1/19/2017

Quantum Theory of Solids

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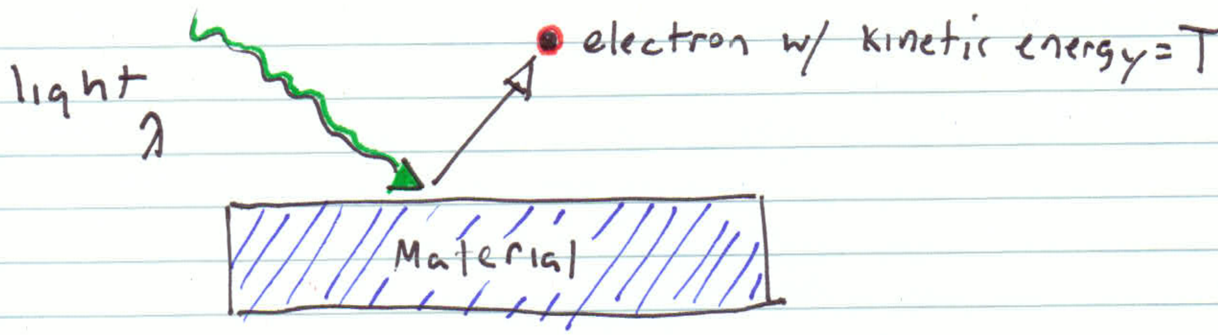
Lecture 3

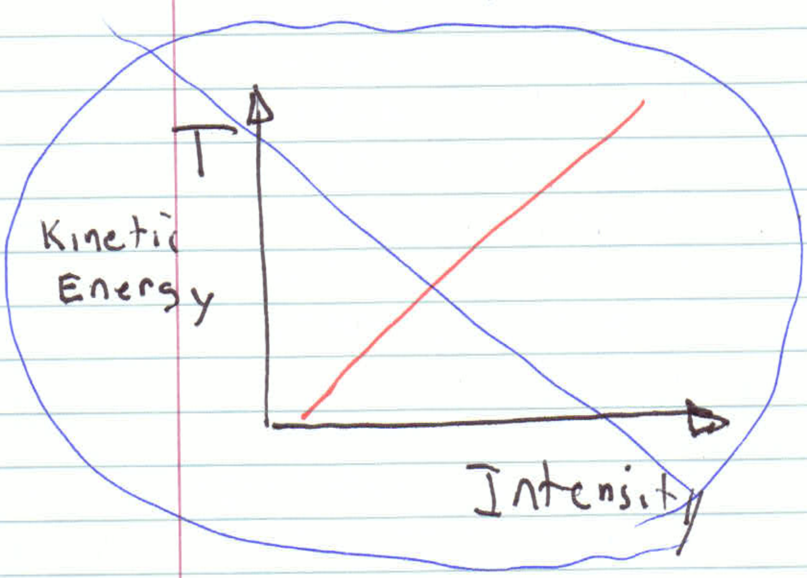
- Around 1900's there were experiments that seemed to not follow classical mechanics
- One notable experiment was the photoelectric effect



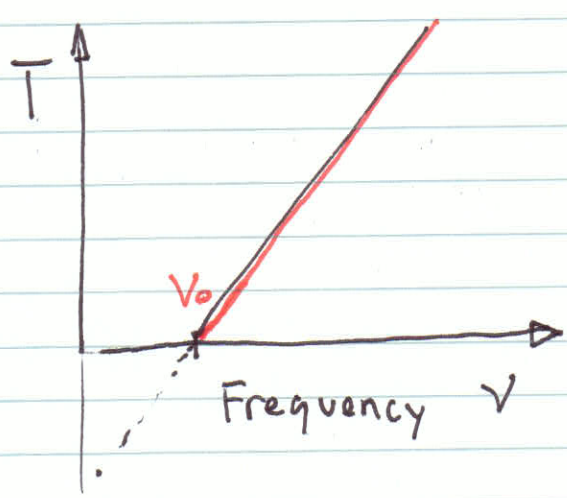
What do we expect?

