Types of molecular / solid bonds

- Ionic bond: electrons hop from one atom to another, creating ions with <more> complete electron shells and opposite charges. Such ions are then held together by Coulumb attraction

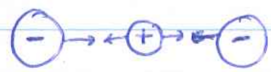
$$Na + Cl \Rightarrow Na^+ + Cl^-$$

$[Ne]+3s^1$ $[Ar]-3p^1$ $\quad$ $[Ne]$ $\quad$ $[Ar]$

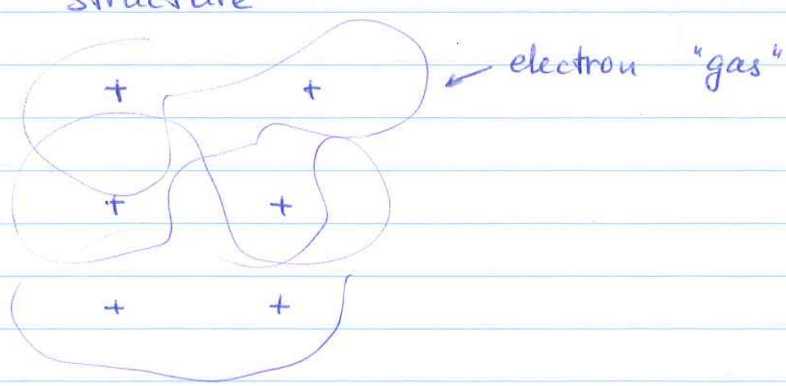
- Dipole - dipole (Van-der-Vaals) bond: attraction b/w atoms (or tightly-bound molecules) with internal or induced dipole moment

short-range weak bound

- Hydrogen bond: Attraction of two negative ions by means of an intermediate hydrogen atom



- Metallic bond (in solids): electrons are delocolized and free to move throughout the material, positive ions are fixed within atomic lattice structure



- Covalent bond: two atoms (often identical) are bound by attraction via shared electrons

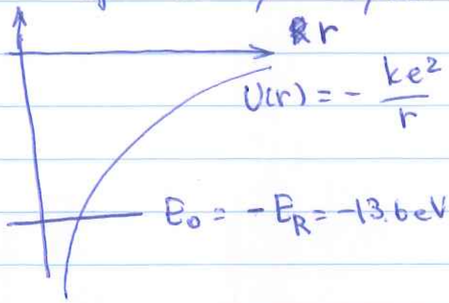
Quantum description of a covalent bond

Our test subject H_2 molecule

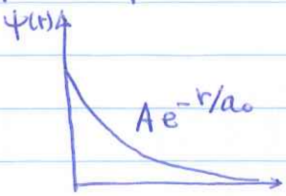
Key word — quantum tunneling

Single H atom in the ground state $n=1, \ell=0, m=0$

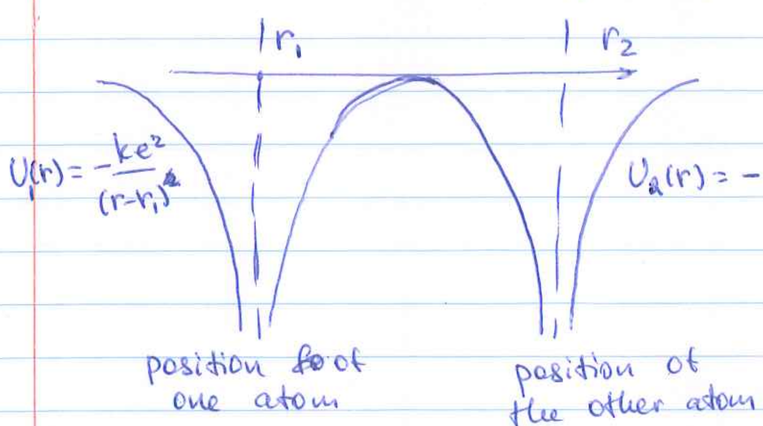
spherically-symmetric state



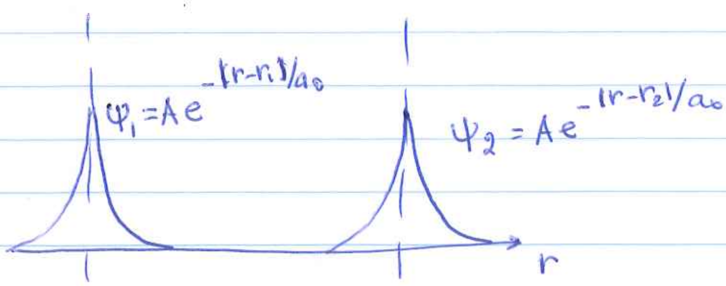
$$\psi(\vec{r}) = \psi(r) = A e^{-r/a_0}$$



To avoid 3-D drawings, I'll cheat and do a "slice" of r-space, which goes from $-\infty$ to $+\infty$



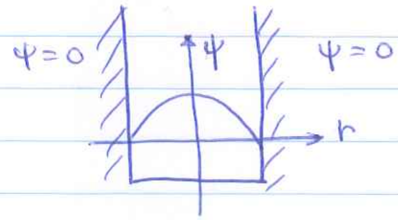
If atoms are far enough apart, each electron is localized at its nuclei position



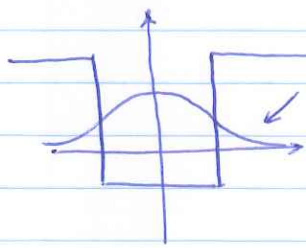
However, as atoms move closer, this localization becomes less and less strict due to tunneling

