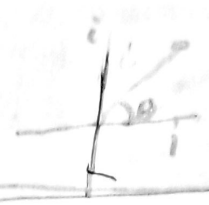
Review Session

3 lectures: 0: Differential equations, ✓
(no specific questions, but used in some)
probability
natural log ln
imaginary #'s i ✓ $\sqrt{-1} = i$ $e^{i\varphi} = \cos\varphi + i\sin\varphi$

$P = |\psi|^2 = \psi\psi^* = (a+ib)(a-ib) = a^2+b^2$

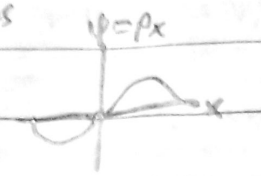
Re Im



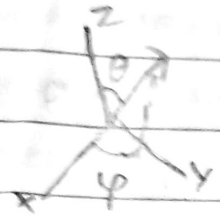
Lecture 4-16: 4 questions, 10 points each, total 40 pts, 20% course grade

Q#1: orbitals → wavefunctions

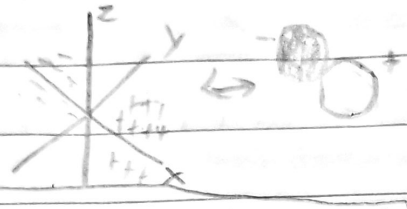
$p_x \propto r e^{-\frac{r}{2a_0}} \sin\theta \cos\varphi$



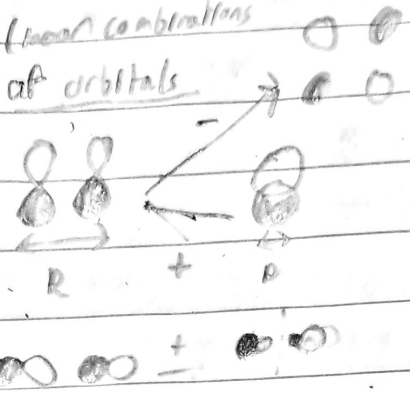
assume $y=0, z=0$ plane



$\cos\varphi =$ ⊖ for $x<0$



linear combinations of orbitals

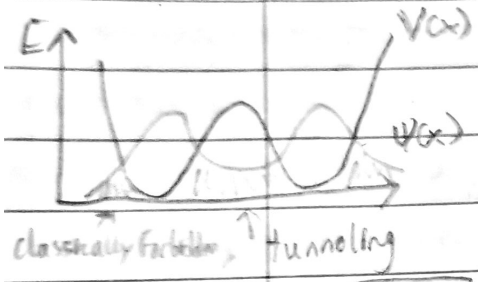


π orbital

σ orbital

(in this case − leads to lower E) →

Q#2: Weird things in QM: $\Delta x \Delta p = \frac{\hbar}{2}$



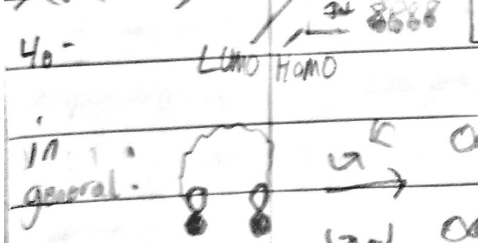
classically $px = xp$
but in QM, $p = \frac{\hbar}{i}\frac{\partial}{\partial x}$
$\hat{p}x \neq x\hat{p}$. This is only true when variables are correlated though.

ex. $p_x \cdot p_x = p \cdot p$ $\quad x \cdot y = y \cdot x$
$p_x \cdot y = y \cdot p_x$ $\quad x \cdot x = x \cdot x$
$\downarrow$
$\frac{\partial}{\partial x} y\,\psi(x,y) = y \frac{\partial}{\partial x}\psi(x,y)$

order matters, no difference

Q#3: Geometry of molecules

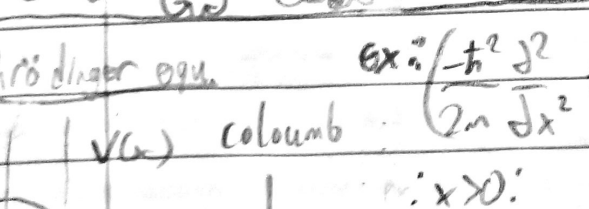
overlap of orbitals.



ex: $y \cdot p_y \neq p_x \cdot y$ → $\frac{\partial}{\partial y} y \cdot y^2 = \frac{\partial}{\partial y} y^3$

say $\psi = y^2$ $\downarrow$ $y \frac{\partial}{\partial y} y^2 = y \cdot 2y = 2y^2 \neq 3y^2$

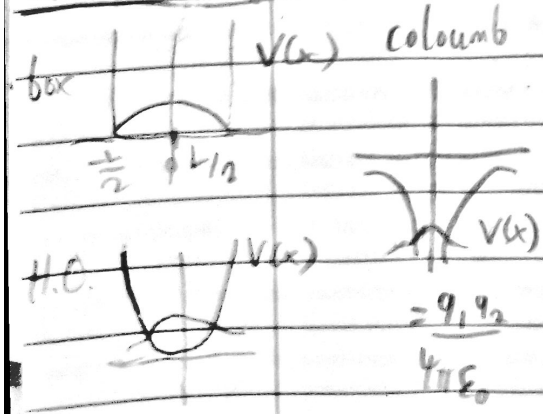
in general:



↳ σ is high E,
↳ σ is low E

sign determined by what HOMO is filled, based on # of e^-

Q4: Schrödinger eqn.



coloumb

ex: $\left(\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}kx^2\right)\psi = E\psi$ $\quad \psi = e^{-|x|}$, is this a wavefunction that satisfies Schrö?

H.O

$x>0$:

$\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}e^{-x} + \frac{1}{2}kx^2 e^{-x} = E\psi$

$\frac{\hbar^2}{2m}e^{-x} + \frac{1}{2}kx^2 e^{-x} = Ee^{-x}$

$x^2 e^{-x} \neq e^{-x}$

No