Chapter 7: Electron Structure of the Atom

October 24, 2022

Chemistry Department, Cypress College

Class Announcements

Lab

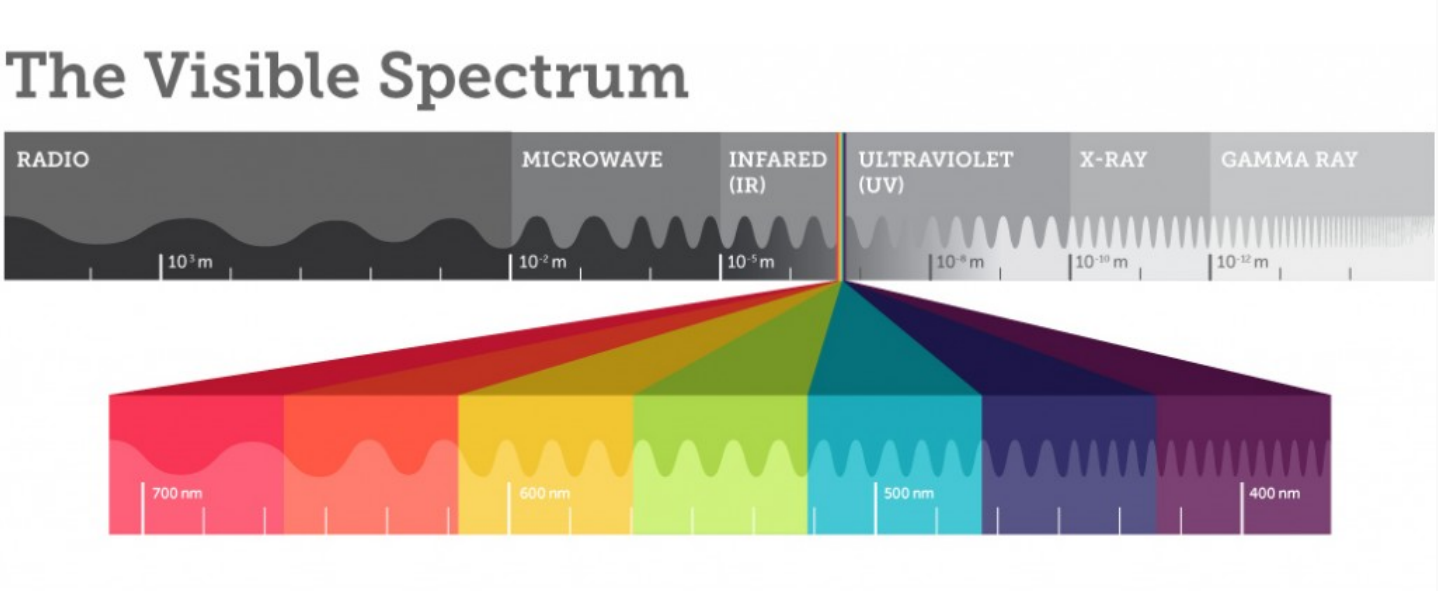
- Experiment 15 - Quantitative Prep of KCl
- Begin the water bath ASAP
- Reminder - Need 70% of laborator points to pass the course

Lecture

- Ch 7 Bonus Lecture - Introduction to Quantum Chemistry
- Go over homework 7 (EC for students who present)
- Quiz and Homework assignment released Fri, Oct 14th at 3pm
- Exam 2 - Weds, Oct 26 at 2:55pm; 2 hours and 8 free response questions

