You should take good notes to save the time reading Quantum Mechanics a book on QM!

* Shrödinger Eq.

\[
\left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})\right] \psi(\vec{r}, t) = i\hbar \frac{\partial}{\partial t} \psi(\vec{r}, t)
\]

\[\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\]

\[\nabla^2 =\]

Meaning of \(\psi(\vec{r}, t)\); Randomness!

1-D case:

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi}{d x^2} + V(x) \psi(x, t) = i\hbar \frac{\partial \psi}{\partial t}\]

Looks similar to a wave equation!

You can guess:

\[\psi(x, t) = \psi(x) e^{-i \frac{E}{\hbar} t} = \psi(x) e^{-i \omega t}\]

\[\frac{\partial \psi(x, t)}{\partial t} = -i \frac{E}{\hbar} \psi(x) e^{-i \frac{E}{\hbar} t}\]

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

It turns out that \(E\) is the energy:

\[E = \hbar \omega\]
This eq. gives us the concept of the stationary states. $\Psi(x)$

A special case — free space

$$\frac{\hbar^2}{2m} \frac{d^2 \Psi}{dx^2} = E \Psi$$

looks like a plane wave.

Guess:

$$\Psi(x) = e^{ikx}$$

$$\frac{d^2 \Psi}{dx^2} = -k^2 \Psi(x)$$

$$\frac{\hbar^2 k^2}{2m} \Psi = E \Psi$$

Wow:

$$p^2 = \hbar^2 k^2$$

$$p = \hbar k = \hbar \frac{2\pi}{\lambda} = \frac{\hbar}{\lambda}$$

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

Notice the difference between this wave and the electromagnetic plane wave.
**EM wave**

\[ f = \frac{c}{\lambda} = c \frac{k}{2\pi} \]

\[ w = ck \]

\[ E = cp \]

\[ E = \hbar w \]

\[ p = \hbar k \]

**De Broglie wave**

\[ E = \frac{p^2}{2m} \]

\[ \hbar w = \frac{\hbar^2 k^2}{2m} \]

\[ w = \frac{\hbar}{2m} k^2 \]

quadratic

\[ v_g \neq v_p \]

\[ v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m} \]
Notice that $p = \hbar k$ \& $E = \hbar kw$ are just two parameters in the solution.

They can assume any value.

For each value, the solution

\[ \psi(x, t) = e^{i(kx - wt)} \]

is called an "eigensate."

In general,

\[ \psi(x, t) = \sum_k c_k e^{i(kx - wt)} \]

We will come back to this later.

Important concept in scattering theory.
For an electron w/ a well defined momentum $p = \hbar k$.

$$|e^{ikx}|^2 = 1$$

It can be anywhere!

**Constant probability!**

A paradox?!

In physical reality, an electron just can't have a well defined $p$.

Wave packet.
\[ \psi(x) = e^{ikx} \quad \Rightarrow \quad \Phi(k) \]

On the other hand, if an electron had a well-defined position,

\[ \psi(x) = \delta(x) \]

\[ \Rightarrow \quad \Psi(k) = e^{-ikx} \]

The momentum can be anything.

A real electron is something between these 2 extremes.

Something call a wave packet.
A Gaussian wave packet.

\[ \psi(x) = e^{-\frac{1}{2} \alpha^2 x^2} \]

\[ |\psi(x)|^2 = e^{-\alpha^2 x^2} \]

\[ \Downarrow \text{Fourier Transform.} \]

\[ \Psi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\frac{1}{2} \alpha^2 x^2} e^{-ikx} \, dx \]

\[ = \frac{1}{\alpha} e^{-\frac{k^2}{2\alpha^2}} \]

\[ |\Psi(k)|^2 = \frac{1}{\alpha^2} e^{-\frac{k^2}{\alpha^2}} \]

\[ \Delta k \sim \frac{1}{\alpha} \]

\[ \Delta x \cdot \Delta k \sim 1 \]
This is the famous uncertainty principle.

\[ x \Delta x \sim 1, \]

\[ \Delta x \Delta p \sim h. \]

Gaussian analysis is just for mathematical convenience.

The conclusion is more general.

Just as in signals & systems,

- time domain vs. freq. domain

\& The momentum is actually special frequency of the wave !!!

