Lecture 15

Monday, September 25, 2023 9:57 AM

Today: More Spectroscopy & tunneling

ex. for the wavefunction of two pi e^-

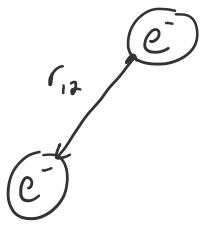
$$\Psi(x_1, x_2) = \pi_+(x_1)\,\pi_-^*(x_2) - \pi_+(x_2)\,\pi_-^*(x_1)$$

(π_+: $m_s = +\frac{1}{2}$)

Note: the actual exact soln. of the Schrödinger eqn

$\mathcal{H}\,\Psi(x_1, x_2) \; E\,\Psi(x_1, x_2)$ are distorted from the simple sum (like $p_A + p_B$).

Reason: e^- e^- repulsion.

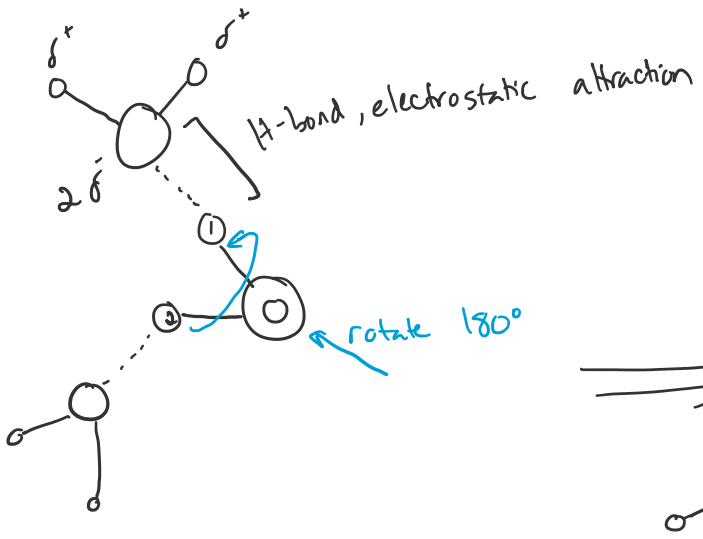


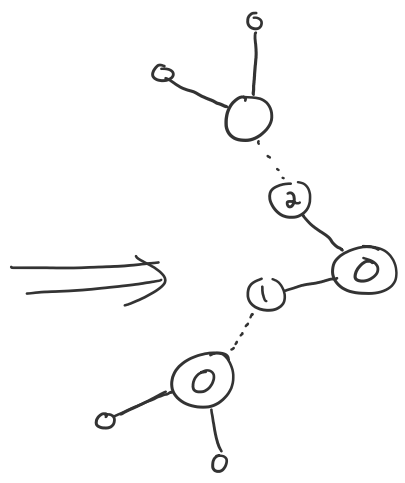
$$V_{repulsion}(r_{12}) = + \frac{e^2}{4\pi\varepsilon_0 r_{12}}$$

"e^- correlation"

Thought Experiment: ~~~> (e^- waves) H_2O

What Rotation Allows a hydrogen bond in water to be broken?





Water has C_2 symmetry

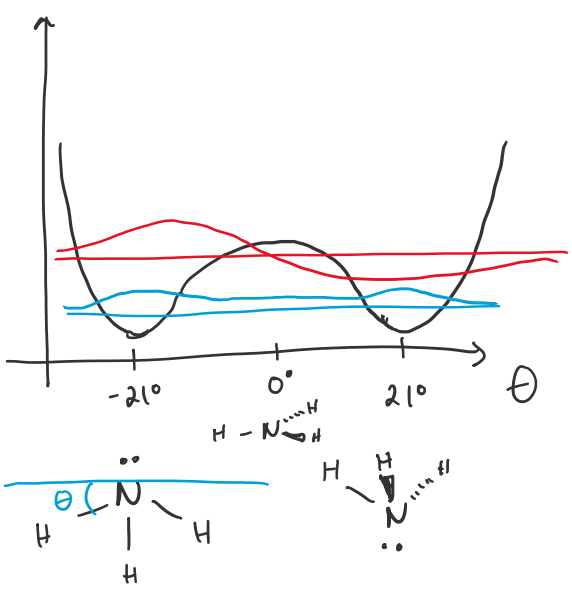
180°

H #1

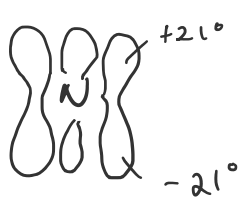
H #2

are exchanged

Tunneling = "ammonia has no structure"



← Stak @ low energy

Ψ: 

more likely to find @ ± 21° than 0°