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CHEM 3420: Physical Chemistry II — Spring 2009

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Lecture 1: Introduction to Quantum Mechanics & Wave Properties

References

1. Levine, *Physical Chemistry*, Sections 17.1–17.5

Key Concepts

- Our main goal this semester is to connect the structure of atoms & molecules to the observed experimental properties of these substances.
- We'd like to try and explain things such as: the periodic table, molecular bonding, and spectroscopy.
- Heart of the quantum mechanical world is wave-particle duality. In the macroscopic world, electrons act like particles. However, on a microscopic/atomic level, they have wave-like properties.
- Classical mechanics works great in the macroscopic world. It is deterministic: given a set of initial conditions, exact predictions about the outcome can be computed using physical laws (ex, Newton's laws of motion).
- Quantum mechanics (QM) is need at small (atomic) length scales where matter (electrons) behaves like waves.
- Quantum mechanics is probabilistic: we can never say what *will* happen, only what is *most likely* to happen.
- Understanding the properties of waves is essential in QM. A general 3-D wave (F) is a function of four variables: $F = F(x, y, z, t)$, where x, y, and z are positional variables in 3-D and t is the time dependence.
- Important parameters to describe waves:
  - Wavelength (λ): measured in cm, m, nm, μm, Å
  - Frequency (ν): measured in s^{-1}
  - Velocity (v): measured in m/s, cm/s. The velocity of liqht is a constant, c equal to 3×10^8 m/s
  - The wavelength and frequency are related through the velocity: $c = \lambda\nu$
  - Period (τ): time for one complete cycle/wavelength, measured in seconds, $\nu = \frac{1}{\tau}$.
  - Wave number ($\overline{\nu}$): the inverse of the wavelength, usually in cm^{-1}
  - Wave vector (k) = $\frac{2\pi}{\lambda}$
- Wave interference (as seen in the double-slit experiment) is a result of constructive and destructive interference of two waves. When they add, they increase their amplitude when the constructively interfere. When they destructively interfere, they subtract from one another and lead to no or very small amplitude.
- The interference of electrons in the double-slit experiment is our first evidence of the need to quantum mechanics to explain an observed phenomena.