$c = \lambda \cdot \nu$

$\lambda = \dfrac{h}{m \cdot v}$

$E_{photon} = h \cdot \nu = \underbrace{\Phi}_{\text{work function (min E required to escape)}} + \frac{1}{2} \cdot m \cdot v^2$

$E_{up} - E_{lower} =$

$\sigma_x \cdot \sigma_{p_x} \geq \dfrac{\hbar}{2}$ | $\hbar = \dfrac{h}{2\pi}$

Shrodinger Equations

Time Dependent: $\dfrac{-\hbar}{i} \cdot \dfrac{\delta}{\delta t} \Psi = -\dfrac{\hbar^2}{2 \cdot m_1} \cdot \left(\dfrac{\delta^2 \Psi}{\delta x^2} + \dfrac{\delta^2 \Psi}{\delta y^2} + \dfrac{\delta^2 \Psi}{\delta z^2} \right) - \ldots + V \cdot \Psi$

↳ 1 Dimentional 1 Particle: $\dfrac{-\hbar^2}{2 \cdot m} \cdot \dfrac{\delta^2 \Psi}{\delta x} + V(x) \cdot \Psi = \dfrac{-\hbar}{i} \cdot \dfrac{\delta \Psi}{\delta t}$ | $\Psi(x, t)$

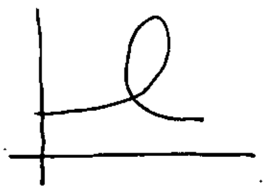
Time Independent: $-\dfrac{\hbar^2}{2 \cdot m} \cdot \dfrac{d^2 \psi}{dx} + V(x) \cdot \psi = E \cdot \psi$ | $\psi(x)$

$\therefore \Psi(x, y, z, t) = e^{-i \cdot E \cdot t / \hbar} \cdot \psi(x, y, z)$

$|\Psi|^2 = |\psi|^2 = \psi^* \cdot \psi$ | $\displaystyle\int_{-\infty}^{\infty} |\psi|^2 \cdot d\tau = 1$ [definite integral across 3 dimensional space]

Well behaved state functions must be....

single valued:

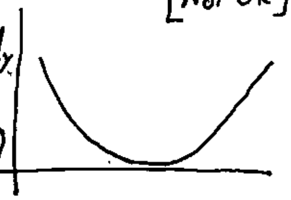


[Not OK]

continuous:

[Not OK]

quadratically integral [$\int |\psi|^2 d\tau = const$]



[Not OK]

Particle in a box

1 dimensional: $\psi(x) = \sqrt{\dfrac{2}{a}} \cdot \sin\left(\dfrac{n \cdot \pi \cdot x}{a}\right)$ | $0 \leq x \leq a$, $n = 1, 2, \ldots$

$E = \dfrac{n^2 \cdot h^2}{8 \cdot m \cdot a^2}$

3 dimensional: $\psi(x, y, z) = \sqrt{\dfrac{8}{a \cdot b \cdot c}} \cdot \sin\left(\dfrac{n_x \cdot \pi \cdot x}{a}\right) \cdot \sin\left(\dfrac{n_y \cdot \pi \cdot y}{b}\right) \cdot \sin\left(\dfrac{n_z \cdot \pi \cdot z}{c}\right)$

$$E = \frac{h^2}{8 \cdot m} \cdot \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

degree of degeneracy = number of states belonging to the same energy level

Operators:

$$(\hat{A}+\hat{B})\,f(x) = \hat{A}(f(x)) + \hat{B}(f(x))$$
$$(\hat{A}\,\hat{B})\,f(x) = \hat{A}(\hat{B}(f(x)))$$

position operator: $\hat{x} = x\cdot$

momentum operator: $\hat{p}_x = \frac{\hbar}{i}\cdot\frac{\delta}{\delta x}$

Linear operator if:

$$\hat{L}(f+g) = \hat{L}(f) + \hat{L}(g)$$
$$\hat{L}(c\cdot f) = c\cdot\hat{L}(f)$$

