HW #4

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1. A Chemical Bond

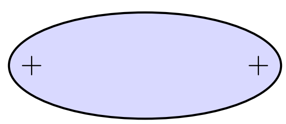
(a) If electrons behaved like bullets (no interference), the total probability is the sum of the individual probabilities:

$$P = |\psi_1|^2 + |\psi_2|^2 = (0.35)^2 + (0.22)^2 = 0.1225 + 0.0484 = \boxed{0.1709}$$

(b) Since electrons behave like waves with constructive interference, we first add the amplitudes, then square:

$$P = |\psi_1 + \psi_2|^2 = (0.35 + 0.22)^2 = (0.57)^2 = \boxed{0.3249}$$

(c) The wave probability (0.3249) is nearly double the classical bullet probability (0.1709). This enhanced electron density between the two positive nuclei creates an electrostatic attraction that holds them together—this is a covalent bond.



Bonding: enhanced e^- density between nuclei

Because of constructive interference, there is a higher probability of finding the electron between the two nuclei, which lowers the overall energy of the system and forms a stable bond.

2. Hydrogen Atom

(a) The Balmer series consists of transitions that end at $n = 2$. The longest wavelength corresponds to the smallest energy difference, which is the $E_3 \to E_2$ transition.

Using the provided energy-level diagram:

$$E_3 = -1.5 \text{ eV}, \qquad E_2 = -3.4 \text{ eV}$$

$$\Delta E = E_3 - E_2 = -1.5 - (-3.4) = 1.9 \text{ eV}$$

$$\lambda = \frac{hc}{\Delta E} = \frac{1241 \text{ eV} \cdot \text{nm}}{1.9 \text{ eV}} \approx \boxed{653 \text{ nm (red)}}$$

(b) Energy difference between E_1 and E_5 (from the provided diagram):

$$E_1 = -13.6 \text{ eV}, \qquad E_5 = -0.54 \text{ eV}$$

$$\Delta E = E_5 - E_1 = -0.54 - (-13.6) = \boxed{13.06 \text{ eV}}$$

(c) Using the Boltzmann distribution:

$$\frac{P(E_5)}{P(E_1)} = e^{-\Delta E/k_B T} = \frac{1}{1000}$$

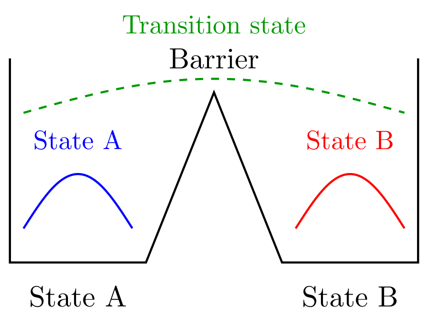
$$-\frac{13.056}{k_B T} = \ln(0.001) = -6.908$$

$$k_B T = \frac{13.056}{6.908} = 1.890 \text{ eV}$$

$$T = \frac{1.890 \text{ eV}}{8.617 \times 10^{-5} \text{ eV/K}} = \boxed{21{,}900 \text{ K}}$$

3. Chemical Reactions

(a) The three standing waves on the double-well potential:



The molecule must pass through the transition state because to convert from A to B, the wave must reorganize from being localized in well A to being localized in well B. This requires enough energy to exist at the top of the barrier, where the wavefunction is spread across both wells. The transition state represents the unstable intermediate configuration during bond rearrangement.

(b) The rate of crossing a barrier is given by:

$$\text{rate} = \nu\, e^{-E_{\text{barrier}}/k_B T}$$

where $\nu \approx 10^{13}$ s^{-1} is the molecular vibration frequency. At body temperature ($T = 310$ K):

$$k_B T = (8.617 \times 10^{-5})(310) = 0.02671 \text{ eV}$$

Barrier = 100 meV = 0.1 eV:

$$\text{rate} = 10^{13} \times e^{-0.1/0.02671} = 10^{13} \times e^{-3.74} = 10^{13} \times 0.024 = 2.4 \times 10^{11} \text{ s}^{-1}$$

$$\text{time} = \frac{1}{\text{rate}} \approx \boxed{4 \times 10^{-12} \text{ s (picoseconds)}}$$

Barrier = 1 eV:

$$\text{rate} = 10^{13} \times e^{-1/0.02671} = 10^{13} \times e^{-37.4} = 10^{13} \times 5.3 \times 10^{-17} = 5.3 \times 10^{-4} \text{ s}^{-1}$$

$$\text{time} = \frac{1}{\text{rate}} \approx \boxed{1{,}900 \text{ s} \approx 32 \text{ minutes}}$$

Barrier = 10 eV:

$$\text{rate} = 10^{13} \times e^{-10/0.02671} = 10^{13} \times e^{-374} \approx 10^{13} \times 10^{-163} = 10^{-150} \text{ s}^{-1}$$

$$\text{time} = \frac{1}{\text{rate}} \approx \boxed{10^{150} \text{ s (far longer than the age of the universe)}}$$

Small barriers allow reactions to occur almost instantaneously at body temperature. Medium barriers take minutes—enzymes can lower these to speed up biological reactions. Large barriers make spontaneous reactions essentially impossible, which is why covalent bonds (like those in DNA) are stable at physiological temperatures.