin \left(\frac{3 \pi x}{L}\right) & 0<x<L \\ 0 & x>L\end{array}\right.$
$\psi(x)=\left\{\begin{array}{cc}0 & x<-L / 2 \\ \cos \left(\frac{\pi x}{L}\right) & -L / 2<x<L / 2 \\ 0 & x>L / 2\end{array}\right.$
We don't know (yet) how to find wave functions for any systems - we'll get there!

This the probability density also tells us about the probability of finding a particle in a certain region of space, say between $x=a$ and $x=b$.

$$
\wp_{a<x<b}=\int_{a}^{b} \wp(x) d x=\int_{a}^{b} \psi *(x) \psi(x) d x
$$

Notation alert: Script P with an argument of $x$ is used for probability density. The same script P with no $x$ argument is used for probability. They have different dimensions!

We will state two things without proof, and you'll see why they are reasonable, later.

1. In the "position representation" or "position basis", the position operator is represented by the variable $x$ :

$$
\hat{x} \doteq x
$$

2. In the "position representation" or "position basis", the momentum operator is represented by the derivative with respect to $x$ :

$$
\hat{p} \doteq-i \hbar \frac{d}{d x}
$$

3. This follows if you accept (2). The energy operator is:

$$
\hat{H}=\frac{\hat{p}^{2}}{2 m}+\hat{V} \doteq-\frac{\hbar^{2}}{2 m} \frac{d^{2}}{d x^{2}}+V(x)
$$

Now think about eigenfunctions of these operators (worksheet)

If the momentum operator operates on a wave function and IF AND ONLY IF the result of that operation is a constant multiplied by the wave function, then that wave function is an eigenfunction or eigenstate of the momentum operator, and its eigenvalue is the momentum of the particle.

$$
\hat{p} \emptyset(x)=\widehat{P}(x) \longrightarrow \text { eigenfunction }
$$

operator

$$
-i \hbar \frac{d \varphi(x)}{d x}=C \varphi(x) \Rightarrow \varphi(x)=A e^{i C x / \hbar}
$$

- not all states are eigenstates - and if they are not, they can be usually be written as superpositions of eigenstates
- if a state is an eigenstate of one operator, (e.g. momentum), that state is not necessarily an eigenstate of another operator (e.g. energy), though it may be.

Look more closely at the momentum eigenfunction or eigenstate:

$$
\varphi_{p}(x)=A e^{ \pm i p x / \hbar}
$$

1. Why did we change $C$ to $p / h b a r$ ? And why the subscript?
2. What is the probability distribution for this state?
3. Is it normalized? Normalizable?
4. It is degenerate (new word, maybe?)
5. What sort of particle would be represented by this function?

Position eigenstates:
This is a useful (but a bit pathological) representation of a position eigenstate:

1. Normalizable? $\varphi_{x^{\prime}}(x)=\delta\left(x-x^{\prime}\right)$
2. Otherwise reasonable?

## BASICS OF QUANTUM MECHANICS REVIEW

- Review language of PH425
- Kets and wave functions
- Probability density
- Operators - position, momentum, energy
- Eigenfunctions
- Mathematical representations of the above