ex.) $\sqrt{}$ is not linear

ex.) $\frac{d}{dx}$ is linear

Hamiltonian operator:

$$\hat{H} = \frac{-\hbar^2}{2\cdot m}\cdot\nabla^2 + V\cdot \quad \Big|\quad \nabla^2 = \frac{\delta^2}{\delta x^2}+\frac{\delta^2}{\delta y^2}+\frac{\delta^2}{\delta z^2}$$
$$\hat{H}\,\Psi = \frac{-\hbar}{i}\cdot\frac{\delta}{\delta t}\,\Psi$$
$$\hat{H}\,\psi = E\cdot\psi$$

Hermetion operator: $\langle M\rangle = \langle M\rangle^*$

$$\int f^*\cdot\hat{M}(g)\cdot d\tau = \int g\cdot(M(f))^*\,d\tau$$
$$\langle f|M|g\rangle = \langle Mf|g\rangle$$

Harmonic Oscilator: $V(x) = \frac{1}{2}\cdot k\cdot x^2$ in time-independent equation

$$E = (v+\tfrac{1}{2})\cdot h\cdot\nu \quad\Big|\quad v = 0,1,2,\ldots$$

$$\psi_v = \begin{cases} e^{-\alpha\cdot\frac{x^2}{2}}\cdot(c_0 + c_2\cdot x^2 + \ldots + c_v\cdot x^v) & v \text{ is even} \\ e^{-\alpha\cdot\frac{x^2}{2}}\cdot(c_1\cdot x^1 + c_3\cdot x^3 + \ldots + c_v\cdot x^v) & v \text{ is odd}\end{cases}$$

$$\alpha = \frac{2\pi}{\hbar}\cdot\nu\cdot m$$

---

2 Particles:

$x = x_2 - x_1$, $y = \ldots$, $z = \ldots$

$X = \frac{m_1\cdot x_1 + m_2\cdot x_2}{m_1+m_2}$, $Y = \ldots$, $Z = \ldots$

$p_x = \mu\cdot v_x$, $p_y = \ldots$, $p_z = \ldots$

$P_X = M\cdot v_X$, $P_Y = \ldots$, $P_Z = \ldots$

$M = m_1 + m_2$

$\mu = \frac{m_1\cdot m_2}{m_1+m_2}$

$$H = \underbrace{\left[\frac{1}{2\cdot\mu}\cdot(p_x^2+p_y^2+p_z^2) + V(x,y,z)\right]}_{\hat{H}_\mu\psi_\mu(x,y,z) = E_\mu\cdot\psi(x,y,z)} + \underbrace{\left[\frac{1}{2\cdot M}\cdot(P_X^2+P_Y^2+P_Z^2)\right]}_{\hat{H}_M\psi_M(X,Y,Z) = E_M\cdot\psi(X,Y,Z)}$$

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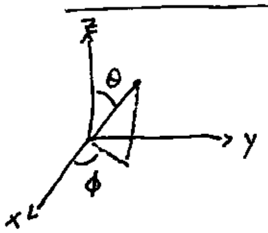
2 Particle Rigid Motor:



for 2 quatum #'s:

Θ_{J,M_J}, Φ_{M_J}

$$E_{rot} = J\cdot(J+1)\cdot\frac{\hbar^2}{2\cdot I}$$

$I = \mu\cdot d^2$

$J = 0,1,2,\ldots$

$M_J = -J, -J+1, \ldots 0, 1, \ldots J-1, J$

[Each rotational level is $2J+1$ fold degenerate]

$e(\text{electron}) = 1.6022 \cdot 10^{-19}\, C$

$\varepsilon_0 = 8.854 \cdot 10^{-12} \frac{C^2}{N \cdot m^2}$

$\frac{1}{4\pi \cdot \varepsilon_0} = 8.988 \cdot 10^{9} \frac{N \cdot m^2}{C}$

$a = \frac{\hbar^2 \cdot 4\pi \cdot \varepsilon_0}{\mu \cdot e^2} \approx 0.5292 \cdot 10^{-10} m$