Outline

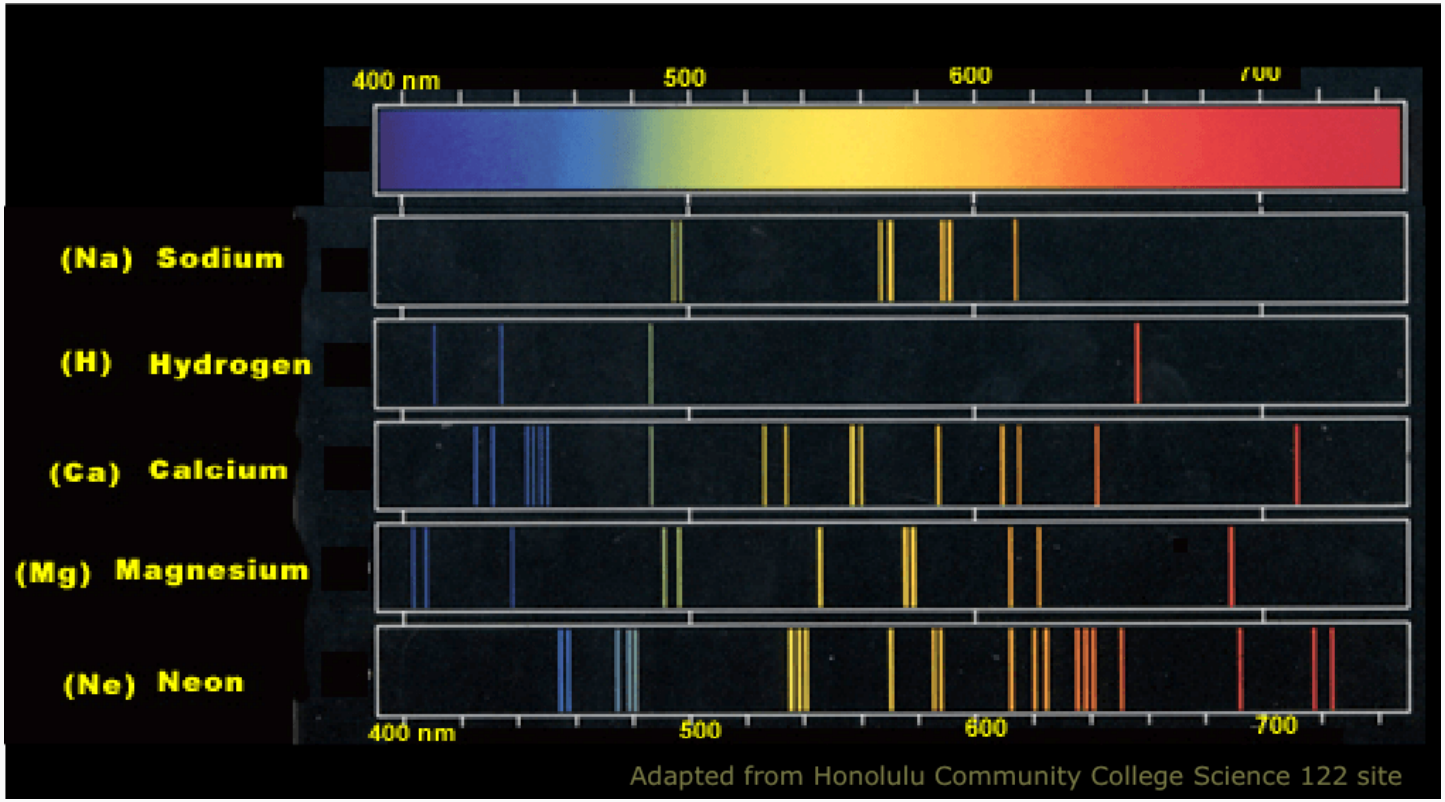
Revisit: Radiation Energy



$$E = \frac{hc}{\lambda} = h\nu \tag{1}$$

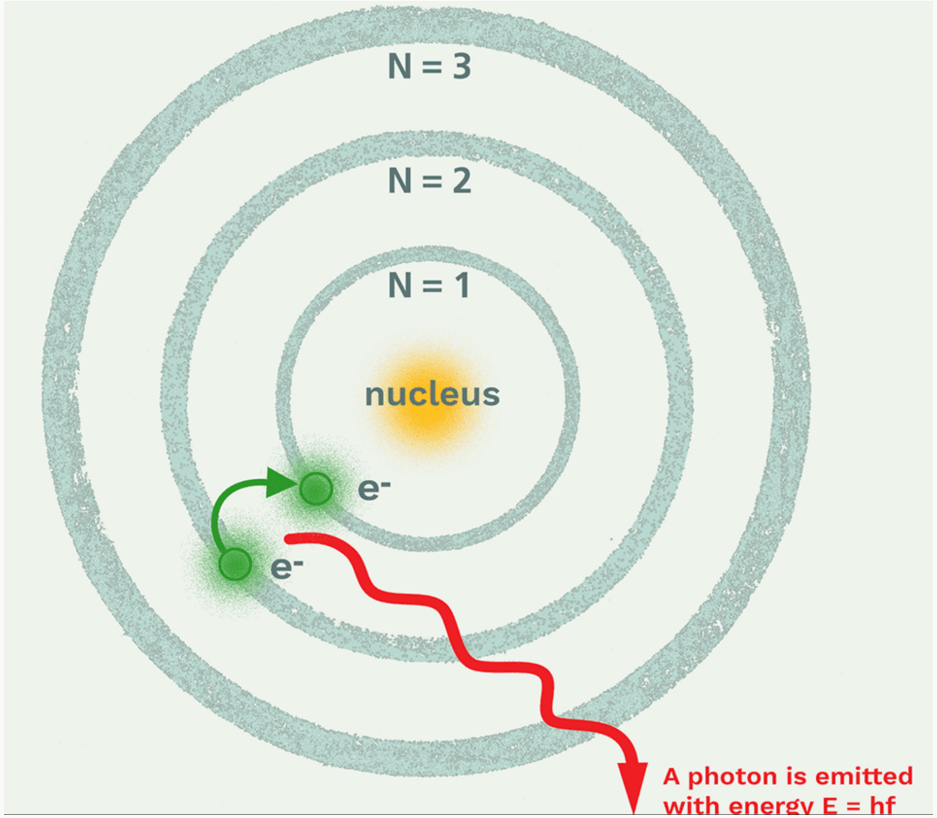
- High frequency and larger wavelengths lead to higher radiation energy
- Energy are contained in packages known as photons; Eqn 1 computes the energy for 1 photon

