Lecture 2 362 January 16, 2019

Paradigm Shift: Development of Current Atomic Theory— Spectroscopy and Energy Levels in Atoms

OR,

"Show me the Electrons!"

Color	Metal Flame Colors
Red	*Carmine*: Lithium compounds. Masked by barium or sodium. *Scarlet or Crimson*: Strontium compounds. Masked by barium. *Yellow-Red*: Calcium compounds. Masked by barium.
Yellow	Sodium compounds, even in trace amounts. A yellow flame is not indicative of sodium unless it persists and is not intensified by addition of 1% NaCl to the dry compound.
White	*White-Green*: Zinc
Green	*Emerald*: Copper compounds, other than halides. Thallium. *Blue-Green*: Phosphates, when moistened with H_2SO_4 or B_2O_3. *Faint Green*: Antimony and NH_4 compounds. *Yellow-Green*: Barium, molybdenum.
Blue	*Azure*: Lead, selenium, bismuth, $CuCl_2$ and other copper compounds moistened with hydrochloric acid. *Light Blue*: Arsenic and come of its compounds. *Greenish Blue*: $CuBr_2$, antimony
Violet	Potassium compounds other than borates, phosphates, and silicates. Masked by sodium or lithium. *Purple-Red*: Potassium, rubudium, and/or cesium in the presence of sodium when viewed through a blue glass.

Atomic Emission (Spectroscopy)

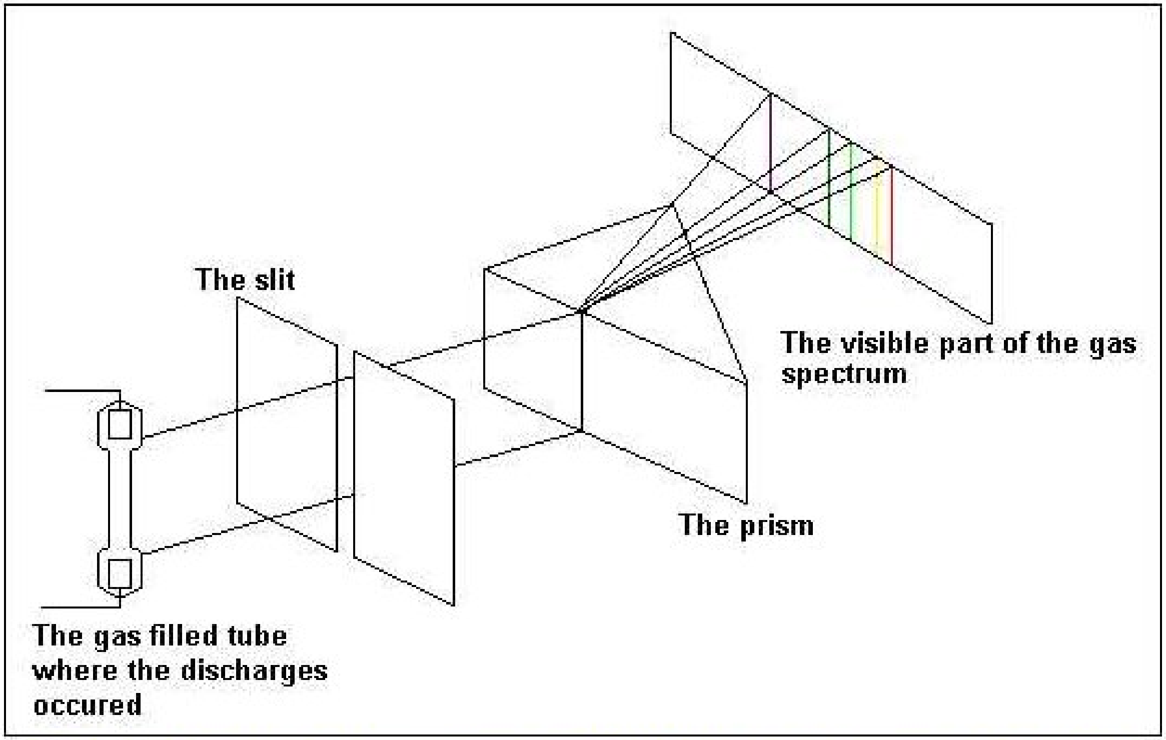
- An emission spectrum requires first the addition of energy to a material.
- The addition of energy promotes electrons of that material from the ground state to the excited state.
- As the electrons "fall" from the excited state to the ground state, they emit the energy they absorbed in the form of electromagnetic radiation (heat, light, etc.)

Comments

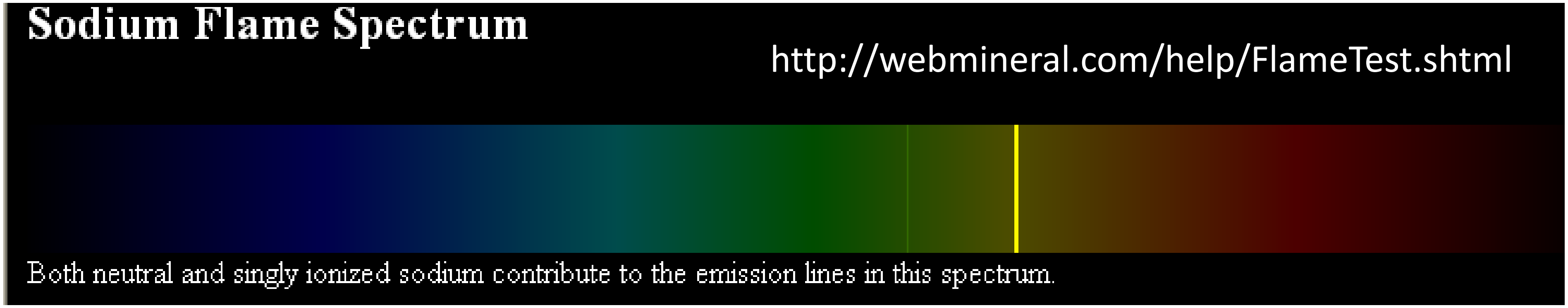
- Atomic emission is used in street lamps, fluorescent lights, and neon signs.
- Two common street lamps using this are the mercury lamp and the sodium lamp.
- "Neon" signs frequently implement the emission spectra of other gases such as argon and krypton.
- Very sophisticated instrumental techniques such as "flame photometry" and "atomic absorption" are based on the principles of atomic emission.

