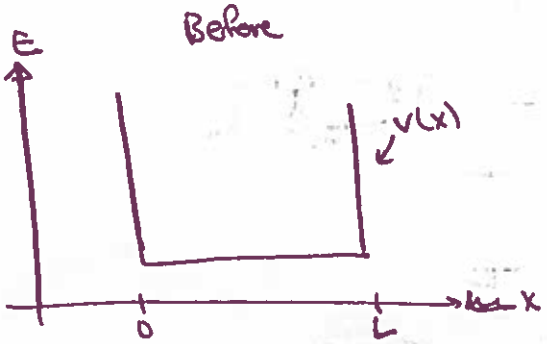
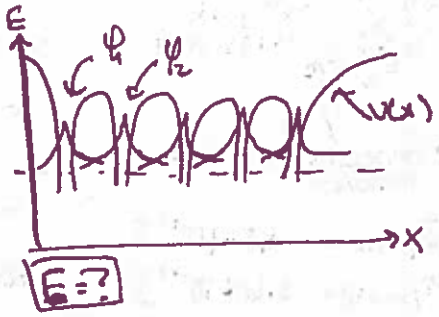
Improve bonding models

Hückel model: PIB w/ tunneling



$$E_n = \frac{h^2 n^2}{8mL^2}$$



Use a basis of 1 function at each atom and ~~diagonal~~ diagonalize

The functions ($\psi_1, \psi_2 \ldots$) don't have to be 1s

ex: 

butadiene: 2p, 4e⁻

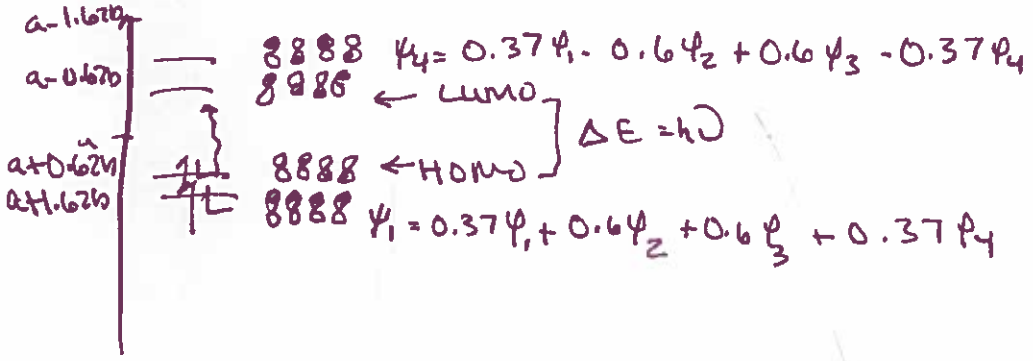
$\langle 3|\hat{H}|4\rangle = b = \langle 1|\hat{H}|2\rangle = \langle 2|\hat{H}|3\rangle < 0$

$\langle 1|\hat{H}|3\rangle \approx 0$ (ψ_1 and ψ_3 are far apart)

$\langle 1|\hat{H}|1\rangle = a \approx \langle 2|\hat{H}|2\rangle = \langle 3|\hat{H}|3\rangle \approx \langle 4|\hat{H}|4\rangle$

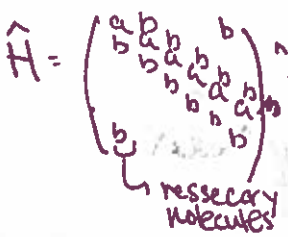
The matrix $\underline{\underline{H}} = \begin{pmatrix} a & b & 0 & 0 \\ b & a & b & 0 \\ 0 & b & a & b \\ 0 & 0 & b & a \end{pmatrix}$ "tridiagonal"

Solving,



ex  benzene, 2D, 6e⁻ in ring-box

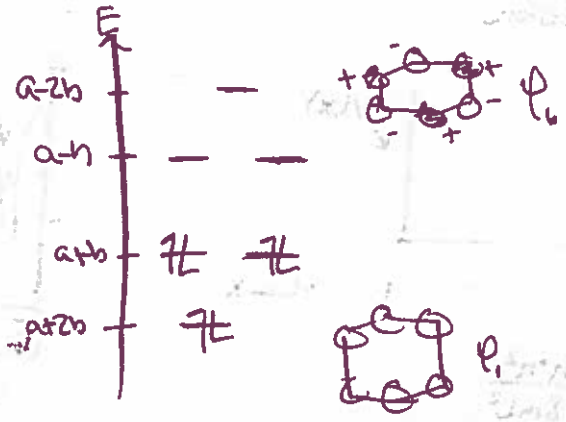
$\langle 1|\hat{H}|2\rangle = b = \ldots \langle 6|\hat{H}|1\rangle$

$\hat{H} =$  not quite tridiagonal

↳ necessary for aromatic molecules

$b \approx -75\ kJ/mole = -4.5 \cdot 10^{-18} J$

$a \approx +400\ kJ/mole = 3.6 \cdot 10^{-17} J$



Comparison to particle in a ring