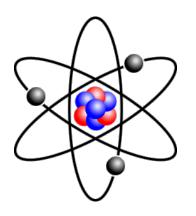
PHY2005 Atomic Physics

Lecturer: Dr. Stuart Sim

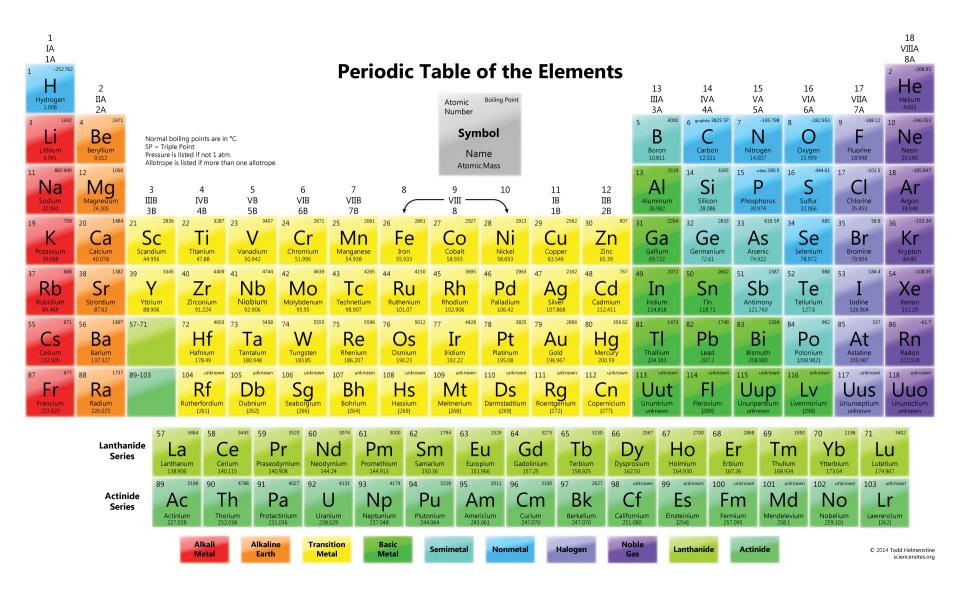
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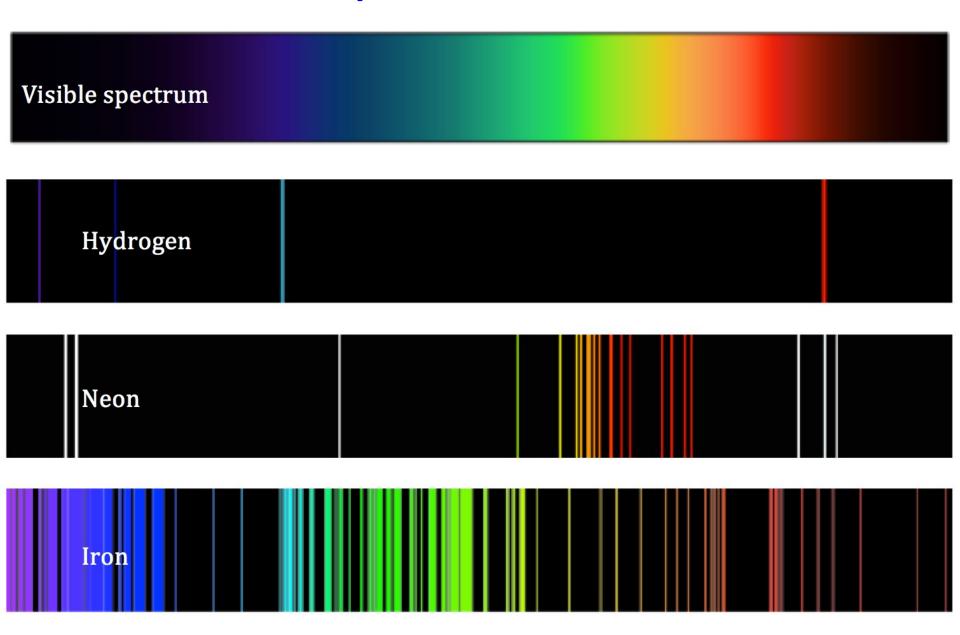
Atoms in physics