Continuous and Line Spectra

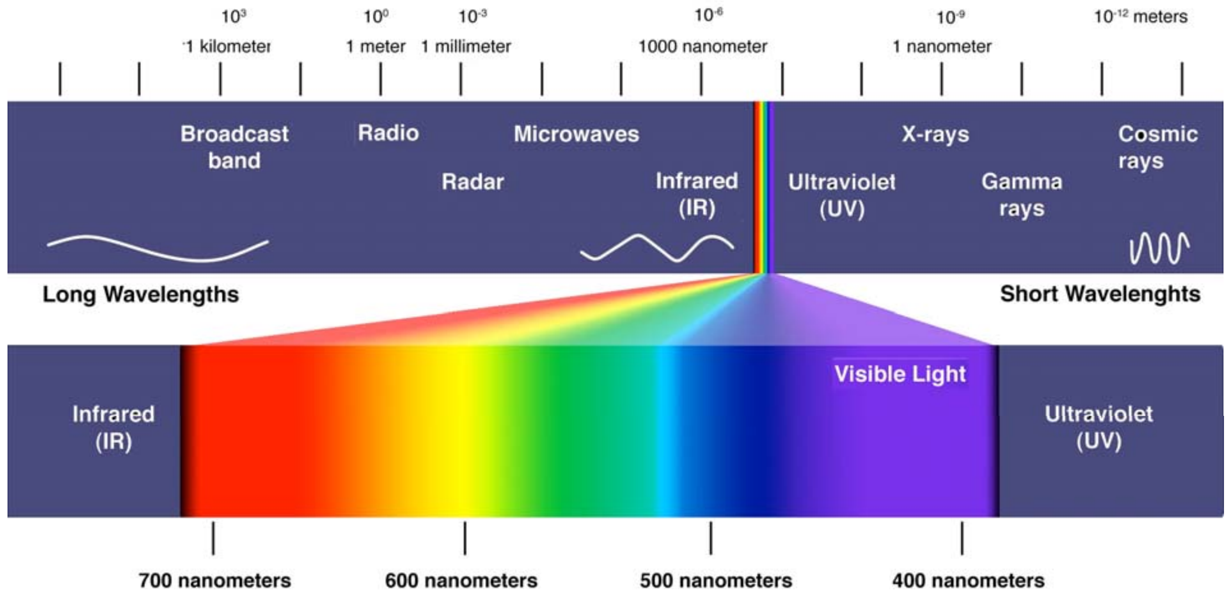
Dark Side of the Moon
Pink Floyd

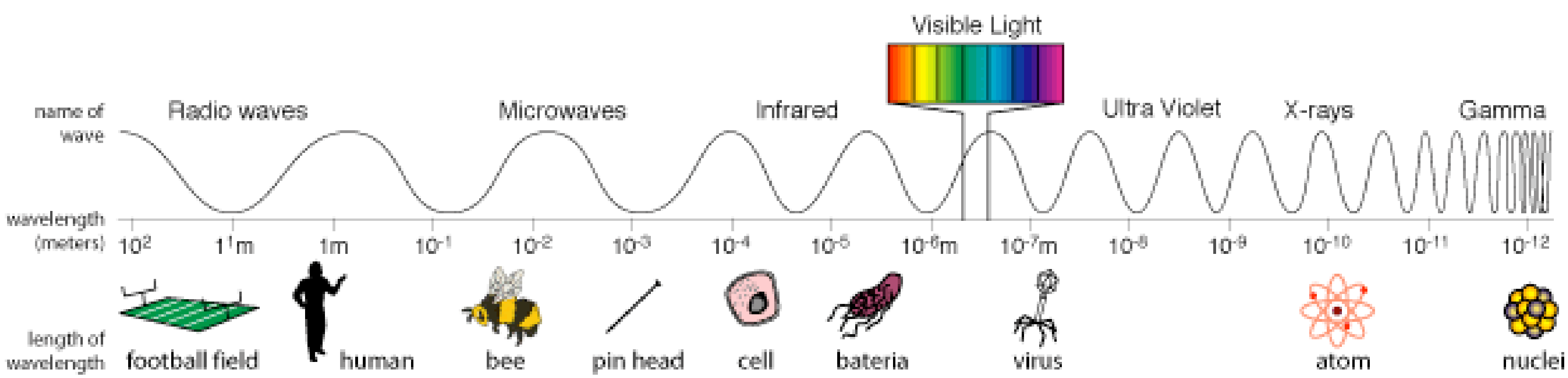


The discharges in the low pressure gas filled tube are the sources of the light which undergo refraction on the prism. We see the line spectrum of the gas.



Electromagnetic Radiation Spectrum





In the news: January 20, 2016: Infer what we cannot see. . .

