Lecture 29, Apr 7, 2022

Time Independent Schrodinger Equation and Hydrogen Orbits

- $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = (E - V)\psi$
- If $E > V$ then this means $\frac{\partial^2\psi}{\partial x^2}$ and ψ have different signs; this means the wavefunction curves towards zero (if $\psi > 0$ then it curves down, if $\psi < 0$ then it curves up)
  - This means we have oscillatory solutions
  - For the simple case where $V = 0$ (free electron), $\psi = \sin(kx)$ or $\cos(kx)$ where $E = \frac{\hbar^2 k^2}{2m}$
- If $E < V$, $\frac{\partial^2\psi}{\partial x^2}$ and ψ have the same sign; the wavefunction curves away from zero
  - This means we have exponential solutions
  - There can be 2 cases, either the solution blows up to infinity, or it decays towards zero
- In the infinite square well, in the well the solution oscillates, and outside the well the solution is always zero
- For the finite square well, in the well the solution still oscillates ($E > V$), but outside the well the solution decays towards zero ($E < V$)
  - There are a finite number of bound states (quantized states), because at some point $E > V$ everywhere
- For the quantum harmonic oscillator ($V = bx^2$):
  - For the $n = 1$ solution it resembles the finite square well
  - Since the potential gets wider as energy increase, increasing n makes the wavefunction wider
  - The place where $E = V$ is the *classical turning point*
  - In this case energy levels are evenly spaced (proportional to n instead of n^2)
- For the hydrogen atom energy is proportional to $\frac{1}{n^2}$; these 3 cases above are the only cases where there is a simple expression for E based on n
- The $2s$ state has a larger radius than the $1s$ state because the classical turning point is further away

Band Theory

- When two finite potential wells are brought near each other (like when two atoms approach each other during bonding), their wavefunctions overlap
  - The $n = 2$ state for hydrogen is bigger so there is more overlap
- Overlapping wavefunctions create bands; with n atoms there will be n bands
- The spacing between bands doesn't arbitrarily increase, so with a very large number of atoms, there is effectively a continuous range of energy levels
- Only valence electron wavefunctions overlap and form bands

Band Structure

- Metals have a partially filled band
  - States above a certain level are unfilled, below that level are filled
  - E_F is the Fermi level, below which all energy states are filled
  - Note there's a potential barrier at the edge of a metal so the electrons don't leak out (the work function Φ)
  - Since there are states immediately above the Fermi level, electrons can easily move in an electric field, so they can conduct electricity easily
- A semiconductor has 2 bands: the valence and conduction bands
  - The valence band is fully occupied at $T = 0$; the conduction band is unoccupied at $T = 0$
  - The band gap sits between the valence and conduction bands
    - The colour of light emitted by LEDs is the photon energy of its band gap

  - Electrons can only move if they have enough energy to cross the band gap and go into the conduction band
  - With enough energy, electrons leave the valence band and move into the conduction band, leaving behind a hole
    - The hole acts like a positive charge and can be a charge carrier
  - E_F for a semiconductor is usually somewhere in the band gap
- An insulator is similar to a semiconductor but the band gap is very large, making it very hard to cross
- A material appears as optically transparent if it does not absorb photons in the visible light range
  - If the band gap is large enough that photons in the visible range cannot excite electrons across the gap, then photons will not be absorbed and the material is transparent
  - For metals and other materials where the band gap is small, photons will be absorbed by electrons which jump to the conduction band, so the material is opaque