

Quantum Mechanics

- Particles are waves $\psi(x,t)$.

$$|\psi(x,t)|^2 = \text{Probability to find a particle at point } x$$

- Position and momentum are operators which act on waves

$$\hat{P} \psi(x,t) = -i\hbar \frac{\partial}{\partial x} \psi(x,t)$$

$$\hat{X} \psi(x,t) = x \psi(x,t)$$

- operators take waves and spit out transformed waves

- The wave function changes in time, physics predicts this change

$$\left(\frac{\hat{P}^2}{2m} + \hat{V}(x) \right) \psi(x,t) = i\hbar \frac{\partial}{\partial t} \psi(x,t)$$

→ The Hamiltonian = KE + PE

The Schrödinger equation:

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

How to Find the average of an operator:

$\langle \hat{X} \rangle$ = average position of particle

$$= \int dx \psi^*(x,t) \hat{X} \psi(x,t)$$

$$\langle \hat{X} \rangle = \int dx x |\psi|^2$$

$\langle \hat{P} \rangle$ = Average momentum of a particle

$$\langle \hat{P} \rangle = \int dx \psi^*(x,t) \hat{P} \psi(x,t)$$

$$= \int dx \psi^*(x,t) -i\hbar \frac{\partial}{\partial x} \psi(x,t)$$

"Eigenstates" of Operators:

$$\hat{\Omega} \phi_{\omega}(x) \propto \phi_{\omega}(x) \quad \text{or} \quad \hat{\Omega} \phi_{\omega}(x) = \omega \phi_{\omega}(x)$$

- certain functions that when you act with an operator you get back the same function times a number
- Example #1, Eigenstates of the Hamiltonian

$$\hat{H} \phi_E(x) = E \phi_E(x)$$

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

↑ Also known as the Schrödinger equation

- Example #2, Eigenstates of momentum

$$\hat{P} \phi_p(x) = p \phi_p(x)$$

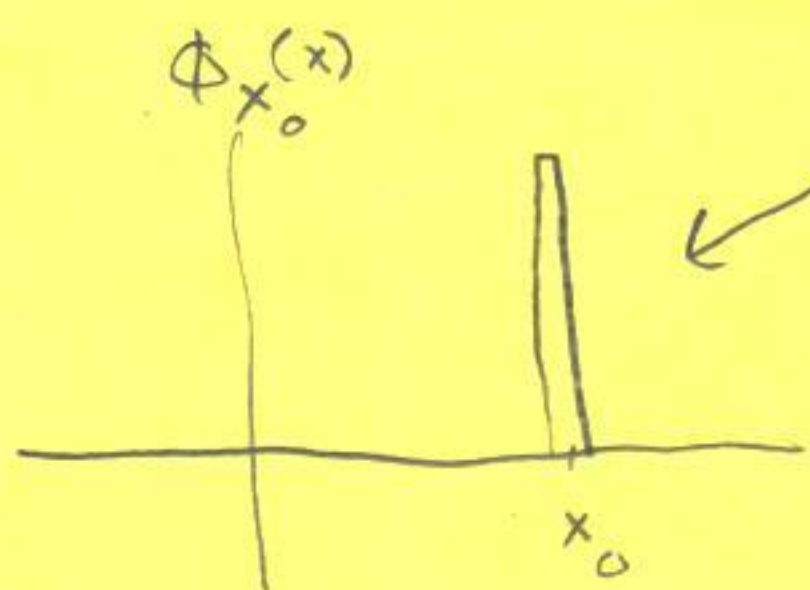
$$-i\hbar \frac{\partial}{\partial x} \phi_p(x) = p \phi_p(x) \quad \leftarrow \text{Differential equation for } \phi_p(x)$$