Atomic Spectra



- Continuous spectra is given at the top and discrete lines are emitted by atoms
- **Q:** Why are there discrete lines for the atomic spectra?

Bohr Model of the H Atom



$$\Delta E = E_{\text{final}} - E_{\text{initial}} \tag{2}$$

Note: Keep in mind of sign conventions ($\Delta E > 0$ and $\Delta E < 0$)

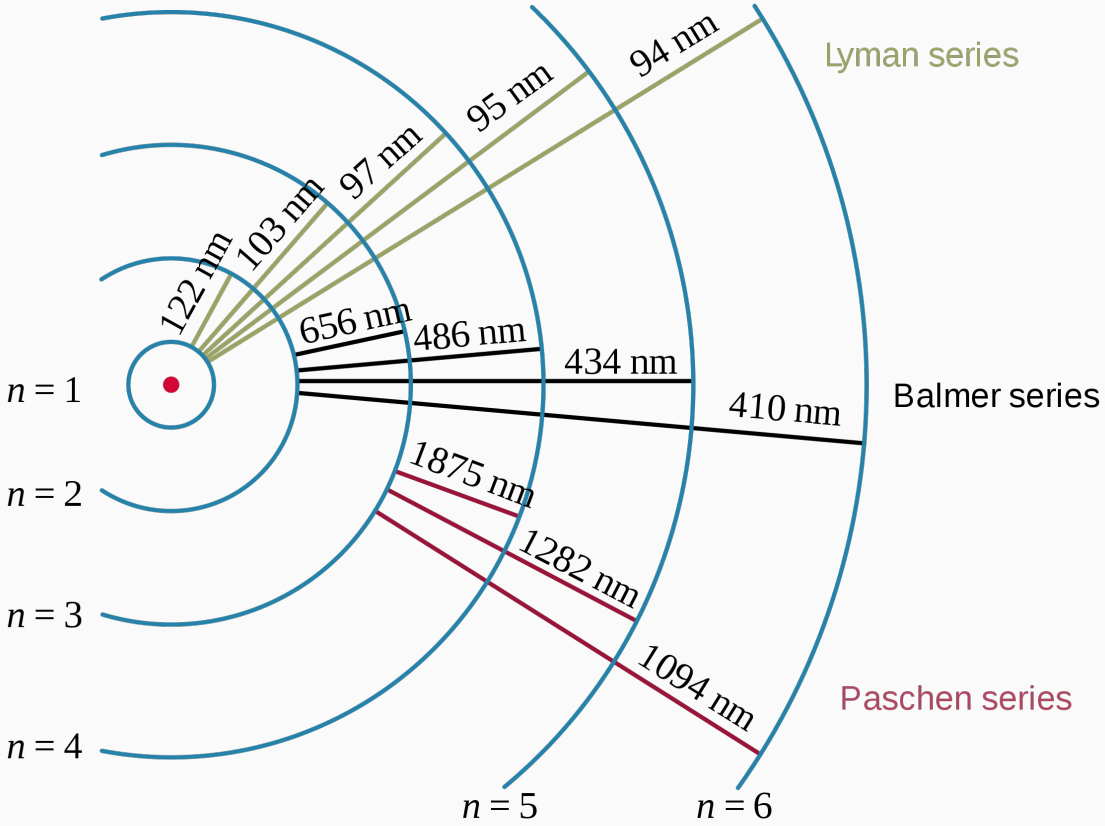
Bohr Model

- Energy is quantized
- Electrons orbit the nucleus in orbits that have a set size and energy
- The energy of the orbit is related to its size; the lowest energy is found in the smallest orbit
- Radiation is absorbed or emitted when an electron moves from one orbit to another