Atom: particles bound by Coulomb potential



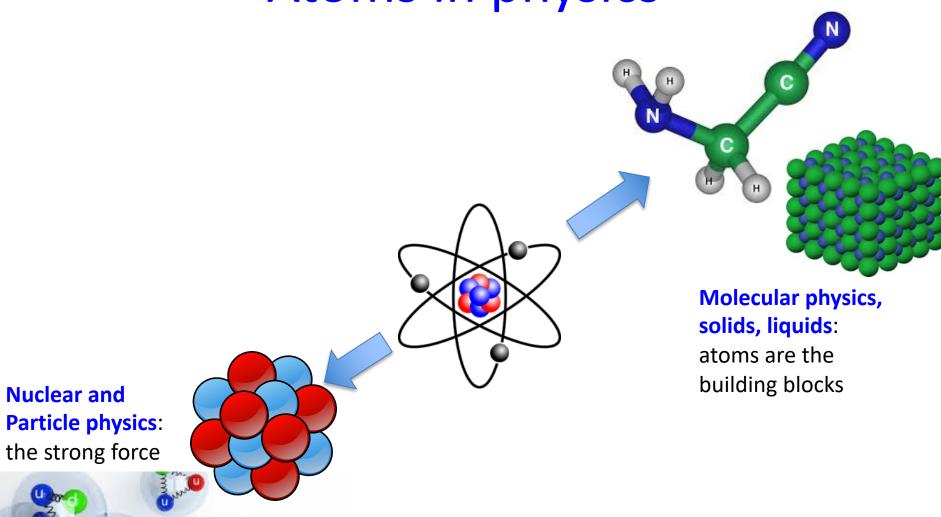
Very testable QM



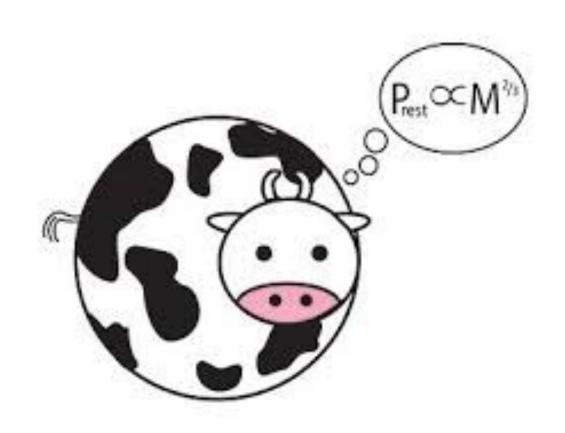
Very testable QM

"The spectrum of the hydrogen atom has proved to be the Rosetta stone of modern physics: once this pattern of lines had been deciphered much else could be understood" – Hänsch, Schawlow & Series (Scientific American, 1979)

Atoms in physics



How physics really works



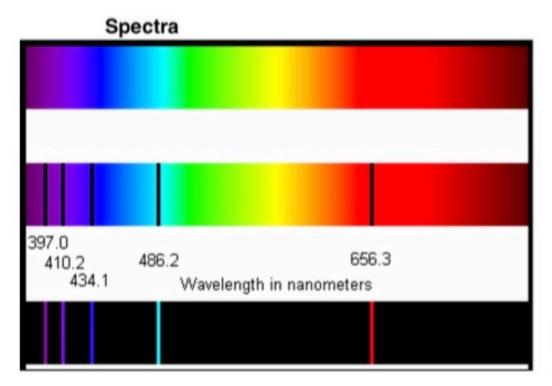
(2) Single-electron atoms

Learning goals

- 1. To revise the observed properties of the spectrum of the hydrogen atom.
- 2. To revise the postulates of the Bohr model, including how quantization is introduced to the model via a quantum number.
- 3. To revise the application of the Bohr model to calculate energy levels (and radii) in single-electron atoms.
- 4. To understand how the Bohr model can be applied to singleelectron atoms with differing nuclear mass and/or differing nuclear charge.
- 5. To assess the quantitative accuracy of the Bohr model.
- 6. To understand limitations of the Bohr/Sommerfeld model of single-electron atoms.

