L6

$\hbar = h/2\pi$

Last Time

① Conjugate variables, e.g. $p = \frac{\hbar}{i}\frac{\partial}{\partial x} \Leftrightarrow \Delta x \Delta p = \frac{\hbar}{2}$

or $E = \frac{\hbar}{i}\frac{\partial}{\partial t} \Leftrightarrow \Delta E \Delta t = \frac{\hbar}{2}$

② Equation of motion: $H\Psi = i\hbar\frac{\partial}{\partial t}\Psi$ (H = energy)

③ Measurement $P(x) = \Psi^*(x)\Psi(x) = |\Psi(x)|^2$

$$\bar{A} = \int dx\, \Psi^*(x) A \Psi(x)$$

④ Two kinds of particles: Spin change ⇒ magnetic field

Fermions. $s = 1/2, 3/2, 5/2, \ldots$ $\Psi_F(1,2) = -\Psi_F(2,$

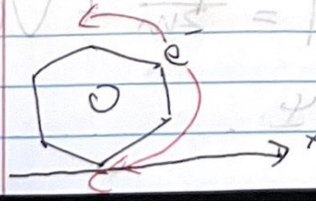
Bosons $s = 0, 1, 2, \ldots$ $\Psi_B(1,2) = +\Psi_B(2,1)$

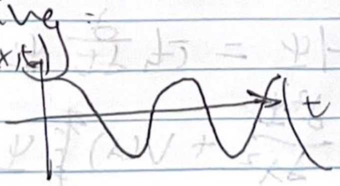
4 rules allow us to calculate all properties of molecules and of chemical reaction. e.g. color, rate, Woodward-Hoffman's rule.

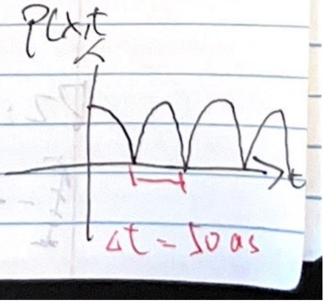
Today: Example of consequence of postulates.

Time-dependance of the wavefunction of an e^-

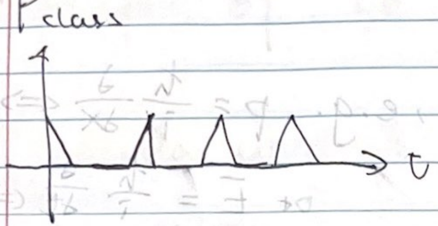
In the benzene ring:





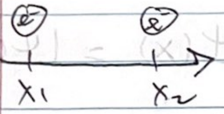


$= 5\times 10^{-17}$ s.



Some electrons in ~~QA~~ QM move a little faster, some a little slower, $\Delta x \underset{\neq 0}{\Delta p} = \frac{\hbar}{2}$.

ex #2 : Pauli exclusion Principle (PEP)



$\Big\}$ P4 $\Rightarrow \Psi(\overset{e^-\#1}{x_1}, \overset{e^-\#2}{x_2}) = -\Psi(\overset{e^-\#1}{x_2}, \overset{e^-\#2}{x_1})$

What happened to $\Psi(x_1, x_2)$ & therefore the probability $P = |\Psi|^2$ when the electron get close together? In the limit $x_1 \to x_2$

$\Psi(x_1, x_1) = -\Psi(x_1, x_1) = 0$.

$P(x_1, x_1) = 0$.

e^- avoid one another, PEP.

$\Downarrow$

objects are solid.

ex #3 The Schrödinger equation:

P1: $p = \frac{\hbar}{i}\frac{\partial}{\partial x} = p^2 = p \cdot p = -\hbar^2 \frac{\partial^2}{\partial x^2}$

$E = i\hbar \frac{\partial}{\partial t}$

P2: $H\Psi = i\hbar \frac{\partial}{\partial t}\Psi$; $H = \frac{p^2}{2m} + V(x)$

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

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\Psi = E\Psi \Rightarrow \overset{\text{energy operator}}{H}\Psi = \underset{\text{eigenvalue}}{E}\,\overset{\text{eigenvector}}{\Psi}$$

ex #4. The order of variables in QM.

HW Q1.3.

CM = $x\cdot p - p\cdot x = 0$

QM = $(x\hat{p} - \hat{p}x)\Psi = \left(x\cdot\frac{\hbar}{i}\frac{d}{dx} - \frac{\hbar}{i}\frac{d}{dx}\cdot x\right)\Psi$

$$\cancel{\neq \left(x\cdot\frac{\hbar}{i}\frac{d\Psi}{dx} - \frac{\hbar}{i}\frac{d}{dx}\right.}$$

$$= \frac{\hbar}{i}\left(x\frac{d\Psi}{dx} - \frac{d(x\Psi)}{dx}\right)$$

$$\frac{d(x\Psi)}{dx} = \frac{dx}{dx}\cdot\Psi + \frac{d\Psi}{dx}\cdot x$$

$$= \underbrace{1\cdot\Psi}_{\text{not cancelled.}} + x\cdot\frac{d\Psi}{dx}$$