$\Psi^*(x,t) \Rightarrow$ complex ...
↳ $|\Psi_x|^2 = \psi(x)\psi^*(x)$

- expection values for the position and momentum
  ↳ electron at x_1 and x_2, probability to find particle at

  x_1:
  $$\Psi(x_1,t)\,\Psi^*(x_1,t)$$

  x_2:
  $$\Psi(x_2,t)\,\Psi^*(x_2,t)$$

- mean value: fool at notes

- $$\bar{x} = \langle x \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\, x\, \Psi(x,t)\,dx$$

- expectation value for momentum or any other value:

$$\bar{p} = \langle p \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t)\,\hat{p}\,\Psi(x,t)\,dx$$
$$=$$
$$-i\hbar \int_{-\infty}^{+\infty} \Psi^* \frac{d\Psi}{dx}\,dx = -i\hbar \int_{-\infty}^{+\infty} \psi^* \frac{d\psi}{dx}\,dx$$

- lect 5 09/06; 3D schrodinger equation
  ↳ 1D case → particles can only propogate in 1 direction
    ↳ following eqns introduced:
    $$\Psi(x,t) = \Psi_0\, \exp(i(px/\hbar - Et/\hbar))$$

→ SE:
$$i\hbar \frac{d}{dt}\Psi(x,t) = \hat{H}\Psi(x,t) \Rightarrow$$

$$\hat{p} = -i\hbar\frac{d}{dx}$$
$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$$

total energy

$$\overbrace{\quad\quad\quad}$$

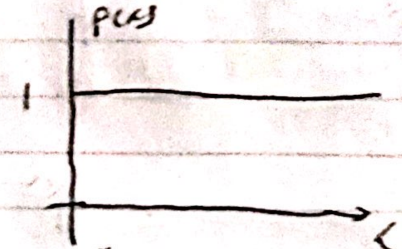
• Hamiliton eq: $H = \frac{p^2}{2m} + U(x)$; for Hamiltonian for QP: constructed if potential energy is 0

↳ $\dot{p} = -\frac{\partial H}{\partial x}$, $\dot{x} = \frac{\partial H}{\partial p}$

$-\frac{\partial U}{\partial x} = \frac{dp}{dt} = F$ ↳ $\frac{dH}{dp} = p/m$

• quantum systems: $\Psi(x,t) = e^{i(kx - \omega t)}$ } → one particle, simplest form

1) position: probability density ⇒ $f(x) = \Psi^*\Psi = 1 = |\Psi|^2$



particle can be found anywhere with equal probability

2) momentum p

$\hat{p} = -i\hbar \frac{\partial}{\partial x}$; $\hat{p}\Psi = (-i\hbar)(ik)\Psi = p\Psi$

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

→ wave function above has well defined momentum but sometimes they do not

→ Position not always defined ⇒ not all wave function can solve all operators ⇒ only well defined p or x

3.5 $\bar{X}, \bar{P}$ and example

↳ expectation values:

$\langle x \rangle = \bar{x}$ ⇒ Ⓐ Ψ_a x_a Ⓑ Ψ_b x_b ⇒ $\Psi_a \Psi_a^* x_a + \Psi_b \Psi_b^* x_b$

• position operator $\hat{x} = x$

→ $P_a = 1/3$ and $P_b = 2/3$] → probability
↳ $\bar{x} = x_a P_a + x_b P_b$; $P_a + P_b = 1$
; $\psi_a^* \psi_a + \psi_b^* \psi_b = 1$

• $\bar{x} = \langle x \rangle = \int \psi^*(x)\, \psi(x)\, x \, dx$; if x is continuous use integral, if x discrete, use definition above

• $\bar{p} = \langle p \rangle = \int \psi^*(x)\, \hat{p}\, \psi(x)\, dx$
• $\bar{E} = \langle E \rangle = \int \psi^*(x)\, \hat{H}\, \psi(x)\, dx$

• $\langle p^2 \rangle = \int \psi^*(x)\, \hat{p}^2\, \psi(x)\, dx$, same for $\langle x^2 \rangle$ and $\langle E^2 \rangle$ for any expectation value

• Schrödinger equation : $i\hbar \frac{\partial \Psi}{\partial t} = \hat{H} \Psi$] → time-dependent