Spectrum of hydrogen

Optical:



Continuous visible spectra

H atom absorption spectra

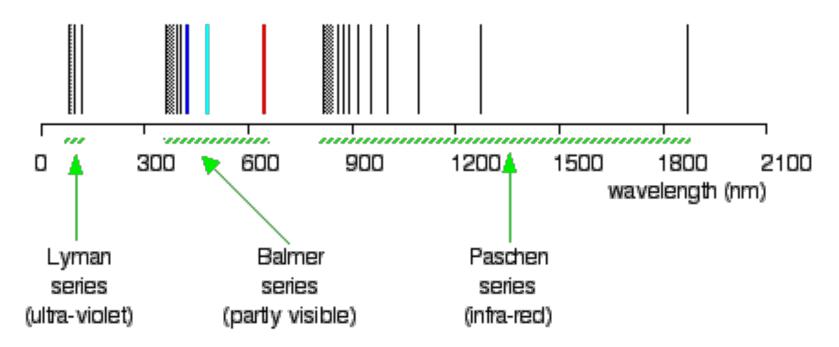
H atom emission spectra

Spectrum empirically matched by Rydberg formula:

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right) \text{ for } n \ge 3$$

Spectrum of hydrogen

Ultraviolet, optical and infrared:



Spectrum matched by Rydberg/Ritz:

$$\frac{1}{\lambda} = R\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right) \text{ for } n_2 > n_1$$

Spectrum of hydrogen

Ultraviolet, optical and infrared:

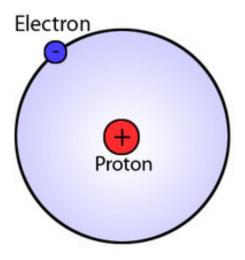
| Series | Region | n_1 | n_2 |
|-----------------|-------------|-------|---------------|
| name | | | |
| Lyman | Ultraviolet | 1 | 2 to ∞ |
| Balmer | Visible | 2 | 3 to ∞ |
| Paschen | Infrared | 3 | 4 to ∞ |
| Brackett | Far IR | 4 | 5 to ∞ |
| Pfund | Far IR | 5 | 6 to ∞ |

Table 1: Series of lines in the hydrogen spectrum.

Transitions within series named using Greek letter $(\alpha, \beta, \gamma \text{ etc.})$, starting from the longest wavelength.

Postulates of the Bohr model

- 1. Electron in "classical" circular orbit
- 2. Orbital angular momentum, L, is quantized
- 3. Electron does not radiate while in allowed state
- 4. Radiation emitted in transitions between states



Bohr formulae

Allowed states specified by principal quantum number, n. Energy and radius in each state obey:

$$E_n = -\left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{m_e Z^2 e^4}{2\hbar^2 n^2} \approx -13.6 \text{ eV} \frac{Z^2}{n^2}$$

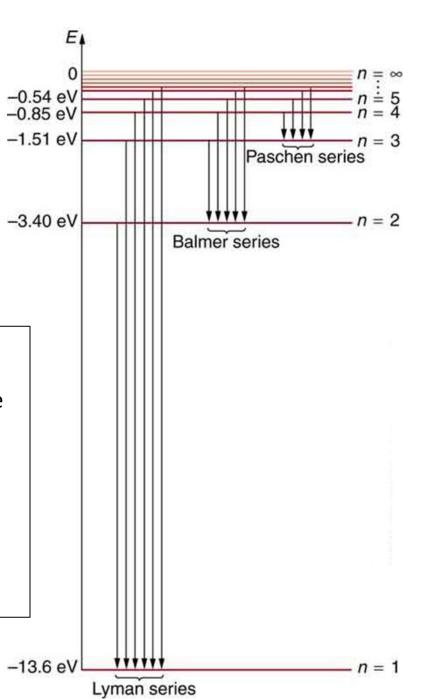
$$r = \frac{4\pi\epsilon_0 n^2 \hbar^2}{m_e Z e^2} = a_0 \frac{n^2}{Z}$$
$$a_0 \approx 5.3 \times 10^{-11} \text{ m}$$

Wavelengths of transitions in the Bohr model

For photons emitted in transition between levels with quantum numbers n_i and n_f :

$$\frac{1}{\lambda} = \frac{\nu}{c} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{m_e Z^2 e^4}{4\pi\hbar^3 c} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R_\infty Z^2 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$
where
$$R_\infty = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{m_e e^4}{4\pi\hbar^3 c}$$

Energy levels and transitions in hydrogen ("energy level diagram")



Note:

- here we are using energy scale "relative to ionization"
- common alternative to take "ground" state as E=0
- definition of energy scale particularly important for multi-electron atoms (later)