$x = r \cdot \sin(\theta) \cdot \cos(\phi)$

$y = r \cdot \sin(\theta) \cdot \sin(\phi)$

$z = r \cdot \cos(\theta)$

$d\tau = r^2 \cdot \sin(\theta) \cdot dr \cdot d\theta \cdot d\phi$

$0 \le r \le \infty$

$0 \le \theta \le \pi$

$0 \le \phi \le 2\pi$

$\mu_{12} = \frac{m_1 \cdot m_2}{m_1 + m_2}$

Hydrogen Atom:

for quantum numbers: $n = 1, 2, \ldots$

$l = 0, 1, \ldots, n-1$

$m = -l, -l+1, \ldots, l-1, l$

$\Psi(r, \theta, \phi) = \underset{n,l}{R}(r) \cdot \underset{l,m}{\Theta}(\theta) \cdot \underset{m}{\Phi}(\phi)$

$E(z, n) = -\frac{Z^2}{n^2} \cdot \underbrace{\frac{e^2}{(4\pi \cdot \varepsilon_0) \cdot 2a}}_{\sim 13.60\, eV}$

(where Z is # protons)

$R_{1s} = 2 \cdot \left(\frac{Z}{a}\right)^{\frac{3}{2}} \cdot e^{\frac{-Z \cdot r}{a}}$

$R_{2s} = \sqrt{2} \cdot \left(\frac{Z}{a}\right)^{3/2} \cdot \left(1 - \frac{Z \cdot r}{2 \cdot a}\right) \cdot e^{\frac{-Z \cdot r}{2a}}$

$R_{2p} = \sqrt{24} \cdot \left(\frac{Z}{a}\right)^{5/2} \cdot r \cdot e^{\frac{-Z \cdot r}{2a}}$

$R_{3s} = 2 \cdot \left(\frac{Z}{3a}\right)^{3/2} \cdot \left(1 - \frac{2 \cdot Z}{3 \cdot a} \cdot r + \frac{2 \cdot Z^2}{27 \cdot a^2} \cdot r^2\right) \cdot e^{\frac{-Z \cdot r}{3a}}$

$\Theta_{s0} = \frac{1}{\sqrt{2}}$

$\Theta_{p0} = \frac{\sqrt{6}}{2} \cdot \cos(\theta)$

$\Theta_{p1} = \Theta_{p-1} = \frac{\sqrt{3}}{2} \cdot \cos(\theta)$

$\Phi_m = \frac{1}{\sqrt{2\pi}} \cdot e^{i \cdot m \cdot \phi}$

radial probability density: $Pr(r \to r+dr) = \underbrace{4\pi \cdot r^2}_{SA_{sphere}} \cdot |\Psi|^2 \cdot dr$

nodes: l angular

$n - l - 1$ radial

Ψ_{2p}: $2p_x$, $2p_y$] m=1 and m=-1; $2p_z$] m=0

Ψ_{3d}: m=+1 and m=-1 [$3d_{xy}$, $3d_{yz}$ | $3d_{x^2-y^2}$, $3d_{xy}$] m = +2 and m = -2; $3d_{z^2}$] m = 0

Angular Momentum: $\vec{L}$

$\hat{L}^2 \Psi = l \cdot (l+1) \cdot \hbar^2 \cdot \Psi$

$\hat{L}_z \Psi = m \cdot \hbar \cdot \Psi$

$|\vec{L}| = \sqrt{l \cdot (l+1)} \cdot \hbar$

$L_z = m \cdot \hbar$

Spin: $\vec{S}$

$|\vec{S}| = \sqrt{s \cdot (s+1)} \cdot \hbar$

$S_z = m_s \cdot \hbar$

$s = \begin{cases} \text{boson: } 0, 1, \ldots \\ \text{fermion: } \frac{1}{2}, \frac{3}{2}, \ldots \end{cases}$