• C.M. ⇒ $H = \frac{p^2}{2m} + U(x)$
• Q.M. ⇒ $\hat{H} = \frac{\hat{p}^2}{2m} + U(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)$
• example:
plane wave: $\Psi(x,t) = e^{i(kx - \omega t)}$
$U(x) = 0$ → free part

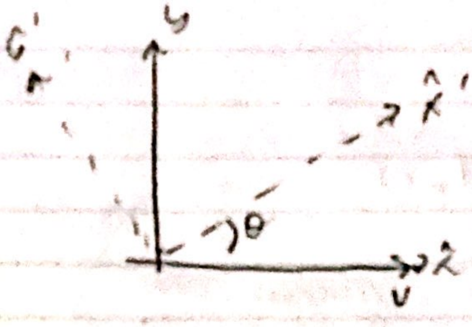
$\hat{H} \Psi = \frac{\hbar^2 k^2}{2m} \Psi = i\hbar(-i\omega) \Psi$

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

↳ $E = E$

applying the

• 3D case:



$x = x' \cos\theta$

$y = y' \sin\theta$

$k_x = k \cos\theta$

$k_y = k \sin\theta$

• phase of wave function, which changes along the x' axis

↳ $kx' \Rightarrow x k_x + y k_y$; $\vec{k}\cdot\vec{r} = x k_x + y k_y + z k_z$

• 3D schrödinger eq: $\Psi(\vec{r},t) = \Psi_0 \exp[\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)]$

↳ $\Psi(\vec{r},t) = \exp[i(\vec{k}\cdot\vec{r} - \omega t)]$; $\vec{k} = \frac{\vec{p}}{\hbar}$

• del operator (reminder):

→ gradient: grad $f = \nabla f$

→ divergence: div $\vec{v} = \nabla\cdot\vec{v}$

→ curl $\vec{v} \Rightarrow \nabla\times\vec{v}$

↳ gradient: $\nabla f = \frac{df}{dx}\hat{i} + \frac{df}{dy}\hat{j} + \frac{df}{dz}\hat{k}$

• 3D eq: $\Psi = \exp(\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et))$

↳ $\nabla\Psi = e_x \frac{d\psi}{dx} + e_y \frac{d\psi}{dy} + e_z \frac{d\psi}{dz}$

$= \frac{i}{\hbar}(p_x e_x + p_y e_y + p_z e_z)\Psi$

$= \frac{i}{\hbar}\vec{p}\,\Psi$; $e_x, e_y, e_z \Rightarrow$ unit vectors

↳ $\hat{p} = -i\hbar\nabla$

• Schrödinger Hamiltonian: $\hat{H} = \hat{T} + \hat{V}$; $\hat{V} = V = V(\vec{r},t)$

↳ $H = \frac{p^2}{2m} + U(x)$

in 3D $\Rightarrow \vec{p} = p_x \vec{e_x} + p_y \vec{e_y} + p_z \cdot \vec{e_z}$

$\Rightarrow p^2 = \vec{p}\cdot\vec{p} = p_x^2 + p_y^2 + p_z^2$

• Q.M. $\Rightarrow \hat{\vec{p}} = -i\hbar\left[\frac{\partial}{\partial x}\hat{e_x} + \frac{\partial}{\partial y}\hat{e_y} + \frac{\partial}{\partial z}\hat{e_z}\right]$

$= -i\hbar\vec{\nabla}$

$(\hat{\vec{p}})^2 = -\hbar^2\nabla^2$; $\hat{H} = \frac{p^2}{2m} + V(x) = \frac{-\hbar^2}{2m}\nabla^2 + V(\vec{r}, t)$

• position operator: $\hat{r} = \vec{r}$ } also stay the <u>same</u>

• 3D schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(\vec{r},t) = \frac{-\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V(\vec{r})\Psi(\vec{r},t) \Big\} !!!$$

• thermal neutrons: $\Rightarrow$ look at posted notes for thermal neutrons for hw
- wavelength: 2 Å
- beam of neutrons shot through Pb container containing flower $\Rightarrow$ used for screening, imaging inside objects
- fission and spallation
- diffraction regime
- reflectometry
- SANS
- imaging
- detecting strain
- internal defects
- magnetic domains