EVIDENCE FOR A DISTANT GIANT PLANET IN THE SOLAR SYSTEM

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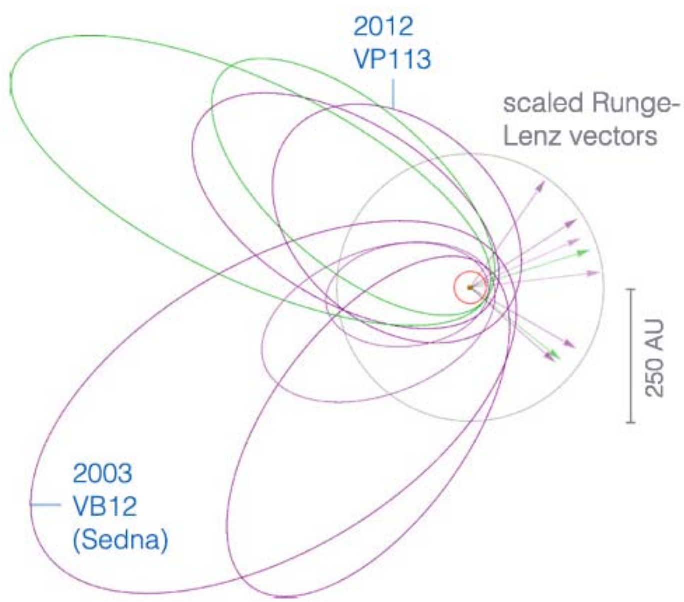
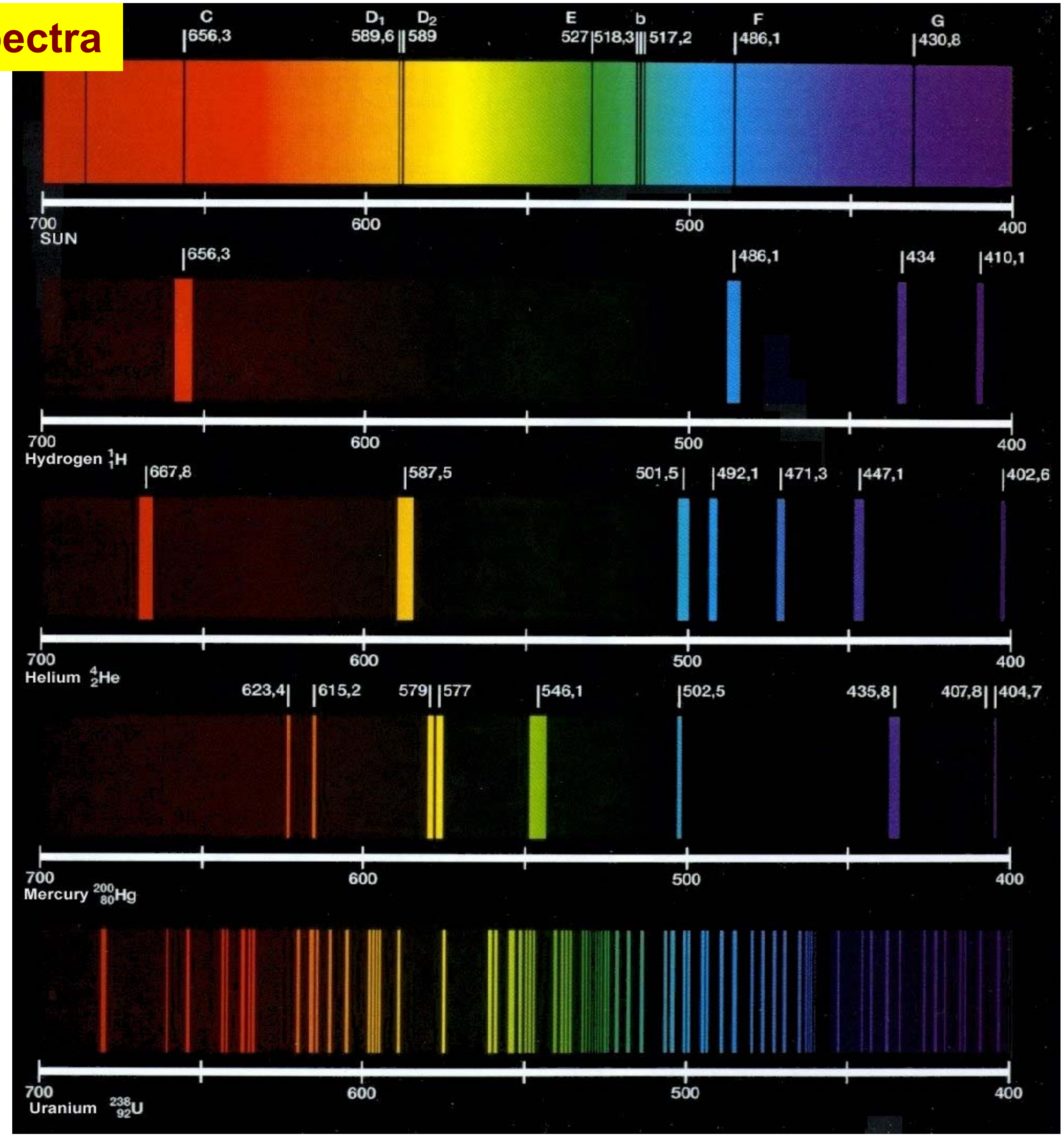
Received 2015 November 13; accepted 2016 January 10; published 2016 January 20

BATYGIN & BROWN



Cumulatively, the presented results offer credence to the hypothesis that the observed structure of the distant Kuiper Belt can be explained by invoking perturbations from an unseen planetary mass companion to the solar system. Simultaneously, the suggestive nature of the results should be met with a healthy dose of skepticism, given the numerous assumptions made in the construction of our simple analytical model. In

Emission Spectra



Sun

Hydrogen

Helium

Mercury

Uranium

700 nm 600 nm 500 nm 400 nm

Complexity increases With size of Element

What do these lines mean?????