$m_s = -s, -s+1, \ldots, s-1, s$

$S_{e^-} = \frac{1}{2}$

$m_{s_{e^-}} = -\frac{1}{2}, \frac{1}{2}$

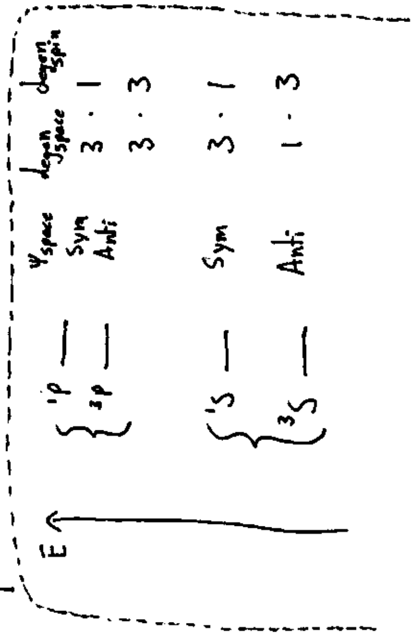
Notation: α is Ψ_{spin} for $m_s = \frac{1}{2}$

β is Ψ_{spin} for $m_s = -\frac{1}{2}$

Helium Atom:

$$\hat{H} = \overbrace{\underbrace{-\frac{\hbar^2}{2m_e}\cdot\nabla_1^2}_{e_1^-} \underbrace{-\frac{\hbar^2}{2m_e}\cdot\nabla_2^2}_{e_2^-}}^{\text{Kinetic Energy Operator}} \overbrace{\underbrace{-\frac{Z\cdot e^2}{4\pi\cdot\varepsilon_0\cdot r_1}}_{\text{Nuc } \& \ e_1^-} \underbrace{-\frac{Z\cdot e^2}{4\pi\cdot\varepsilon_0\cdot r_2}}_{\text{Nuc } \& \ e_2^-} \underbrace{+\frac{e^2}{4\pi\cdot\varepsilon_0\cdot r_{12}}}_{e_1^- \& \ e_2^-}}^{\text{Potential Energy Operator}}$$

assuming
e_1^- & e_2^- interaction = 0 : $E \approx E_1 + E_2$ $\quad \Psi \approx \Psi_1 \cdot \Psi_2$



e^- spin symetry:

symetric	$\alpha(1)\cdot\alpha(2)$	switching e^- $\Psi \to \Psi$
	$\beta(1)\cdot\beta(2)$	
	$\frac{1}{\sqrt{2}}\cdot[\alpha(1)\cdot\beta(2)+\beta(1)\cdot\alpha(2)]$	
anti-symetric	$\frac{1}{\sqrt{2}}\cdot[\alpha(1)\cdot\beta(2)-\beta(1)\cdot\alpha(2)]$	switching e^- $\Psi \to -\Psi$

Poly-electron Atoms:

Total L $(\vec{L}_T) = \sum \vec{L}_i$

Total S $(\vec{S}_T) = \sum \vec{S}_i$

Term Symbol: ^{2S+1}L

Slater determinant:

same Ψ_{space} & Ψ_{spin} ↓

$$\Psi = \frac{1}{\sqrt{\#_{e^-}!}}\cdot\begin{vmatrix} \sim & \sim \\ \sim & \sim \end{vmatrix} \leftarrow \text{same } e^-$$

ex.)

$$\Psi_{1s2s} \approx \frac{1}{\sqrt{3!}}\cdot\begin{vmatrix} 1s(1)\cdot\alpha(1) & 1s(1)\cdot\beta(1) & 2s(1)\cdot\alpha(1) \\ 1s(2)\cdot\alpha(2) & 1s(2)\cdot\beta(2) & 2s(2)\cdot\alpha(2) \\ 1s(3)\cdot\alpha(3) & 1s(3)\cdot\beta(3) & 2s(3)\cdot\alpha(3) \end{vmatrix}$$