Remember: At that time "light is a wave"

Classical Expectation



Actual Experiment



- Experimental observation of photo-electric effect

1. No electrons are ejected for $\nu < \nu_0$.
2. The kinetic energy proportional to frequency.
3. At low intensities, electrons are still ejected so long as $\nu \geq \nu_0$

- Einstein suggested electron is ejected from a collision with a particle-like ~~~~ projectile
  - The projectile carries enough energy to eject the electron from the material
  - If the projetile is ~~an~~ a photon with energy $h\nu$ then by conservation of energy $T = \frac{1}{2}m_e v^2 = h\nu - \Phi$

    where Φ is the work function

- Thus a beam of light is a collection of photons each with energy $h\nu$

Wave particle Duality

- DeBroglie then wonder if particles also behaved like waves,

Relativity

$$E = mc^2 = \sqrt{p^2c^2 + m_0^2c^4}$$

Kinetic energy — Rest mass energy

Kinetic term $E = pc$

we also know $E = h\nu$

equating $h\nu = pc$

$$\frac{hc}{\lambda} = pc \rightarrow \boxed{\lambda = \frac{h}{p} = \frac{h}{mv}}$$

Thus particles can indeed act like waves!

Quantum Numbers

- Quantum numbers describe a conserved quantity
- In classical physics conserved quantanties are continuous

Classical	Quantum (Numbers)
Energy	Principle Quantum Number (n)
Angular Momentum	Azimuthal QN (ℓ)
Magnetic Fields	Magnetic QN (m) or (m_ℓ)
	Spin QN (s) or (m_s)

- The major diffence is that in Quantum systems the conserved quantanties are "quantized", i.e. they come in discrete amounts.

Quantum Mechanics

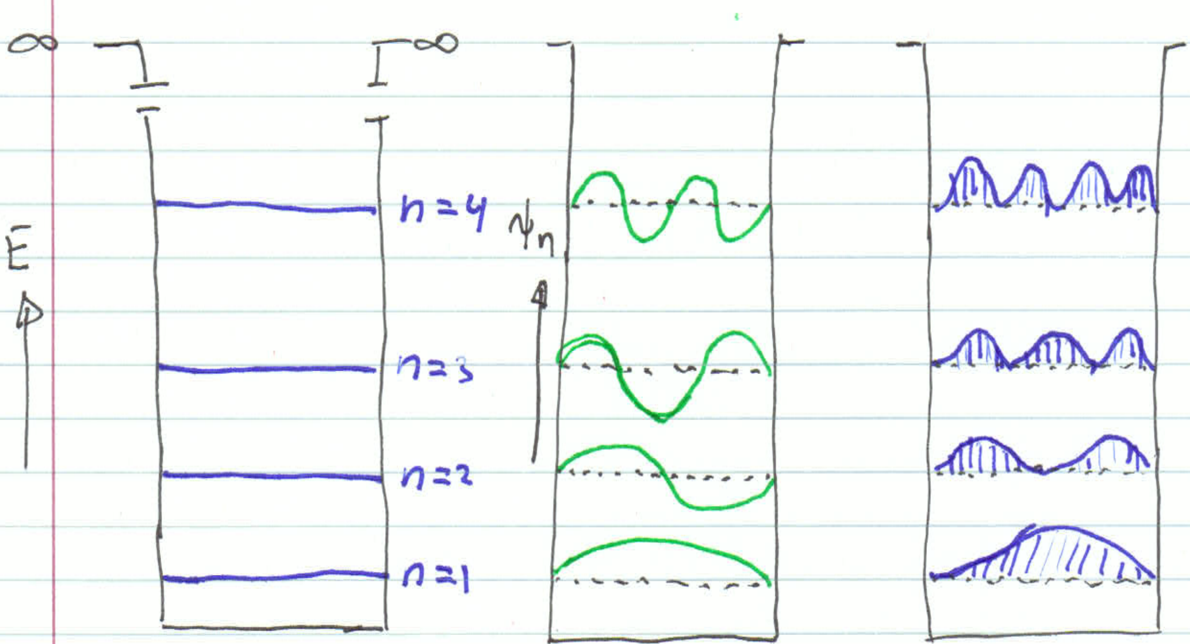
Main governing equation: 1D Schrodinger's equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V(x)\Psi(x,t) = j\hbar\frac{\partial \Psi}{\partial t}$$

where: $\hbar = \frac{h}{2\pi}$ and $j = \sqrt{-1}$

- Ψ is called the wave function
- It contains all the information about a systems dynamical properties.
- Ψ is often labelled with the quantum numbers