A Bit of History

TABLE 2.1 Discoveries in Atomic Structure

1896	A. H. Becquerel	Discovered radioactivity of uranium
1897	J. J. Thomson	Showed that electrons have a negative charge, with charge/mass $= 1.76 \times 10^{11}$ C/kg
1909	R. A. Millikan	Measured the electronic charge as 1.60×10^{-19} C; therefore, mass of electron $= 9.11 \times 10^{-31}$ kg
1911	E. Rutherford	Established the nuclear model of the atom: a very small, heavy nucleus surrounded by mostly empty space
1913	H. G. J. Moseley	Determined nuclear charges by X-ray emission, establishing atomic numbers as more fundamental than atomic masses

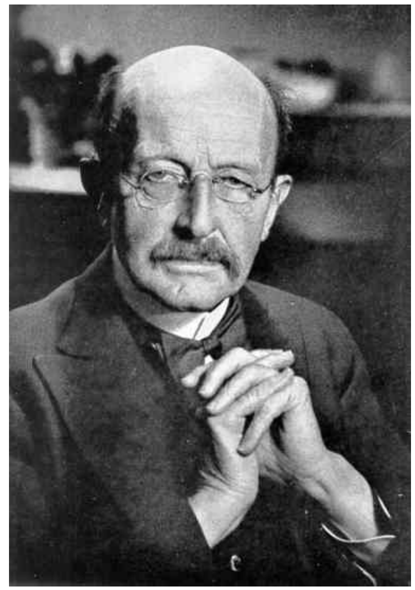
$$^{A}_{Z}E$$

Z = No. protons in nucleus, Atomic number
A = Mass number; no. of protons + neutrons in nucleus

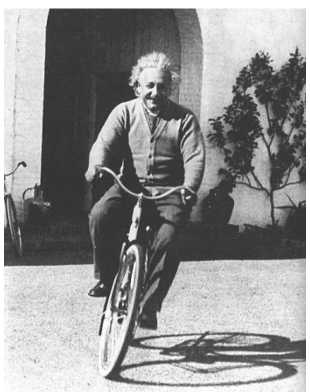
Marie Curie—1867-1934

So how to connect the physical properties of elements to the Periodic Table? Physicists! The current model of the atom belongs to Physicists!


DeBroglie


Planck


Schrodinger


Einstein


Heisenberg


Bohr

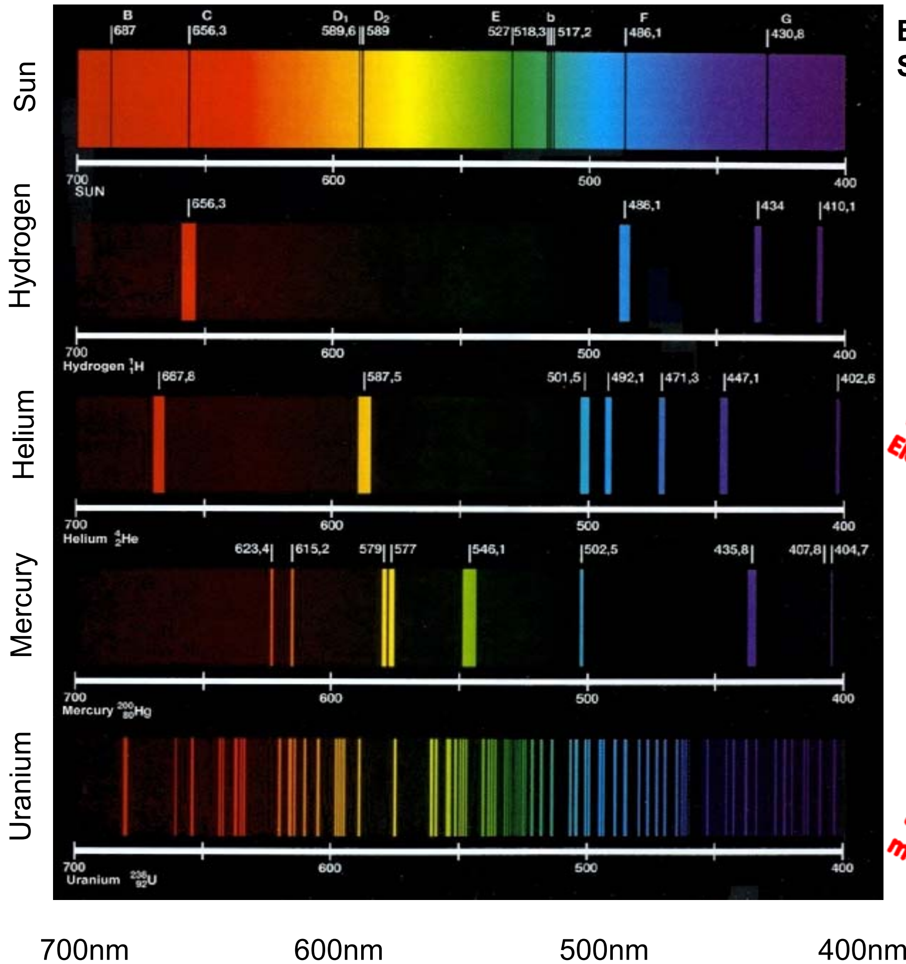
Pauli

Niels Bohr and wife Margrethe around 1930

Taken from John L. Heilbron's "History: The Path to the quantum Atom", Nature 498, 27-30, (06 June 2013)

Taken from John L. Heilbron's "History: The Path to the quantum Atom", Nature 498, 27-30, (06 June 2013)