$Z_{eff} = Z - s$ | s is screening constant by other e^-

Hartree-Fock: $\hat{F}\phi_i = \varepsilon_i \cdot \phi_i$

Problem: $\hat{F}$ depends on ϕ_i

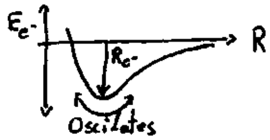
Solution: iterative
↳ start with a guess for wavefunction
↳ vary coefficients of basis functions to minimize energy of Slater deteminant

Configuration Interaction:

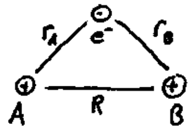
- allow e^- to temporarily move into excited empty orbitals

Hamiltonian for molecule: $\hat{H} = \underbrace{\hat{K}_N} + \hat{K}_{e^-} + \hat{V}_{N,N} + \hat{V}_{N,e^-} + \hat{V}_{e^-,e^-}$

Born-Openheimer aproximation: $\hat{K}_n$ is dropped because $m_N >> m_{e^-}$ ∴ fixed nucler distance



H_2^+ Molecule: $\hat{H}_{e^-} = \frac{-\hbar^2}{2\cdot m_{e^-}} \cdot \nabla^2 - \frac{e^2}{4\pi\cdot\varepsilon_o\cdot r_A} - \frac{e^2}{4\pi\cdot\varepsilon_o\cdot r_B} + \frac{e^2}{4\pi\cdot\varepsilon_o\cdot R}$



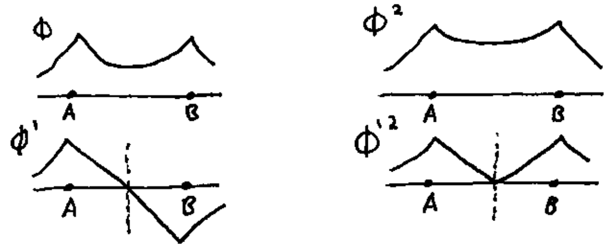
$1s_A = a_o^{-3/2} \cdot \pi^{-1/2} \cdot e^{-r_A/a_o}$

$1s_B = a_o^{-3/2} \cdot \pi^{-1/2} \cdot e^{-r_B/a_o}$

$S = e^{-R/a_o} \cdot \left(1 + \frac{R}{a_o} + \frac{R^2}{3\cdot a_o}\right)$ ∴ @ $R=0 \to S=1 \to$ overlap
@ $R=\infty \to S=\emptyset \to$ no overlap

bonding: $\Phi = (2-2\cdot S)^{-1/2} \cdot (1s_A + 1s_B)$

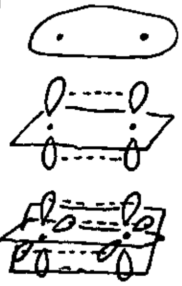
anti-bonding: $\Phi' = (2-2\cdot S)^{-1/2} \cdot (1s_A - 1s_B)$



Bonding:

- bond type depends on the absolute value of the magnetic quantum number $|m|$

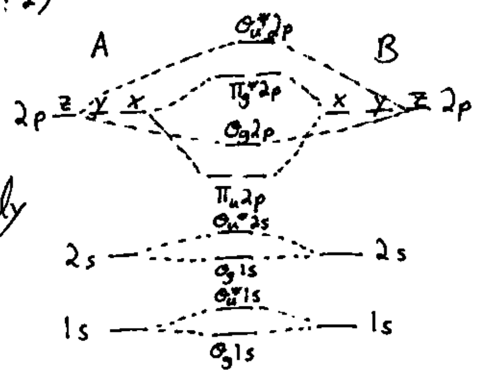
# nodal planes parralel to bond axis	symbol
$\lvert m\rvert = \emptyset$	σ
$\lvert m\rvert = 1$	π
$\lvert m\rvert = 2$	δ



