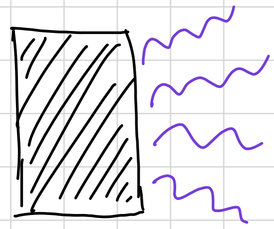
Lecture #3 Quantum Theory of Solids (Band structure)

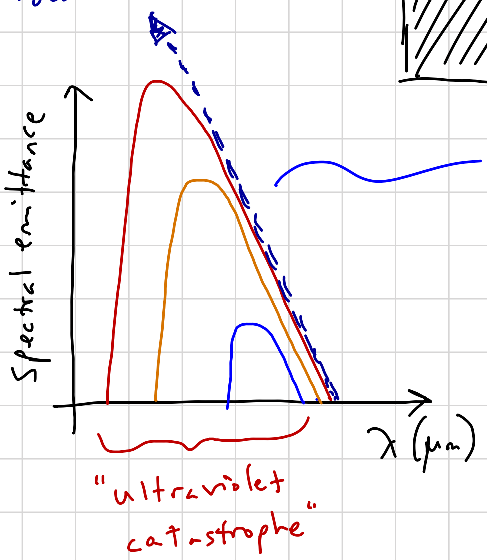
First, reminder of some key aspects of atoms learned over time:

① Blackbody Radiation

an ideal radiator



when "heated" (above Ø K), emits radiation
→ everything does!



19th century models good at long λ, but not at short

→ Max Planck came up with answer (1901)

→ vibrating atoms can only radiate (or absorb) energy in discrete (quantum) packets

→ For oscillating frequency, ν, energy was restricted to:

$$E_n = nh\nu = n\hbar\omega \qquad \hbar = \frac{h}{2\pi}$$

quantum number $n = 0, 1, 2, 3, \ldots$

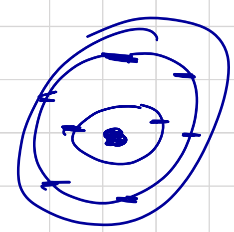
Planck's constant $= 6.63 \times 10^{-34}$ J·s

Take away?

→ In atomic scale systems, quantized (or discrete) allowed energy exists, rather than a continuum.

② Bohr atom

e^-s (electrons) in discrete energy levels in atoms



③ Wave-particle duality

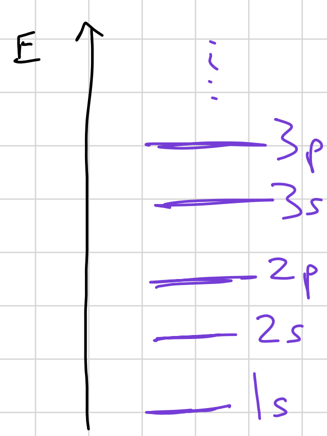
Einstein postulated in 1905 to explain photoelectric effect

→ Energy of impinging light: $E = h\nu = mc^2$ — speed of light; "mass" of a photon

→ momentum: $\boxed{p = h/\lambda} = mc$ — the de Broglie hypothesis ≡ wave-like nature of matter!

④ Wave-mechanical atom model

e^-s fill orbitals defined by quantum numbers



orbitals, subshells, magnetic, and spin

n ℓ m_ℓ m_s

Quantum Mechanics

→ Needed explanation of how expt data was at odds with classical mechanics / law of physics

→ 1926, Schrödinger developed wave mechanics for describing micro & macro universes