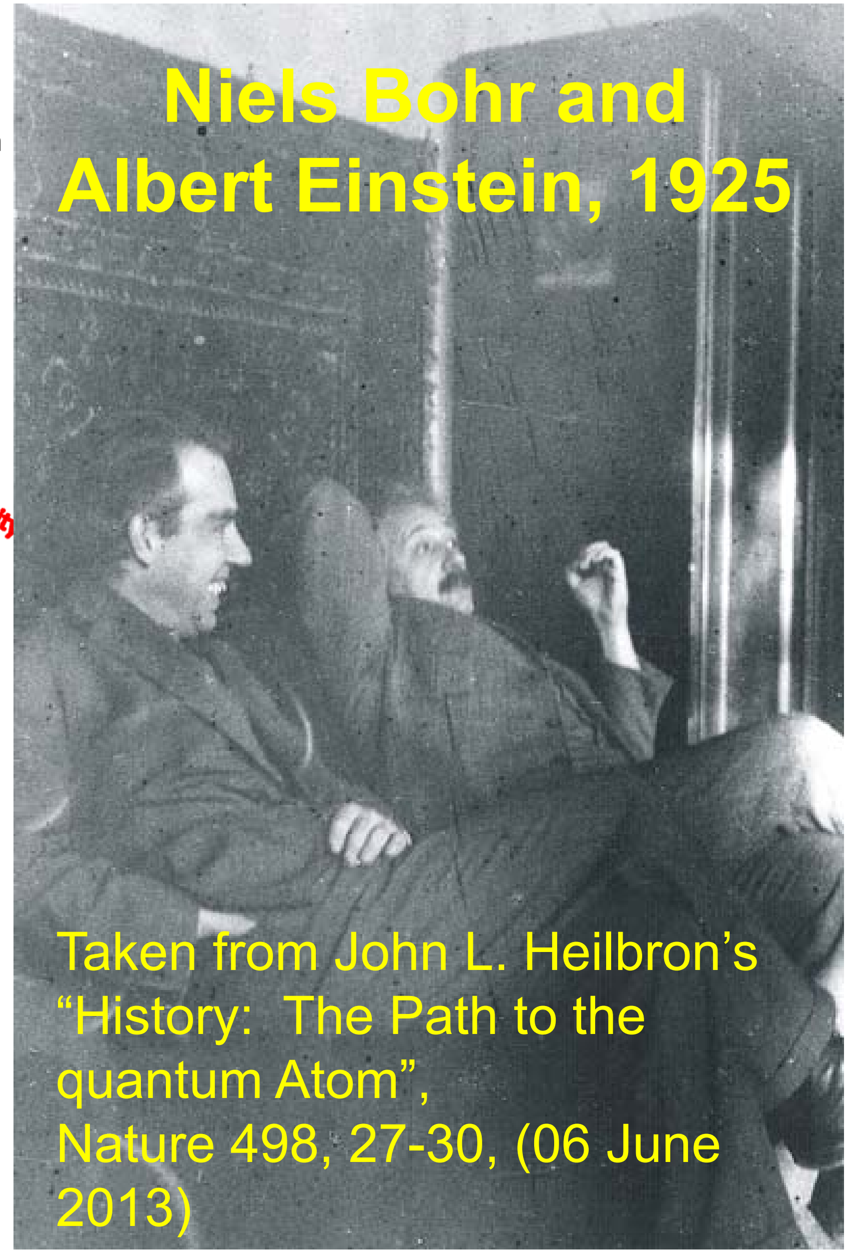
To develop his model, Bohr followed an analogy to the radiation theory of Max Planck (right). ". . . Bohr had developed a doctrine of multiple partial truths, each of which contained some bit of reality, and all of which together might exhaust it. "There exist so many different truths I can almost call it my religion that I think that everything that is of value is true."



Emission Spectra

Complexity increases With size of Element

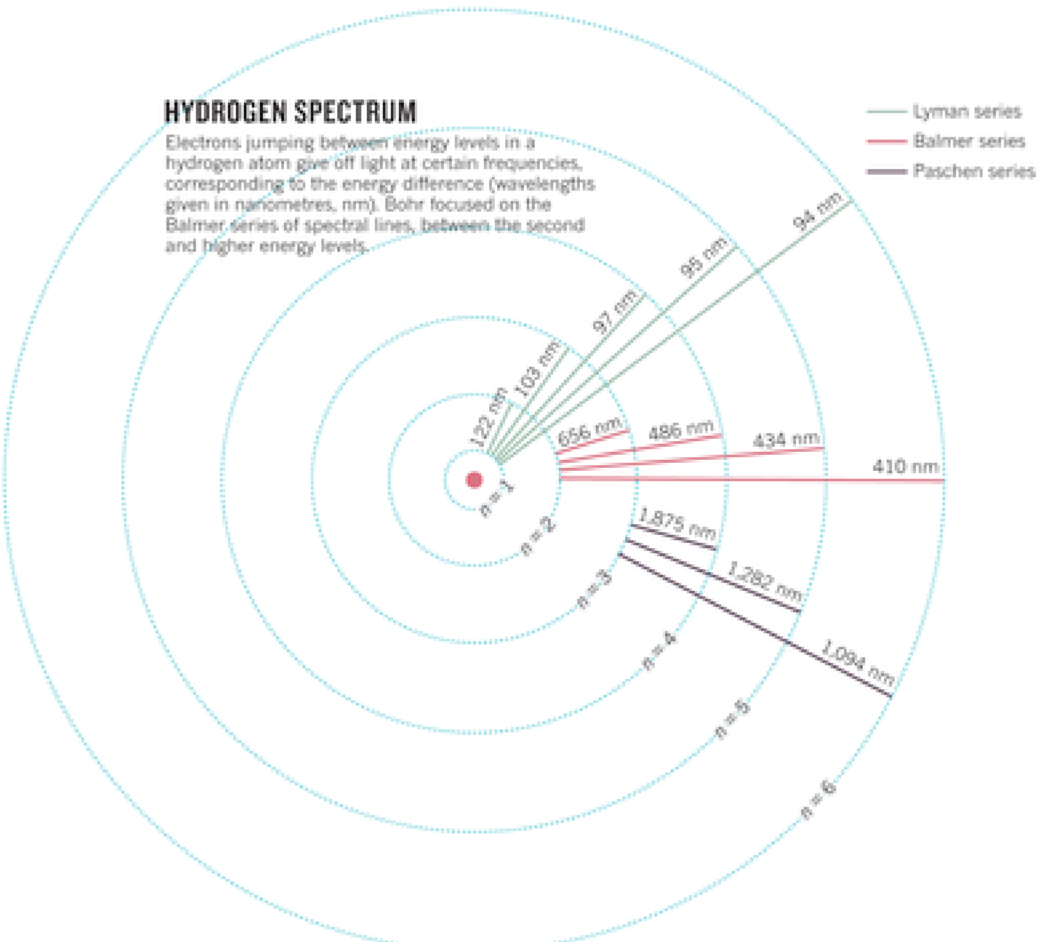
What do these lines mean????



