



CHEM 1035 – Lecture 23

Quantum Theory of Matter

The energy changes that accompany chemical reactions are an important part of chemistry. Much of the Chemistry field is devoted to using chemical reactions to efficiently extract energy.

Light is shown to have either a wave description or a particle description. These principles can also be extended to particles, leading to a wave-particle duality of matter. The wave-particle duality of matter leads to the Quantum Mechanical description of atoms.

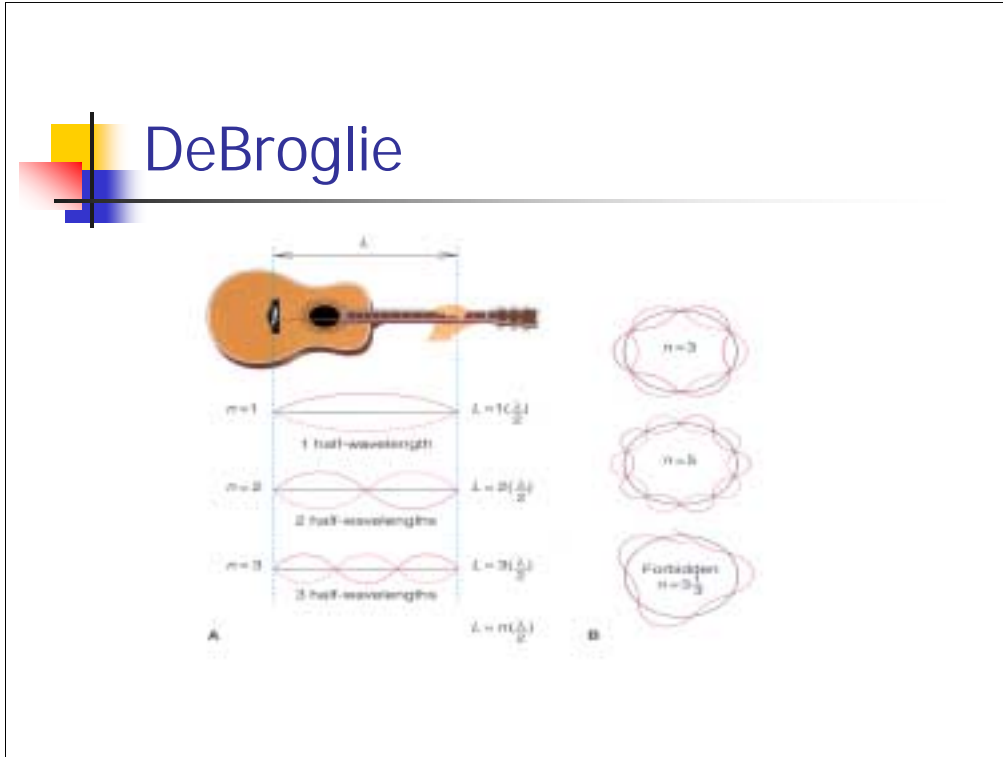


Bohr Atom

The Bohr model of the Hydrogen atom correctly predicts the Atomic Spectrum observed for Hydrogen. This model, however, is not successful in describing the behavior of any other atom.

Bohr's hypothesis is important to the development of modern chemistry because it was the first application of the idea that energy can only take discrete values to the atom. Because the energy emitted by atoms can only have discrete values, that also says that the energy contained by the atoms must also be discrete.

DeBroglie



DeBroglie hypothesized that if light can be described as both a wave and a particle, perhaps things that are traditionally thought of as particles could then also be described by wave behavior. Knowing:

$$E = h\nu \quad \text{and} \quad E = mc^2$$

$h\nu = mc^2 \rightarrow hc/\lambda = mc^2 \rightarrow \lambda = h/mc$ This is known as the DeBroglie wavelength, and it says that wavelength is inversely proportional to the particle mass.

What does this say about the wavelength of very large particles? Does this make sense with our experience?

Particles, therefore, should display wave-properties (e.g. diffraction and refraction)

mc in the denominator (mass x velocity) is the momentum of the particle. If light is a particle, then it has momentum given by the DeBroglie wavelength.

Calculate the wavelength of a large object?



Heisenberg Uncertainty Principle

Consider a beam of light.

- Wave description tells us that it is an oscillating wave
- Particle description tells us that it is a stream of particles

Where does the wave exist? How about the particle? With a particle, it is simple to identify where it is in space. With a wave, however, we can't pin-point the location because the wave exists spread out in space. DeBroglie's hypothesis tells us that all matter can be described as either a particle or a wave. How can we reconcile this?



Heisenberg Uncertainty Principle

The Heisenberg Uncertainty Principle says that it is impossible to know simultaneously the position and momentum of a particle simultaneously

$$\Delta x \cdot m\Delta u \geq \frac{h}{4\pi}$$

This tells us that, contrary to Bohr's hypothesis, we cannot assign a fixed position for the electron in an atom.



Quantum Mechanics

- Planck's Description of Blackbody Radiation
- Einstein's Explanation of the Photoelectric effect
- Bohr's model of the Hydrogen atom
- DeBroglie's Hypothesis of wave-particle duality for all matter
- Heisenberg's Uncertainty Principle.

