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

Quantum Mechanics... a book on QM!

- Schrödinger Eq.

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

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

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

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

1-D case:

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

Looks similar to a wave equation:

You can guess:

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

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

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

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

\[
E = \hbar \omega
\]
This equation 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.

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

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

$$(kx - \omega t)$$

$$\psi(x, t) = e$$

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

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

\[ w = ck \]

\[ E = cp \]

\[ E = \hbar w \]

\[ p = \hbar k \]

**De Broglie wave**

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

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

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

quadratic

\[ v_g \neq v_p \]
Notice that $p = \hbar k$ & $E = \hbar k w$ 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 "eigenstate."

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 $p = \frac{\hbar}{k}$.

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

It can be anywhere!

A constant probability!

A paradox?!

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

Wave packet.
\( \Psi(x) = e^{ikx} \) Fourier Transform \( \Psi(k) \)

If an electron had a well-defined position,

\( \Psi(x) = \delta(x) \)

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

On the other hand, the momentum can be anything.

A real electron is something between these two extremes.

Something call a wave packet
A Gaussian wave packet

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

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

\[ \downarrow \text{Fourier Transform} \]

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

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

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

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

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

\[ \Delta x \Delta k \approx 1 \]

\[ \Delta x \Delta p \approx \hbar \]

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 spatial frequency of the wave!!!

Bare this in mind!
**Bound states**

\[ \int \left| \psi(\vec{r}) \right|^2 d^3\vec{r} = 1 \]

*all space*

Note: Normalize

\[ |\psi|^2, \]

not \( \psi \) per se.

atoms, Coulomb

**Unbound states**

\[ \int_{-\infty}^{\infty} e^{ikx} = \infty \]

Confine it in \( L \)

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

\[ \int_{-L}^{L} \left| \frac{1}{\sqrt{L}} e^{ikx} \right|^2 = 1 \]
in 3-D.

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

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

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

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

In QM, we study the spatial part more → stationary states.

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

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

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

\[-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = E \Psi\]

Let take a guess

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

Kinetic energy = \[\frac{p^2}{2m}\]

Treat the operator as a multiplying factor.

If \[p = i\hbar \nabla\]

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

Now we define operators

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

\[\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r})\]
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.

\( \Psi \) 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 $|C_n(t)|^2$.

\[ \begin{pmatrix} a \\ b \end{pmatrix} = a \left( \begin{array}{c} 1 \\ 0 \end{array} \right) + b \left( \begin{array}{c} 0 \\ 1 \end{array} \right) \]

\[ = a \left| \uparrow \right> + b \left| \uparrow \downarrow \right> \]

right hand rule

\[ |a|^2 + |b|^2 = 1 \]

Guess, for $\left( \begin{array}{c} 1 \\ 0 \end{array} \right)$, $\left( \begin{array}{c} 0 \\ 1 \end{array} \right)$ and $\frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ 1 \end{array} \right)$, what are the P's?
Solid State Physics is about many-body problems.

The equation for 3 particles:

\[ \psi = \psi (\vec{r}_1, \vec{r}_2, \vec{r}_3) \]

\[ \vec{r}_0 = x \hat{x} + y \hat{y} + z \hat{z} \]

\[ -\frac{\hbar^2}{2m} \left( \nabla_1^2 + \nabla_2^2 + \nabla_3^2 \right) \psi \]

\[ + \frac{1}{4\pi \varepsilon_0} \left( \frac{\phi_1 \phi_2}{|\vec{r}_1 - \vec{r}_2|} + \frac{\phi_2 \phi_3}{|\vec{r}_2 - \vec{r}_3|} + \frac{\phi_3 \phi_1}{|\vec{r}_3 - \vec{r}_1|} \right) \psi \]
Quiz for next class mtg.

Other special cases:

1-D infinite well

1-D finite well

1-D harmonic oscillators

1-D general well

3-D general well

Barrier tunneling
Crystal structure.

Bravais lattices

\[ \vec{R} = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \]

1D

The unit cell is any segment \( \vec{a} \) of length \( a \).

2D

The unit cell is any area \( \vec{a} \times \vec{b} \).
3D