- subscript$_g$: even ∴ $f(-x,-y,-z) = f(x,y,z)$
- subscript$_u$: odd ∴ $f(-x,-y,-z) = -f(x,y,z)$
- superscript^b: bonding ∴ charge density between atoms
- superscript*: anti-bonding ∴ node ⊥ to bond axis

Homo nuclear Diatomic (H_2):

- ⊙ Z is now bond axis
- $\hat{V}_{e^-,e^-}$ makes $\hat{H}_{e^-}\Psi_{e^-} = E_{e^-}\cdot\Psi_{e^-}$ difficult to solve exactly
- Pauli repulsion: e^- with same spin repel one another because Ψ for fermions (e^-) must be antisymetric



H_2 ground state: $\Psi_{space} = \sigma_g 1s(1) \cdot \sigma_g 1s(2)$

H_2 1st excited state: $\Psi_{space} = \frac{1}{\sqrt{2}} \cdot (\sigma_g 1s(1) \cdot \sigma_u^* 1s(2) + \sigma_g 1s(2) \cdot \sigma_u^* 1s(1))$

− for anti-symetric

Ψ_{space} for homonuclear diatomics:

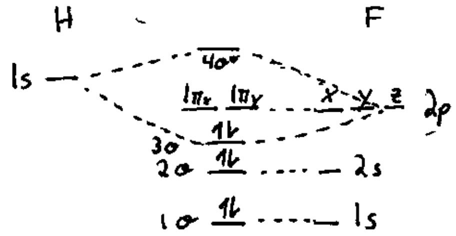
$(\sigma_g 1s)^2 \cdot (\sigma_u^* 1s)^2 \cdot (\sigma_g 2s)^2 \cdot (\sigma_u^* 2s) \cdot (\pi_u 2p)^4 \cdot (\sigma_g 2p)^2 \cdot (\pi_g^* 2p)^4 (\sigma_u^* 2p)$

.....

F is more electronegative

Heteronuclear Diatomic:

ex.) HF



* in actuality, all bonds of equal |m| contribute
  ↳ <u>minimum basis set</u>: set of contributing atomic orbitals for ~~molec~~ atoms in molecule

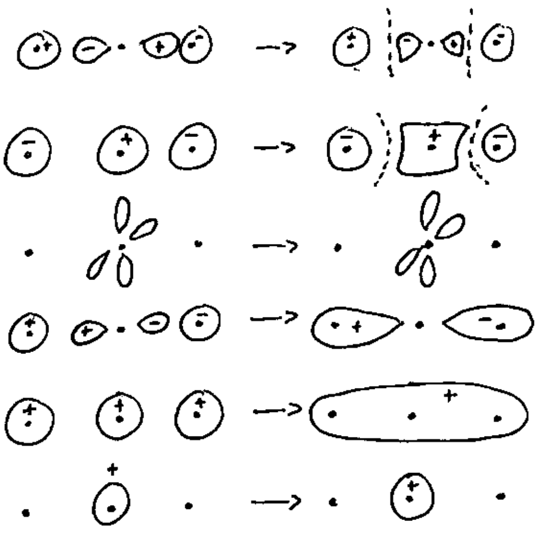
• bond order = (# bonding ≠ # anti-bonding) / 2

Polyatomic:

NOTE: bond number ($2\sigma_g$) increases for antibonding (*)