Niels Bohr and Albert Einstein, 1925

Taken from John L. Heilbron's "History: The Path to the quantum Atom", Nature 498, 27-30, (06 June 2013)

The Bohr Atom: electrons in concentric rings



The Balmer formula expresses the frequencies of some lines in the spectrum of hydrogen in simple algebra:

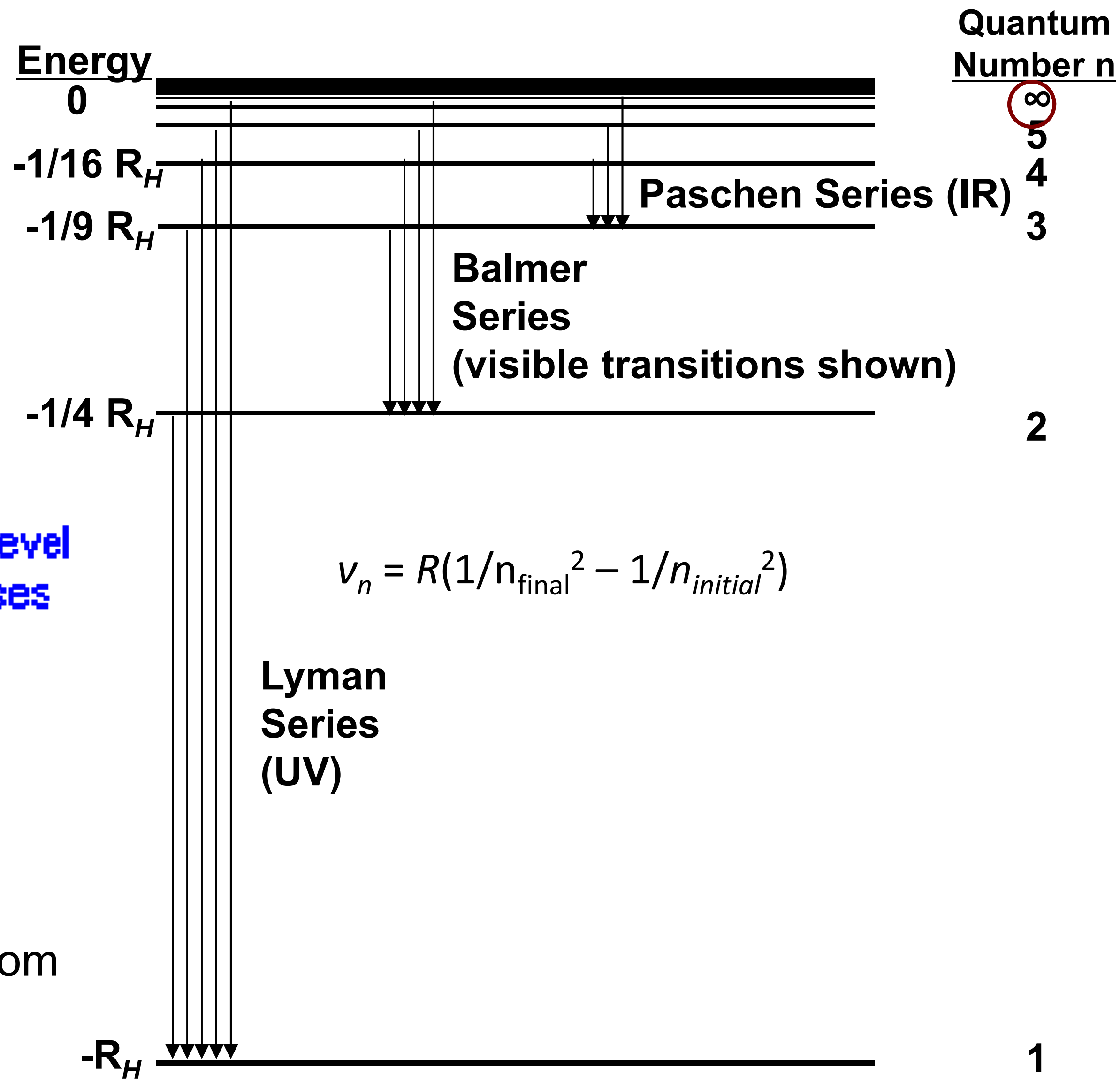
$$v_n = R(1/2^2 - 1/n^2)$$

where v_n is the *n*th Balmer line and *R* is the universal Rydberg constant for frequency, named in honour of the Swedish spectroscopist Johannes Rydberg, who generalized Balmer's formula to apply to elements beyond hydrogen.