Bare this in mind!
More on wave packets

View an electron as a wave packet.
The electron moves at the group velocity of the wave packet.
Recall that

$$v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m} = \frac{p}{m}$$
Review of Semiconductor Physics

**Quantum mechanics**

A few more things:

- Bound states
- Atoms; Coulomb potential
- Normalization of bound state wavefunctions
- Unbound states
- Difficulty of normalization of unbound states and the way around it
- $i$ vs. $j$; physics vs. EE
- More quantum mechanics jargons you need to know
  - Eigenstates
  - Operators, eigenvalues
    - Solving Shrödinger Eq is to find the eigenvalues of the Hamiltonian operator.
- Spin
  The electron has an **intrinsic** angular momentum, with a value $\hbar/2$. Along any direction, spin has two eigenvalues, $\pm \hbar/2$. 
**Bound states**

\[ \int_{\text{all space}} |\psi(\vec{r})|^2 d^3\vec{r} = 1 \]

Note: Normalize \( |\psi|^2 \), not \( \psi \) per se.

Atoms, Coulomb

**Unbound states**

\[ \int_0^\infty e^{ikx} dx = \infty \]

Confine it in \( L \)

\[ \psi(x) = \frac{1}{L} e^{ikx} \]

\[ \int_0^L \left( \frac{1}{L} e^{ikx} \right)^2 dx = 1 \]
in 3-D.

\[ \Psi (\vec{r}) = \frac{1}{\sqrt{V}} e^{i \vec{k} \cdot \vec{r}} \]

notice \( \vec{k} \) is a vector!

\[ \int_{V} \frac{1}{\sqrt{V}} e^{i \vec{k} \cdot \vec{r}} \, d^3r = 1 \]
i vs. j

To describe a plane wave
\( e^{+i(kx - wt)} \)
\( e^{-i(kx - wt)} \) are ok.

In QM, we study the spatial part more
\( \rightarrow \) stationary states

People don't like carrying the neg sign around. So we use
\( e^{i k x} \) or \( e^{i k r} \)

In EE, we deal more with the time part.
we use \( e^{jut} \)

If you say \( j = -i \), you can almost always reconcile physics & EE books.
A solution of the stationary Schrödinger equation is an energy eigenstate:

\[-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r}) \psi = E \psi\]

Let take a guess:

\[\left[-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\vec{r})\right] \psi(\vec{r}) = E \psi(\vec{r})\]

Kinetic energy = \(\frac{\vec{p}^2}{2m}\)

Treat the operator as a multiplying factor.

If \(\vec{p} = i\hbar \nabla\)

\[\frac{\vec{p}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2\]

Now we define operators

\[\hat{\vec{p}} = i\hbar \nabla\]

\[\hat{\mathcal{H}} = \frac{\vec{p}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})\]
Now, the stationary Schrödinger equation can be written as

$$\hat{H} \psi (\vec{r}) = E \psi (\vec{r})$$

To find the Eigenvalues for the Hamiltonian operator $\hat{H}$.

Later, when talk about Bloch, mention that only for free space, $\hat{H}$ & $\hat{p}$ have simultaneous eigenstates.

If a system is described by $\hat{H}$, it can only exist in linear superpositions of eigenstates of $\hat{H}$.

$$\psi (\vec{r}, t) = \sum_n c_n(t) \Psi_n (\vec{r})$$

$$\hat{H} \Psi_n (\vec{r}) = E_n \Psi_n (\vec{r})$$
When you measure the energy, you will get any $E_n$. But you never know what you'll get. You can only know the probabilities $|C_n(t)|^2$.

Spin:

$$\begin{pmatrix} a \\ b \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix} + b \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$= a \ket{\uparrow} + b \ket{\downarrow}$$

Right hand rule:

$$|a|^2 + |b|^2 = 1$$

Guess: for (0), (1), and $\frac{1}{\sqrt{2}} \ket{\uparrow}$, what are the P's?
Review of Semiconductor Physics

Quantum mechanics

Homework

Solve the Shrödinger eq for the following special cases:
1. 1D infinitely deep well
2. 1D finite well
3. 1D harmonic oscillator (optional)
4. 3D infinitely deep and finite well
5. Barrier tunneling

For 1., complete the math, visualize results, draw analogy with the electromagnetic resonant cavity (e.g. short or open terminated transmission line segments).
For 2., find and read thru the math in a book, visualize results, compare to the dielectric cavity (or a general transmission line)
For 3., find and read thru the math in a book, visualize results; compare to the above and get some sense of how energy level spacing is related to the shape of the potential.
For 4., generalize and visualize as much as you can. Also compare to optical (or EM cavities).
For 5., visualize results and discuss physical meanings.