NOTE: + and − in pictures denote the sign of ψ

where: $H_g \equiv H1s_A + H1s_B$, $H_u \equiv H1s_A - H1s_B$



$2\sigma^*_u$ → $c_1 \cdot Be2p_z - c_2 \cdot H_u$

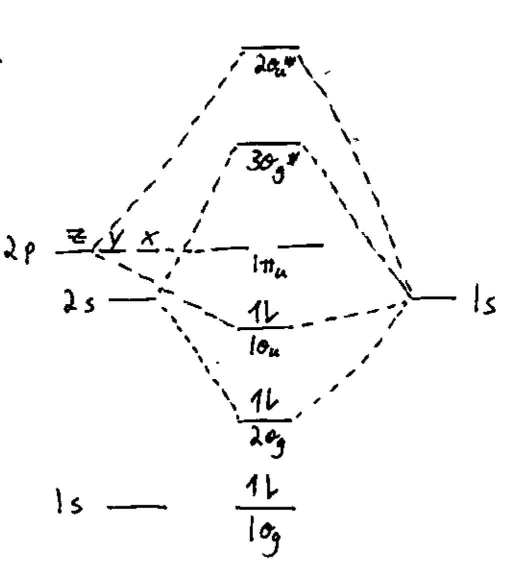
$3\sigma^*_g$ → $c_1 \cdot Be2s - c_2 \cdot H_g$

$1\pi_u$ → $Be2p_{x,y}$

$1\sigma_u$ → $c_1 \cdot Be2p_z + c_2 \cdot H_u$

$2\sigma_g$ → $c_1 \cdot Be2s + c_2 \cdot H_g$

$1\sigma_g$ → Be1s



$$\psi = \frac{1}{\sqrt{\#_{e^-}!}} \cdot \begin{vmatrix} 1\sigma_g(1)\cdot\alpha(1), \ldots \beta(1), \ldots \text{other orbitals} \\ \vdots \text{ other } e^- \end{vmatrix}$$

$$\psi_{Hybrid} = \frac{1}{\sqrt{6!}} \cdot \begin{vmatrix} 1\sigma_g(1)\cdot\alpha(1), \ldots \beta(1), \ldots \overbrace{(2\sigma_g(1)\cdot\alpha(1) + 1\sigma_u(1)\cdot\alpha(1))}^{b_1}, \ldots \\ \vdots \quad \ddots \end{vmatrix}$$

<u>localized orbitals</u>: combine molecular of same |m|

• bonding (b)
• anti-bonding (*)
• non bonding
  ↳ lone pair (l)
  ↳ inner shell (i)

ex.) BeH_2: $b_1 = \frac{1}{\sqrt{2}} \cdot (2\sigma_g + 1\sigma_u)$

$b_2 = \frac{1}{\sqrt{2}} \cdot (2\sigma_g - 1\sigma_u)$

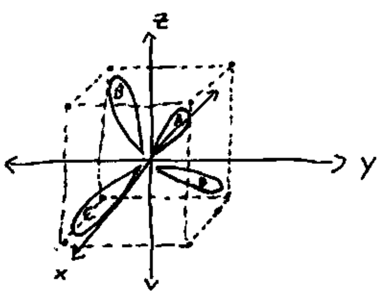
* but b_1 & b_2 are not eigan fuctions $\hat{Fock}$

<u>Hybridization</u>: combine <u>atomic</u> orbitals on the <u>same atom</u> to make localized orbitals

---

VSEPR (Valence Shell Electron Pair Repulsion) Theory:

1. $\#_{e\ pair}$ around atom in lewis structure
2. use ideal geometry to maximize distance
3. account for: $\theta_{l,l} > \theta_{l,b} > \theta_{b,b}$ | l: lone pair, b: bonding e^-

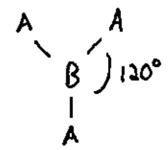
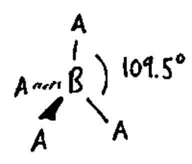


A: $\frac{1}{2} \cdot (s + (p_x + p_y + p_z))$

B: $\frac{1}{2} \cdot (s + (-p_x - p_y + p_z))$

C: $\frac{1}{2} \cdot (s + (p_x - p_y - p_z))$

D: $\frac{1}{2} \cdot (s + (-p_x + p_y - p_z))$

type	structure	hybridization: shorthand	used	not used
linear	A – B – A (180°)	sp	s, p_z	p_x, p_y
trigonal planar		sp^2	s, p_y, p_z	p_x
tetrahedral		sp^3	s, p_x, p_y, p_z	—