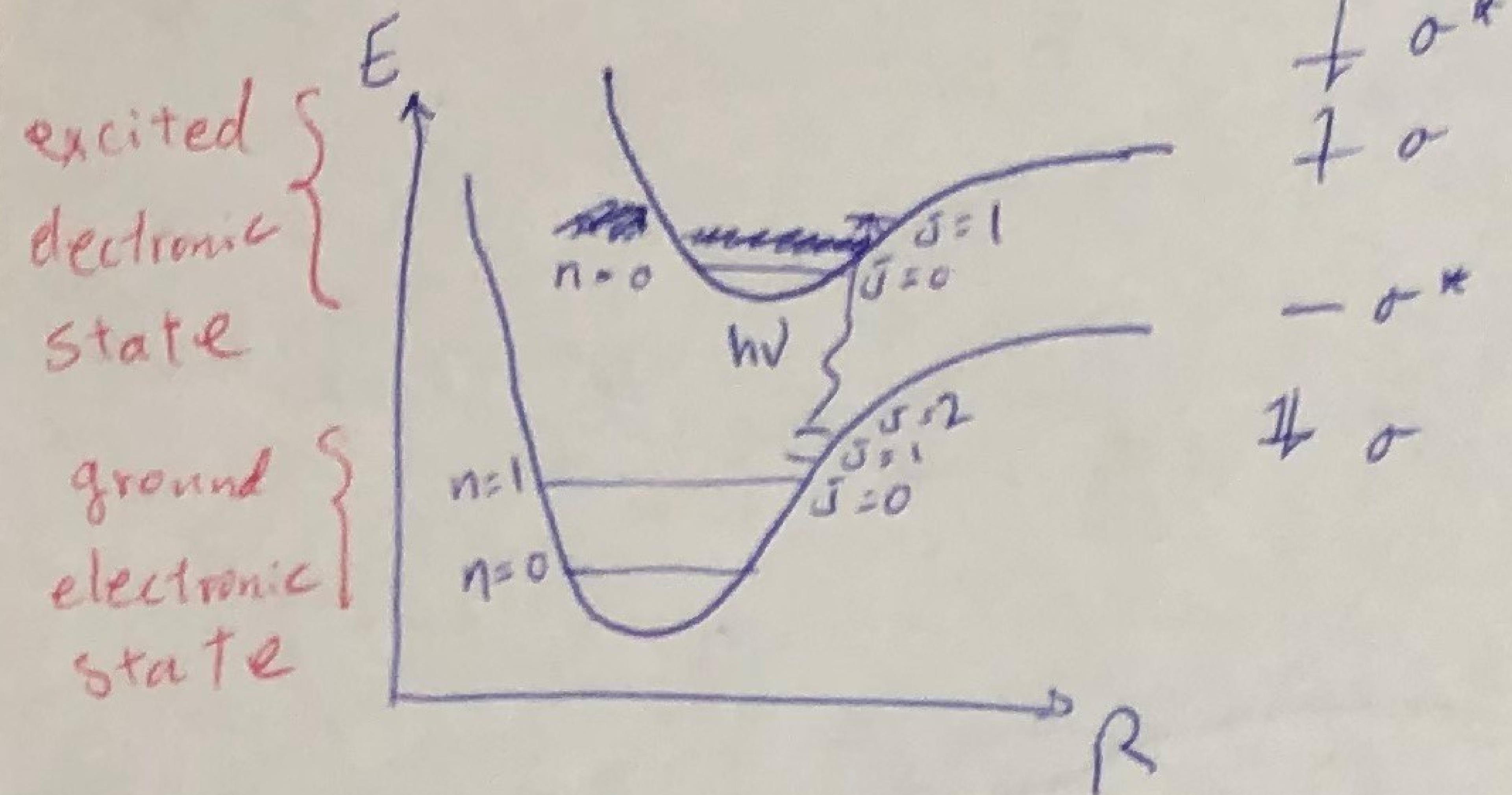
L 15: review

Potential surfaces



Transition $\Delta E = E(\sigma\sigma^*, n=0, J=1) - E(\sigma^2, n=1, J=2)$

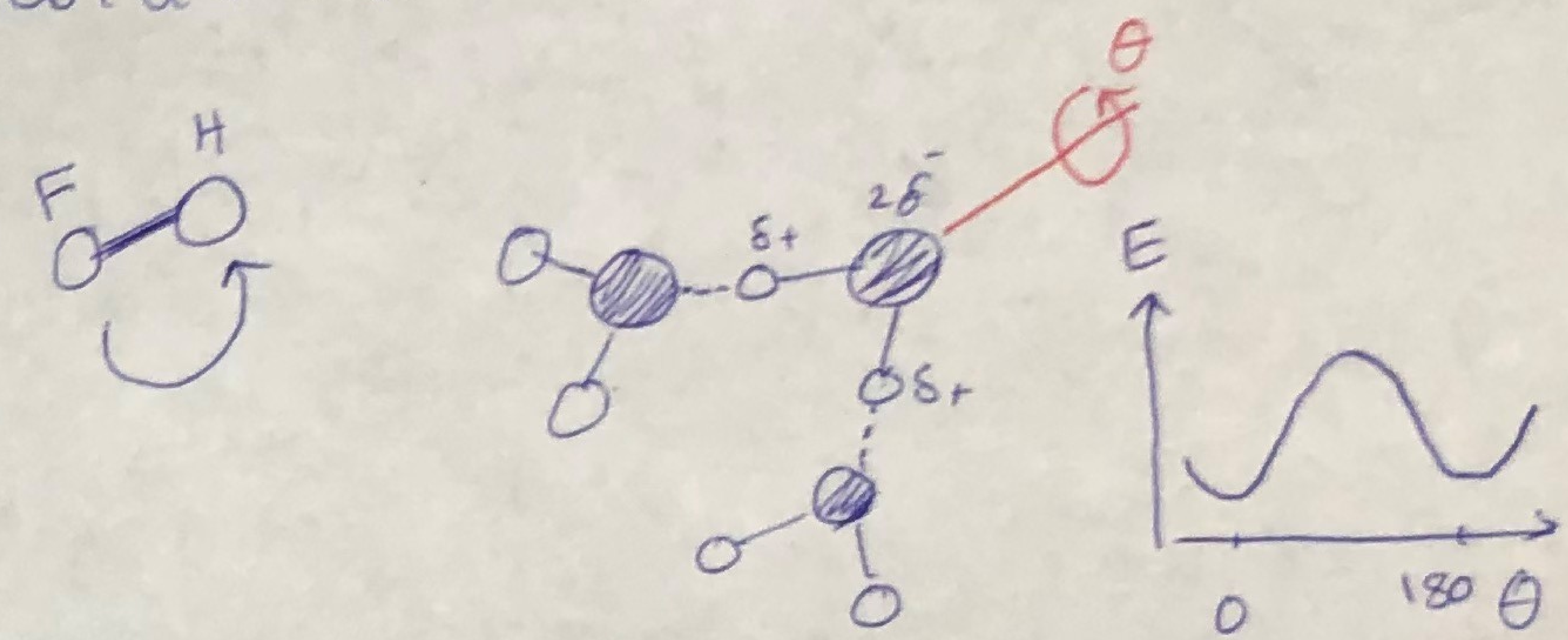
$= h\nu$

* Intensity ~ dipole • electric field

* vibrational states are denoted by n and the rotational states are denoted by J.

* dipole moment dictates absorption intensity: molecular oxygen, O_2, has dipole moment = 0, therefore O_2 does not absorb light (very well); however CO_2 upon bending adopts a dipole moment so it absorbs light.