Particle In a Box



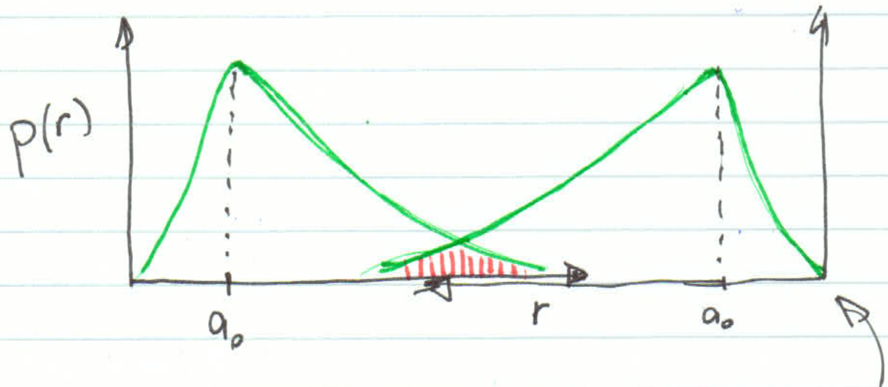
Allowed energy levels — Corresponing wave functions — probability function

- Max Born postulated that $|\Psi|^2 dx$ is the probability of finding the particle between x and x+dx at a given time
- Thus $|\Psi|^2$ is a probability density function

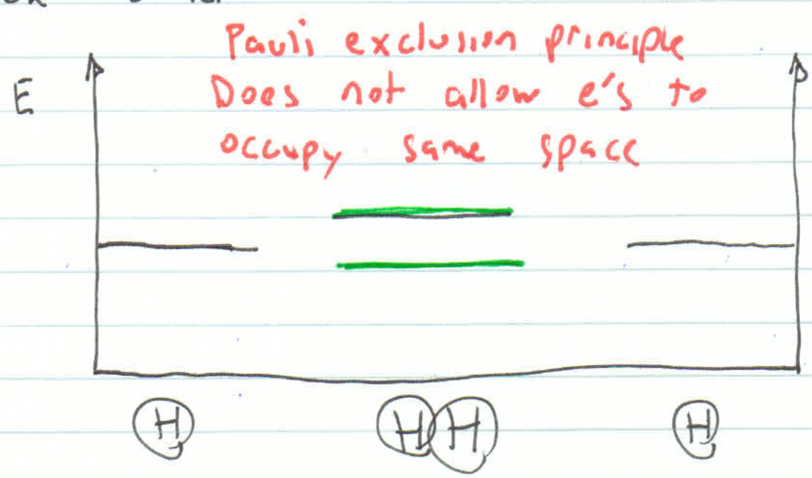
where $|\Psi|^2 = \Psi \cdot \Psi^*$

Energy Bands

- Let's consider a hydrogen atom that is not interacting with anything else
- The radial probability density function $p(r)$ will look like,



- If we have two hydrogen in proximity to each other



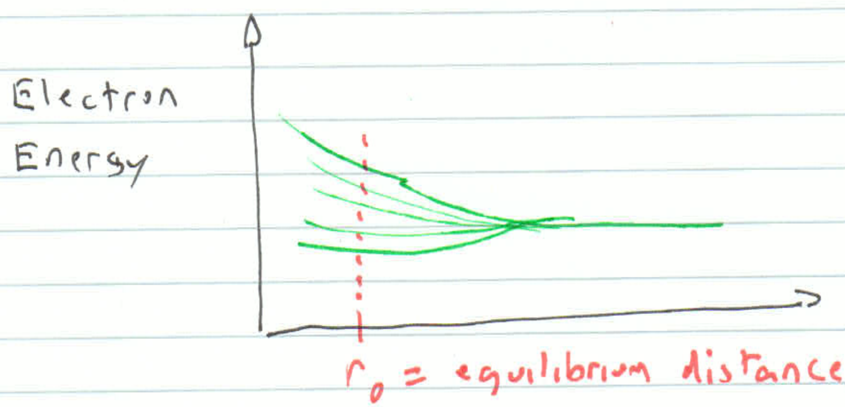
- The wave functions overlap + the e's interact.
- This results in a splitting of the energy levels

Pauli Exclusion Principle

- Two identical Fermions (e.g. electrons) cannot occupy the same quantum state within a quantum system.

- For 2 e's in the same orbital, if their n, l, and m_l quantum numbers are identical, then m_s must be different.

○ For a periodic lattice of hydrogen atoms, a plot of the electron energy as a function of a, i.e. the unit cell length looks like



- The end result is that we obtain bands of allowed energy states.