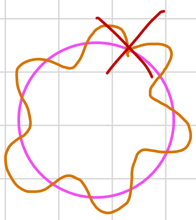
Quantum Mechanics

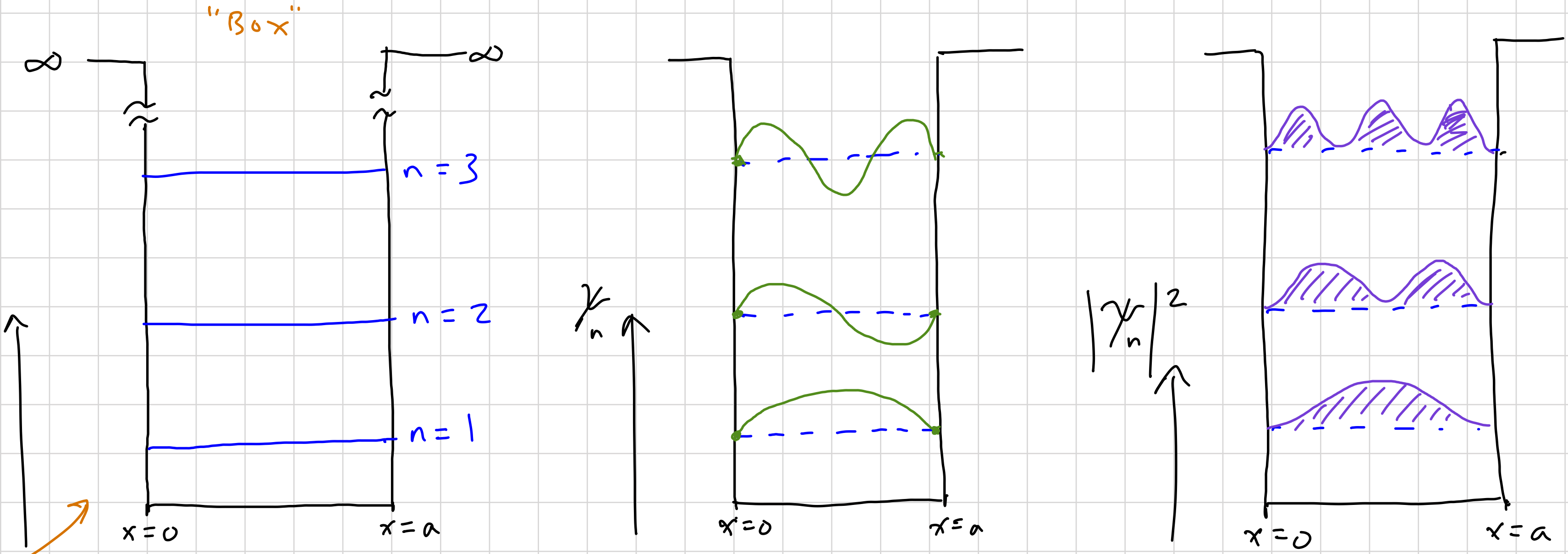
Schrödinger's Equation

principle governing eqn. : $-\frac{\hbar^2}{2m}\nabla^2\psi + U(x,y,z)\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}$

potential energy — $U(x,y,z)$; mass — m; wave function — ψ

- most basically applied to "a particle in a box" (1D)





Allowed Energy Levels

Look familiar? Same concept as e^-'s bound in atoms!

Wavefunctions at the first 3 discrete energy levels

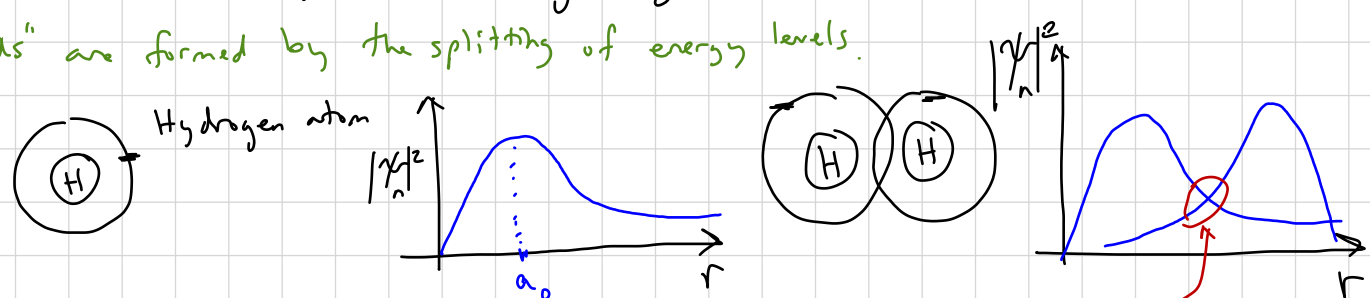
Proportional to the probability of finding the e^- at a certain point in the box/well.

Energy Bands

What happens when atoms are brought close enough together to have their e^- orbitals overlap?

"Energy Bands" are formed by the splitting of energy levels.

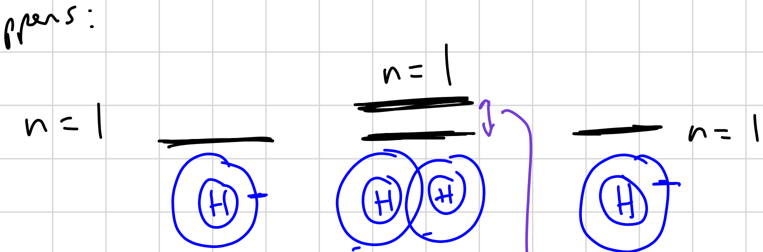
Example:



★ nonzero probability of 2 e^-'s occupying the same space!

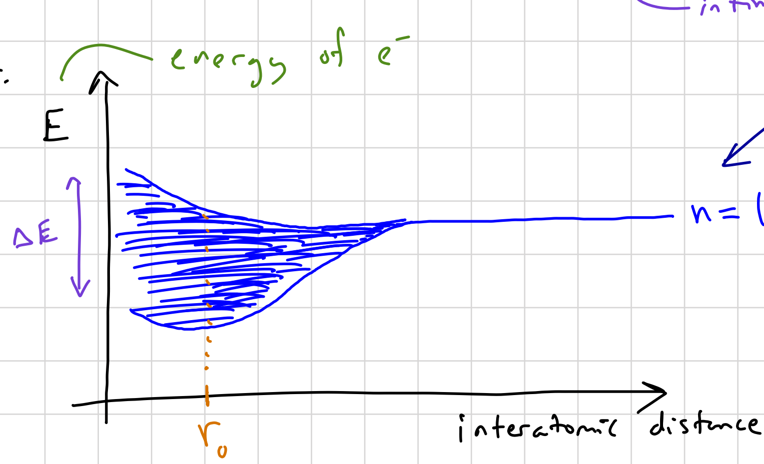
⇒ Pauli exclusion principle says, "No!"

What happens:



infinitesimally small E between them

Summary:



NOTE: This will happen for each e^- orbital, forming "bands" of allowed energy states throughout crystal instead of orbitals in atoms