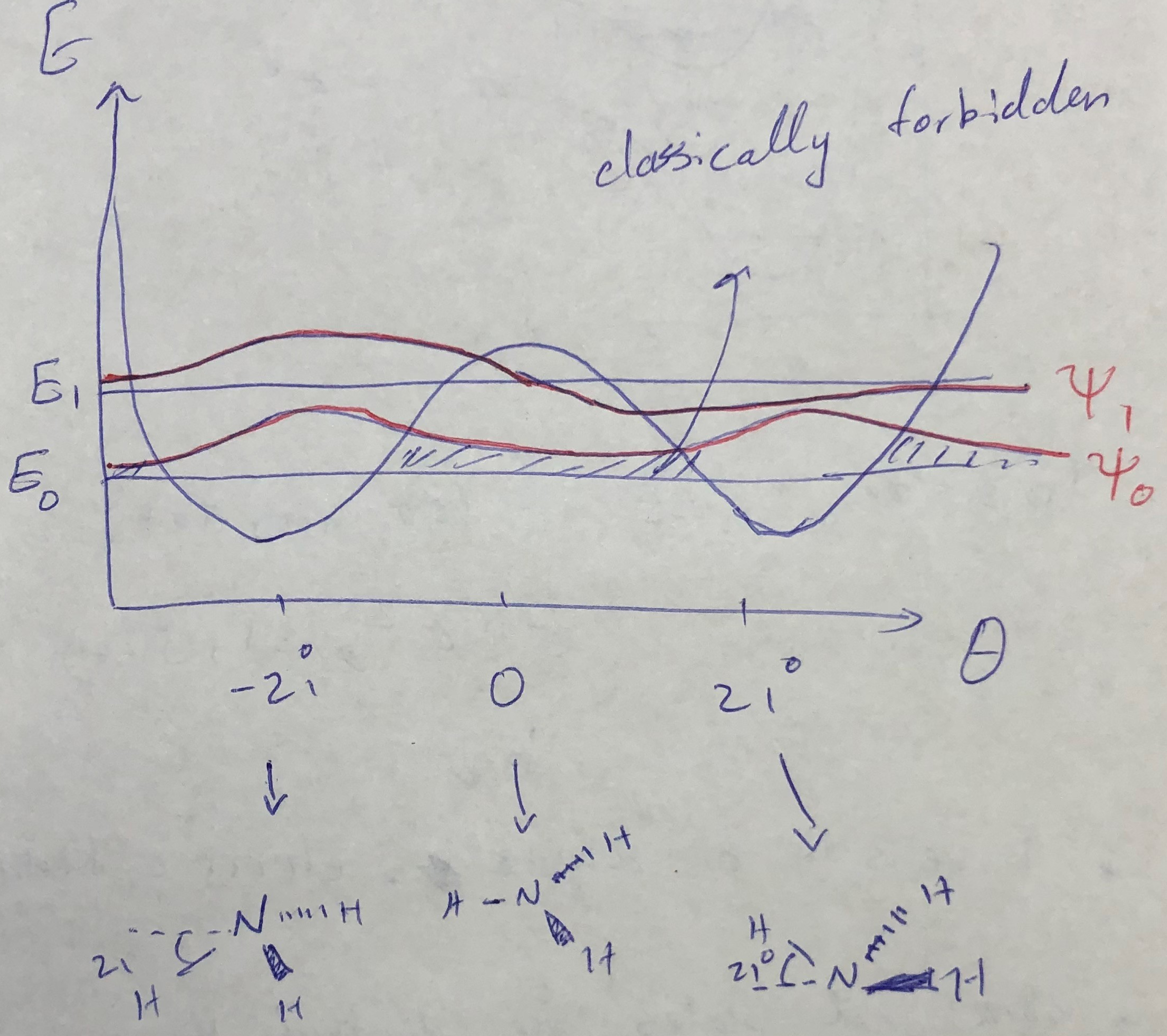
Rotational motion



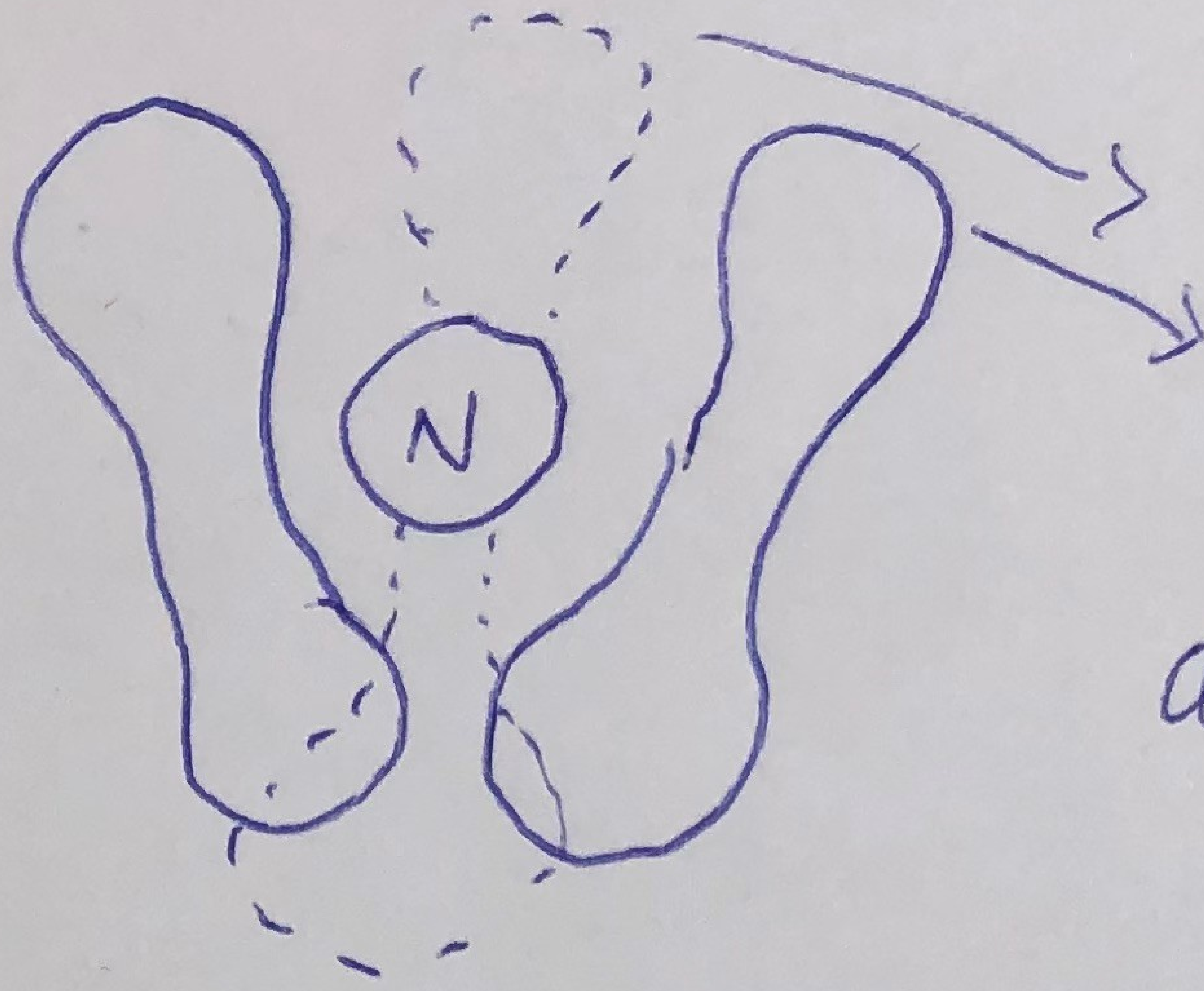
* In the language of group theory objects like water molecule have "C_2 symmetry" because a 180° rotation is identical to the system befor rotatior

(IQmol demo for HF)