$$\text{So } \phi_p(x) = C e^{-ip \cdot x / \hbar}$$

↑ we will come back to the normalization in a bit

Example 3

- Eigenstates of \hat{X}

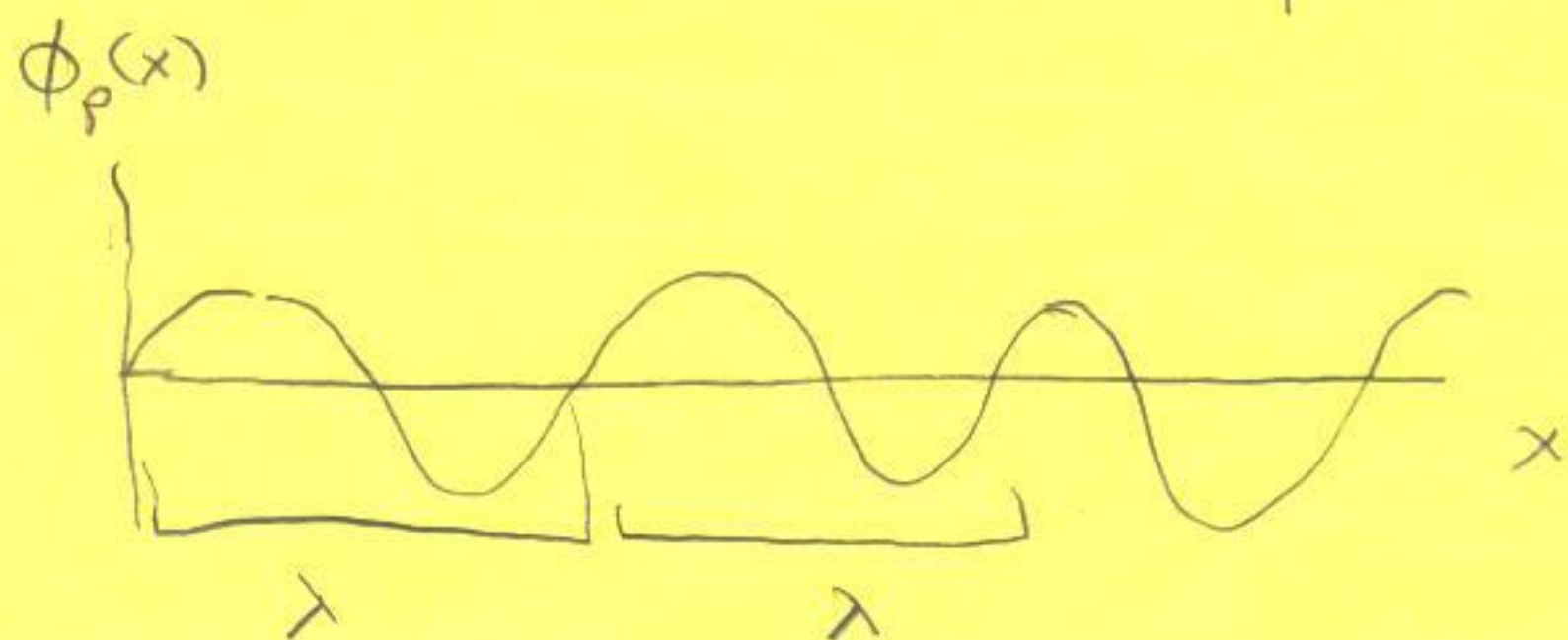


Very sharply peaked function at x_0

$$\hat{X} \phi_{x_0}(x) = x \phi_{x_0}(x) \approx x_0 \phi_{x_0}(x)$$

Then

- Take position \hat{X} , functions which are eigenstates $\phi_{x_0}(x)$ have definite position, x_0 .
- Take momentum \hat{P} , $\phi_p(x) = C e^{i \frac{p_0 x}{\hbar}}$



$\phi_p(x)$ has definite wave length λ

(most functions don't)



$$\lambda = \frac{2\pi \hbar}{p}; \quad \text{definite wavelength} = \text{definite momentum}$$

de Broglie

$$\lambda = \frac{h}{p}$$

Why do we care about Energy Eigenstates?

Suppose that at time $t=0$ we are in a energy eigenstate $\phi_E(x)$

$$\psi(x, t_0) = \phi_E(x)$$

Then at later times we try to solve the Schrödinger Equation

$$\hat{H} \psi(x, t) = i\hbar \frac{\partial \psi(x, t)}{\partial t}$$

Ansatz:

$$\psi(x, t) = \phi_E(x) c(t) \quad c(t_0) = 1$$

$$\hat{H} \psi(x, t) = i\hbar \frac{\partial \psi}{\partial t}$$

$$\hat{H} \phi_E c(t) = i\hbar \phi_E \partial_t c$$

$$E \phi_E c(t) = i\hbar \phi_E \partial_t c(t)$$

$$E c(t) = i\hbar \partial_t c(t)$$

Solution $c(t) = e^{-\frac{iE}{\hbar}(t-t_0)}$

$$\psi(x,t) = \phi_E(x) e^{-iE\Delta t/\hbar}$$

$$|\psi^2(x,t)|^2 = \underbrace{\phi_E^* e^{+iE\Delta t/\hbar}}_{\psi^*(x,t)} \underbrace{\phi_E(x) e^{-iE\Delta t/\hbar}}_{\psi(x,t)}$$

$$= \phi_E^*(x) \phi_E(x)$$

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

↑ independent of time

Energy eigenstates are stable don't change in time

Fourier Series:

Consider a Periodic Function



Any periodic function can be expanded in
sin's and cos's

Completeness

$$f(x) = C_0 + B_1 \sin \frac{2\pi}{L} x + B_2 \sin \frac{2\pi}{L} \cdot 2x + B_3 \sin \frac{2\pi}{L} \cdot 3x + \dots$$
$$+ A_1 \cos \frac{2\pi}{L} x + A_2 \cos \frac{2\pi}{L} \cdot 2x + A_3 \cos \frac{2\pi}{L} \cdot 3x + \dots$$

$$f(x) = C_0 + \sum_{k>0} A_k \cos kx + B_k \sin kx$$

$$k = \frac{2\pi}{L} n \quad n = 1, \dots, \infty$$

$$\cos kx = \frac{e^{+ik \cdot x} + e^{-ikx}}{2}$$

$$\sin kx = \frac{e^{+ikx} - e^{-ikx}}{2i}$$

$$= C_0 + \sum_{k>0} \left(\frac{A_k - iB_k}{2} \right) e^{+ik \cdot x} + \left(\frac{A_k + iB_k}{2} \right) e^{-ik \cdot x}$$

Then we have

$$C_k = \frac{A_k - iB_k}{2} \quad k > 0$$

$$C_{-k} = \frac{A_k + iB_k}{2}$$

$$f(x) = c_0 + \sum_{k>0} C_k e^{ikx} + \sum_{k>0} C_{-k} e^{-ikx}$$

$$f(x) = \sum_k C_k e^{ikx}$$

$$k = \frac{2\pi n}{L} \quad n = -\infty, \dots, \infty$$

How to find the coefficients:

• Orthogonality:

$$\int_{-L/2}^{L/2} e^{-i\frac{2\pi n'}{L}x} e^{+i\frac{2\pi n}{L}x} = 0$$

for $n \neq n'$
because it oscillates

$$= L$$

for $n = n'$

So

$$\int_{-L/2}^{L/2} e^{-ikx} f(x) = \int_{-L/2}^{L/2} \left(\sum_{k'} C_{k'} e^{+ik'x} \right) e^{-ikx}$$

$$= \sum_{k'} \delta_{kk'} L C_{k'} = C_k L$$

$$C_k = \frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} f(x)$$

We will rewrite this:

- $\Phi_k = \frac{e^{ik \cdot x}}{\sqrt{L}}$ $\int_{-L/2}^{L/2} \Phi_{k'}^* \Phi_k = \delta_{kk'}$
- $f(x) = \sum_k f(k) \Phi_k$
- $\int_{-L/2}^{L/2} dx \Phi_k^* f(x) = f(k)$ $f(k) = \sqrt{L} c_k$

Can also do it in terms of sines and cos's:

$$c_k = \frac{1}{L} \int_{-L/2}^{L/2} e^{-ikx} f(x)$$

$$c_{-k} = \frac{1}{L} \int_{-L/2}^{L/2} e^{+ikx} f(x)$$

$$A_{|k|} = c(k) + c_{-k} = \frac{1}{L} \int_{-L}^L (e^{-ikx} + e^{+ikx}) f(x)$$

$$A(k) = \frac{2}{L} \int_{-L/2}^{L/2} \cos kx f(x)$$

$$B_k = \frac{2}{L} \int_{L/2}^{L/2} \sin kx f(x)$$

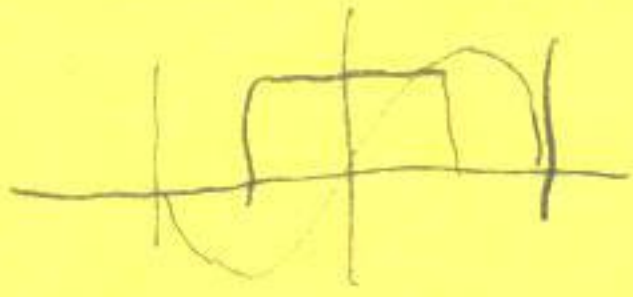
$$C_0 = \frac{1}{L} \int_L f(x) dx$$

$$A_k = \frac{1}{L} 2 \sin \frac{ka}{2}$$

$$k = \frac{2\pi n}{L}$$

$$n = 0, \dots, \infty$$

$$B_k = \frac{1}{L} \int_{-L/2}^{L/2} f(x) \sin \frac{2\pi n x}{L} dx = 0$$



→ To see how well this works for a given # of terms see links on web

$$C_k = \frac{A_k - iB_k}{2} = \frac{1}{2L} \frac{\sin ka/2}{ka/2} \quad k > 0$$

$$C_{-|k|} = \frac{A_{|k|} + iB_{|k|}}{2} = \frac{1}{2L} \frac{\sin ka}{ka/2} \quad k > 0$$

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