Reduced mass

To account for finite mass of nucleus, replace electron mass with *reduced mass* given by

$$\mu = \frac{m_e M}{m_e + M}$$

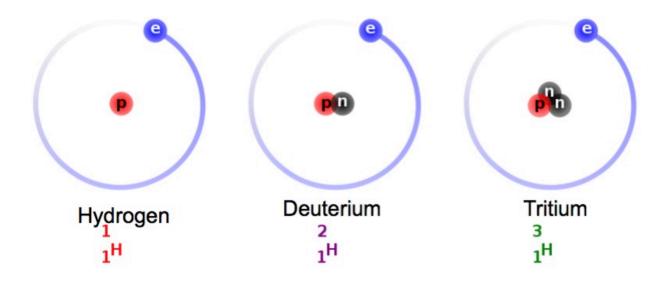
Equivalent to replacing the Rydberg constant with

$$R_M = \frac{\mu}{m_e} R_{\infty} = \frac{M}{m_e + M} R_{\infty}$$

Reduced mass

Although the effect of reduced mass is small (the proton mass is about 2000 times larger than the electron mass), it is measureable in spectra.

It is clearly seen as an isotope shift e.g. between the isotopes of hydrogen (differing number of neutrons in the nucleus).



Other single-electron atoms

The Bohr model can be applied to single-electron atoms, provided that the nuclear charge Z and the reduced mass μ are properly taken into account.

$$\frac{1}{\lambda} = \left(\frac{1}{4\pi\epsilon_0}\right)^2 \frac{\mu Z^2 e^4}{4\pi\hbar^3 c} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

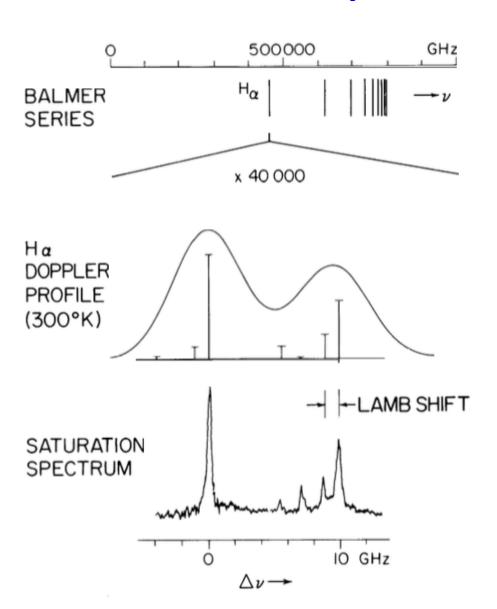
Includes single-electron ions, and exotic examples like positronium.

Table 2: Some single-electron ions and their nuclear charge.

| single-electron ion | nuclear charge |
|---------------------|----------------|
| He ⁺ | Z=2 |
| Li^{2+} | Z = 3 |
| $\mathrm{Be^{3+}}$ | Z = 4 |

Limitations of Bohr theory

Transitions of hydrogen have observed fine structure, which is not explained by the simple theory:



Limitations of Bohr theory

Transitions of hydrogen have observed fine structure, which is not explained by the simple theory:

| Transition | principle quantum | Fine-structure | Bohr theory |
|----------------|-----------------------|-----------------|-------------|
| | number change | components (nm) | (nm) |
| Balmer α | $n=3\rightarrow n=2$ | 656.4522552 | 656.4696 |
| | | 656.4537684 | |
| | | 656.4584404 | |
| | | 656.466464 | |
| Balmer β | $n=4 \rightarrow n=2$ | 486.264130281 | 486.2737 |
| | | 486.264488967 | |
| | | 486.265465436 | |
| | | 486.265570391 | |
| | | | |

Limitations of Bohr theory

Model can be extended (Sommerfeld) to elliptical orbits accounting for special relativity, allowing fine structure to be incorporated, up to a point.

However, such semi-classical treatments were superseded by more complete formulations of quantum mechanics, which are now well accepted.

In the next sections we will revise the quantum treatment of the single-electron atom and then consider multi-electron atoms.

Summary/Revision

- The spectra of single-electron atoms consist of regular series of lines with wavelengths described by the Rydberg formula.
- Bohr's semi-classical model describes the *quantized* energy and radii of electron orbits in the hydrogen atom and introduces a *quantum number*, *n*.
- The pattern of spectral lines predicted by the Bohr model agrees with the general observed properties of the hydrogen spectrum very well.
- The Bohr model makes simple, testable predictions for how the spectra of other single-electron atoms will behave, depending on the reduced mass and the nuclear charge.
- The simple Bohr model does not account for all properties of the hydrogen spectrum, however. In particular, more sophisticated approaches are need to understand *fine structure* in the spectral lines.