Limitation of the Bohr Model

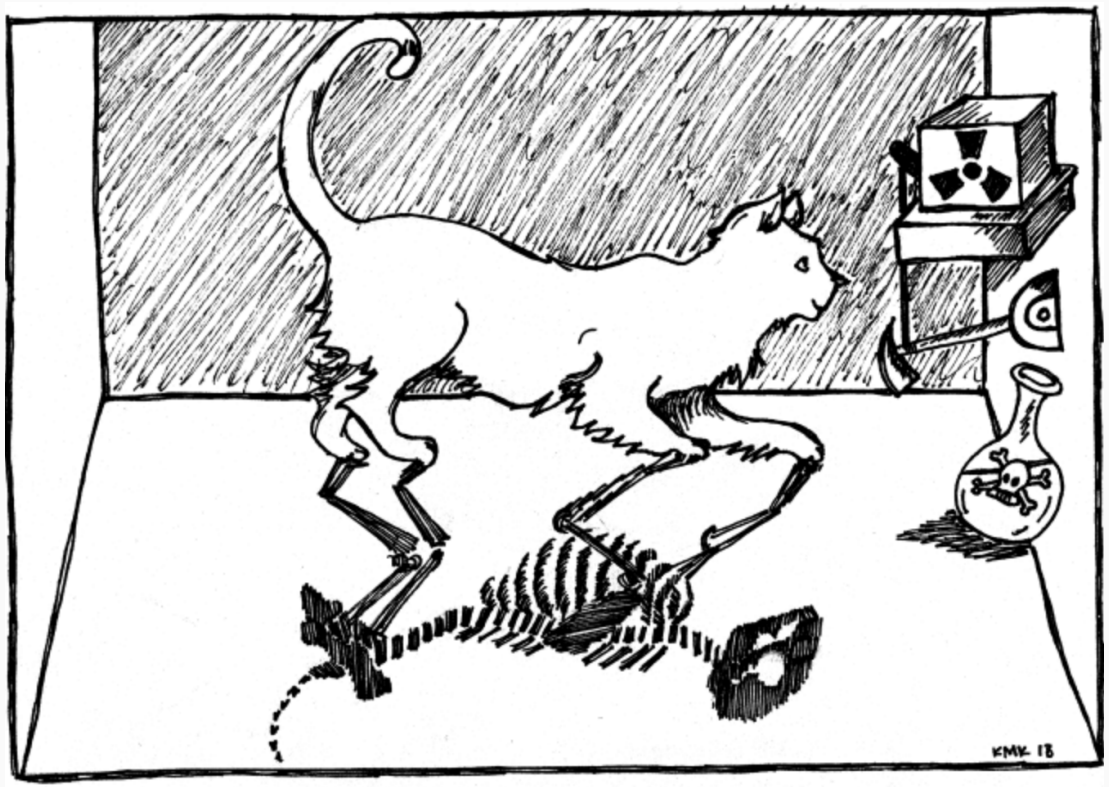
- Violates the Heisenberg Uncertainty Principle
- Poor predictions regarding the spectra of larger atoms
- Does not predict the relative intensities of spectral lines

Example: H atom spectra



Outline

Schrödinger's Cat - Thought Experiment



The world that we know is deterministic, however, dealing with electrons or small subatomic particles, we have to think of it in terms of probabilities

The Wavefunction Ψ

Schrödinger's Equation

$$\hat{H}\Psi = E\Psi \tag{3}$$

where $\hat{H}$ is the Hamiltonian, E is the energy, and Ψ is the wavefunction

- Equation that explain everything about your system
- Chemical and physical properties can be determined from the Ψ

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- Ψ should be continuous and single-valued
- Probability distribution in three dimensions is established using the $|\Psi|^2$
- The probability of finding a particle if it exists is 1.

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- For every observable, there corresponds a Hermitian operator in quantum mechanics
- In any measurement of the observable associated with operator $\hat{A}$, the only values that will ever be observed are the eigenvalues a, which satisfy the eigenvalue equation

$$\hat{A}\Psi = a\Psi \tag{4}$$

Postulates of Quantum Mechanics

- If a system is in a state described by a normalized wave function Ψ, then the average value of the observable corresponding to $\hat{A}$ is given by

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- Total wavefunction must be antisymmetric with respect to the interchange of all coordinates of the electrons

$$\Psi(-x) = -\Psi(x) \tag{7}$$

Atomic Orbitals