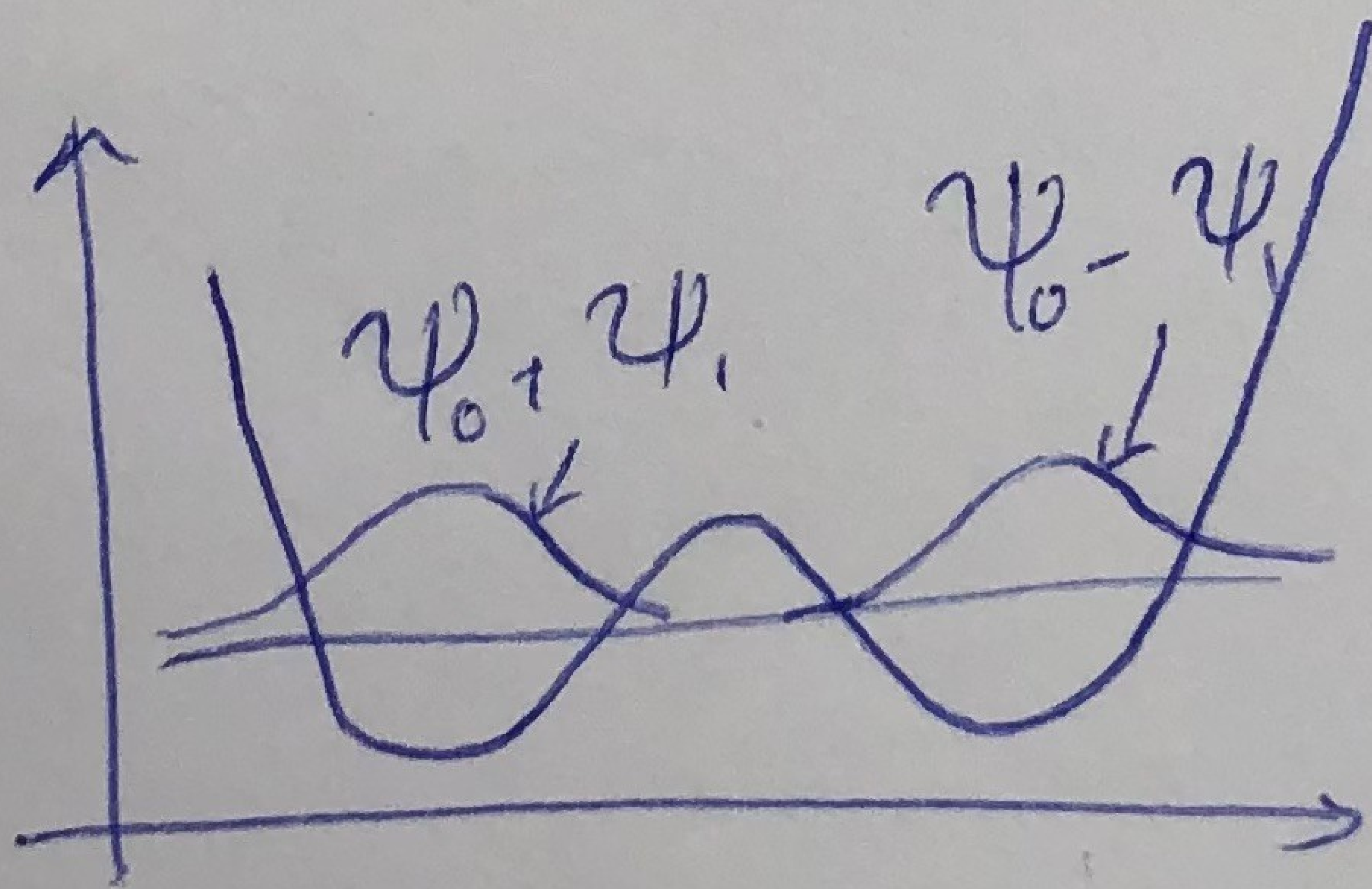
Ammonia



* ammonia is simultaneously pointing up and down (in Ψ_0) and does so by tunneling through a classically forbidden region.



what would more "classical" wavefunction look like? (Ans: linear combination of ψ_0 and ψ_1)



$$\Delta E \cdot \Delta t = \frac{\hbar}{2}$$

$$\Delta t = \frac{\hbar}{2\Delta E} = \frac{1.05 \times 10^{-34}\ \text{J.s}}{2 \times 2 \times 10^{-23}\ \text{J}}$$

$$\approx 2.6\,\text{ps}\ (2.6 \times 10^{-12}\ \text{s})$$