Brief reminder of tunneling

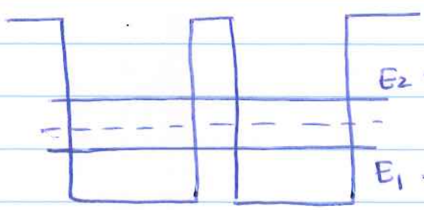
Infinite square well – electrons are completely ~~[illegible]~~ localized within a well



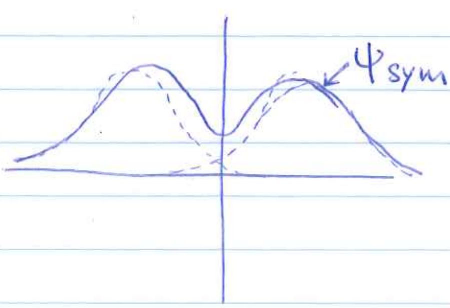
Non-infinite square well — electrons can "leak" outside

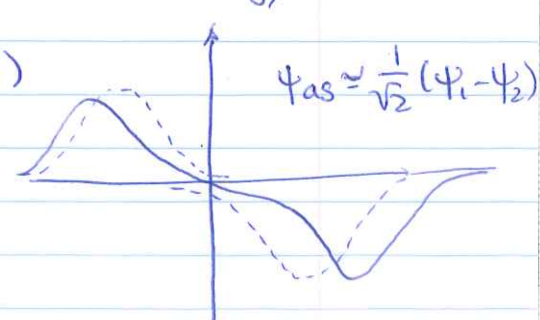


Two wells next to each other: a particle can now tunnel between the two sites.



~~The~~ When we look for the <u>stationary</u> energy states, we have to take into account that if the potential is symmetric (two identical atoms), the resulting wavefunctions will be also either symmetric or antisymmetric. One can show that a symmetric one will corresponds to the lower energy case.



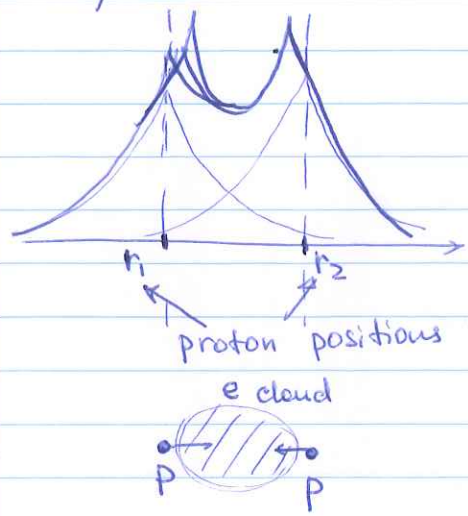


electron density is higher close to the center

electron density is higher farther from center

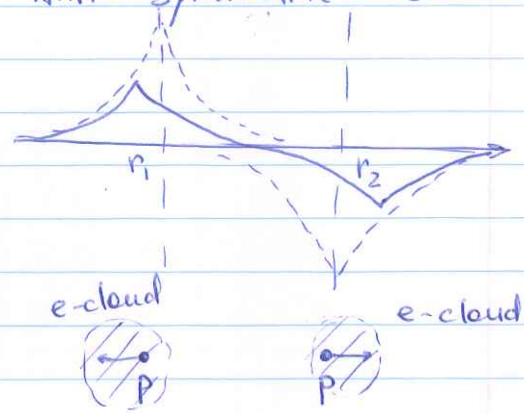
Let's get back to H_2 molecule
we will also find two possible state:
a symmetric one (with the lowest energy) and an antisymmetric one

Symmetric state

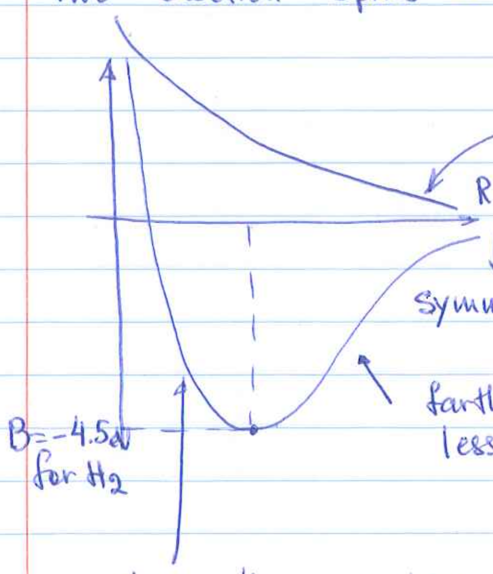


Two protons are attracted toward negatively charged electrons b/w each other, bonding to a stable molecule
Two electron spins are ↑↓

Anti-symmetric state



Electrons are more likely to be at the "outside", away from the intermediate region, pulling protons further apart.
Two electron spins are ↑↑



anti-symmetric case
↑↑ total spin = 1, triplet state (P-state or Π-state)

↓↑ – total spin = 0, singlet state (S-state) or Σ state
symmetric state $U(r_2 - r_1)$

farther from equilibrium separation – less efficient tunneling, less effective attraction

closer than equilibrium separation – p-p coulumb repulsion, pauli exclusion principle

To break up the molecule it is enough to flip a spin
Photo dissociation