These Hypothesis and Models all lead to the Dual Nature of Matter and energy (e.g. described as both a wave and a particle) – leading to the field of Quantum Mechanics - a field of study focused on the wave motion of matter on the atomic scale.



Schrödinger Equation

A mathematical expression that describes the wave behavior of atomic particles (esp. electrons).

$$H\Psi = E\Psi$$

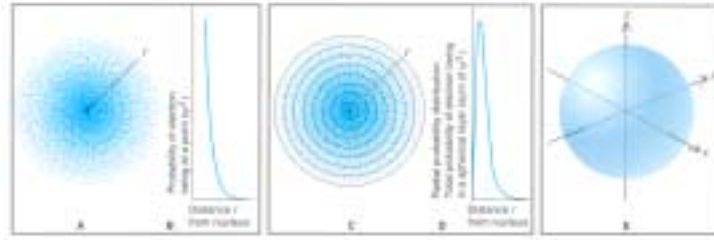
Where H is the Hamiltonian (a mathematical operator), E is the energy of the atom, and Ψ is the “wave function”

The wave function is the description of the electron in terms of the wave properties.



Solution to Schrödinger Equation

Solving the Schrodinger Equation results in an Electron Density Probability Distribution.



Solution of the Schrodinger equation leads to a probability distribution. This shows where the electron density is most likely found. This is most commonly illustrated with a probability contour – this represents the volume within which the electron spends 90% of its time.



Atomic Orbitals

The solutions of the Schrodinger Equation have different “probability contours”. These contours are termed “Atomic Orbitals” and the Atomic Orbitals have characteristic shapes and orientations.

Atomic orbitals are characteristic 90% probability contours for different solutions to the Schrodinger Equation. These Atomic Orbitals (solutions to Schrodinger’s equation) are specified by 3 unique “Quantum Numbers”. These quantum numbers provide information about the size, shape, and orientation of the atomic orbital. Ultimately, the quantum numbers represent the energy of the orbital.

Orbital is an unfortunate term because it implies the planetary model of the Bohr atom. The contour represents a volume within which the electron is most likely (but not necessarily) will be found.



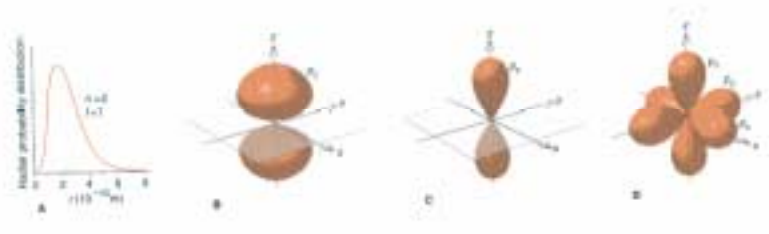
Quantum Numbers

Integer values that represent the Atomic Orbitals

- Principal Quantum Number (n)
- Angular Momentum Quantum Number (l)
- Magnetic Quantum Number (m_l)

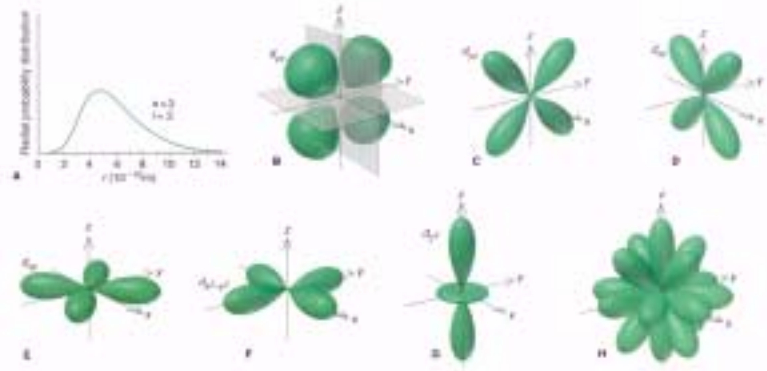
1. Principle Quantum number (n), takes a positive integer value (1,2,3,...) This is representative of the relative size of the orbital. The greater the number, the further from the nucleus the probability contour extends.
2. Angular Momentum Quantum number (l), takes a value ranging from 0 to ($n-1$). This number is representative of the shape of the atomic orbital. If $n = 0$, then the orbital shape is spherical. If $n = 1$, then l can only be 0. If $n = 3$, then $l = 0, 1, \text{ and } 2$. Note that the value of n limits the values available for l
3. Magnetic Quantum Number (m_l), this takes a value ranging from $-l$ to $+l$. This represents the spatial orientation of the orbital. If $n=1$, then $l=0$ and $m_l=0$, this represents a sphere and the sphere is oriented equally distributed in all directions.

$l=1$, p-orbitals



P-orbitals are dumb-bell shaped.
What are the values of m_l ?

$l=2$, d-orbitals



D- orbitals have these shapes. Notice that the d_{z^2} has a different shape.

What values are available m_l ? -2, -1, 0, 1, 2