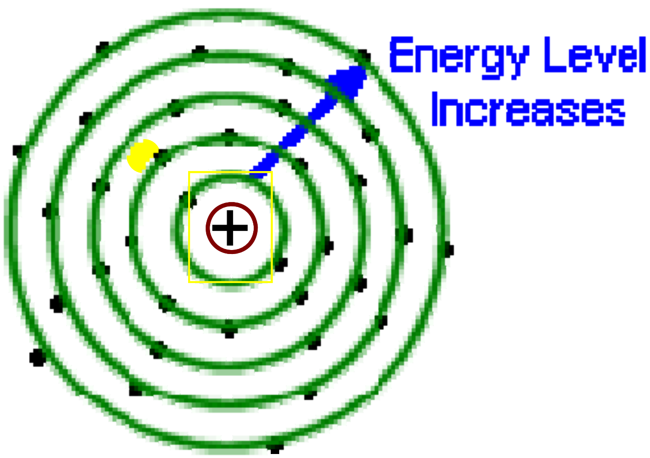
Taken from John L. Heilbron's "History: The Path to the quantum Atom",
Nature 498, 27-30, (06 June 2013)

Each level can accommodate
$2\ n^2$ electron:
Periodic Table Rows

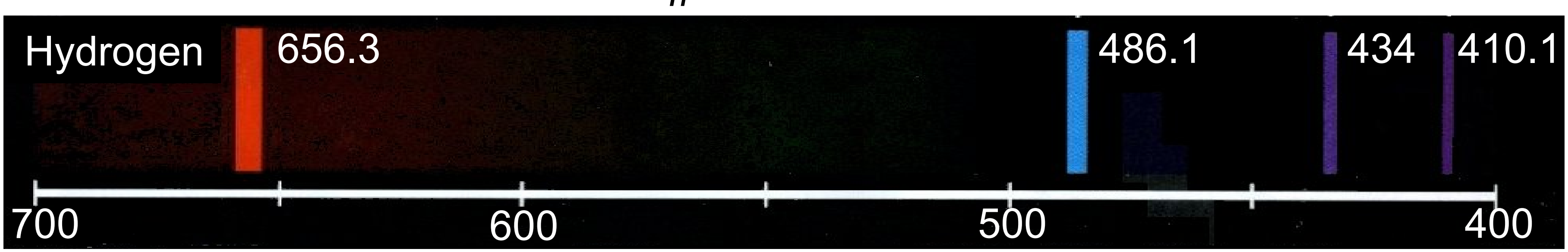
The Hydrogen Atom Spectrum and Energy Levels

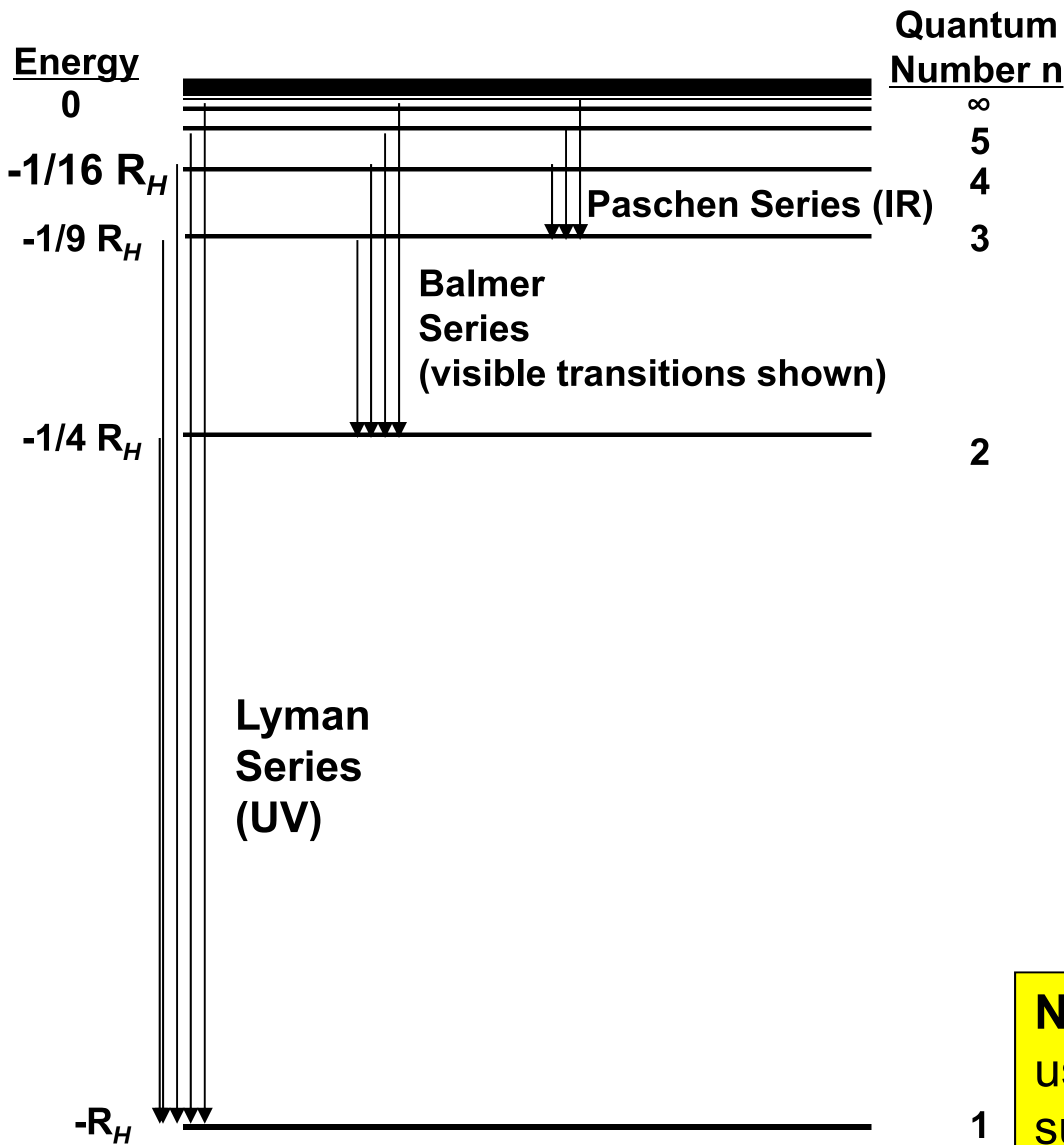


$$\nu_n = R(1/n_{final}^2 - 1/n_{initial}^2)$$



Niels Bohr's view of the atom





For Hydrogen:

$$E = \frac{-R_H}{n^2}$$

Rydberg constant for hydrogen, R_H

$$R_H = \frac{m_e e^4}{8\,\varepsilon_o^2 h^2} = 2.179 \times 10^{-18} J$$

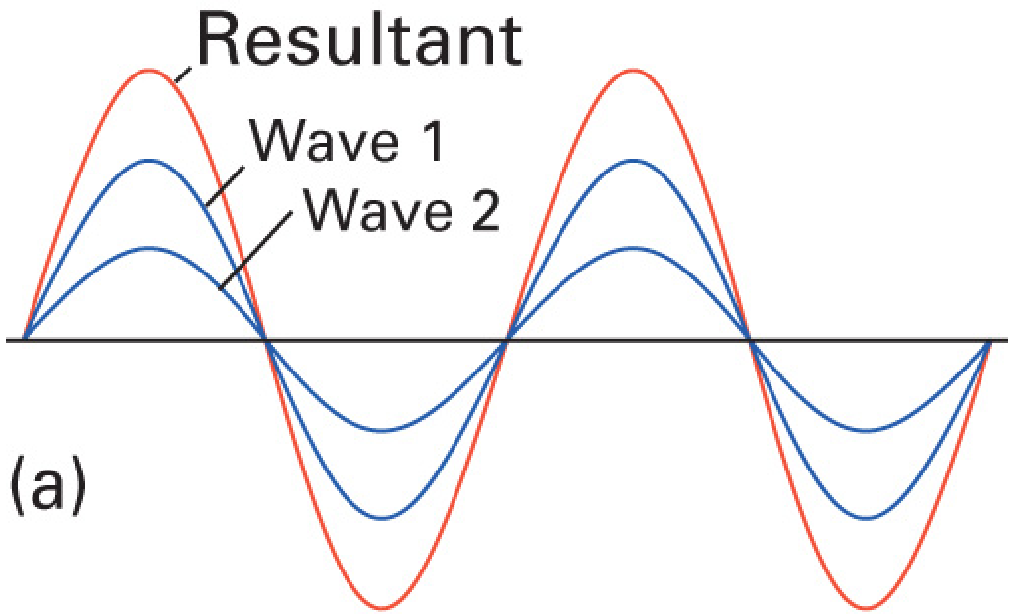
$$= 13.6\ eV$$

General equation for Rydberg constant for any element

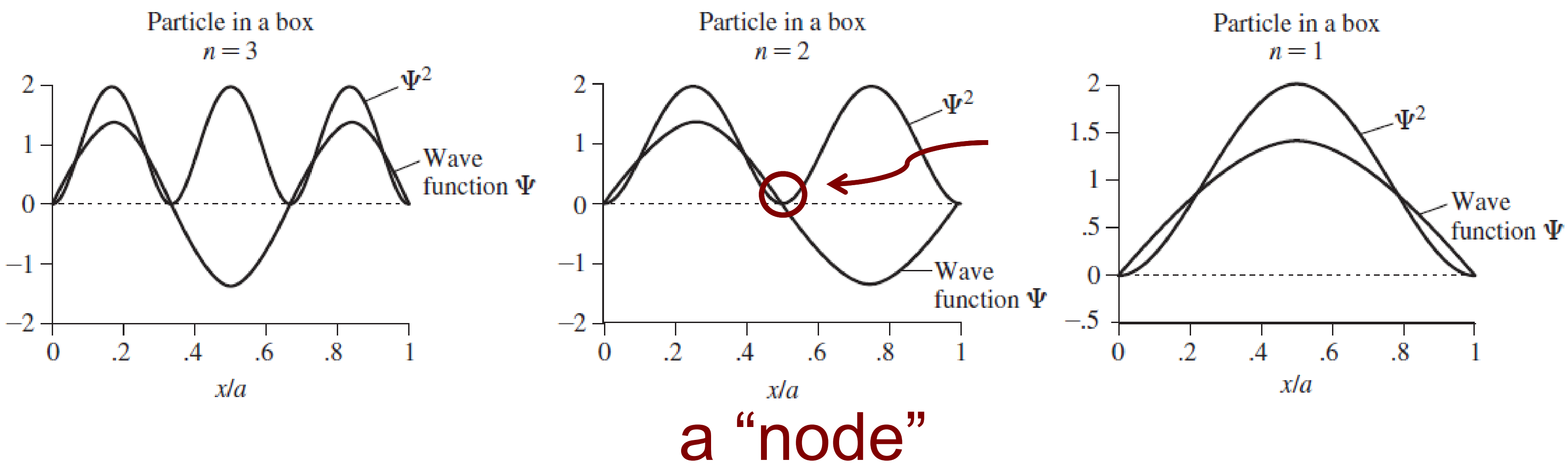
$$R = \frac{-\mu Z^2 e^4}{8\,\varepsilon_o^2 h^2}$$

Note: The predicted emission spectra using the Rydberg constant was only successful for simple elements such as H and failed for heavier atoms due to the limitations of the Bohr view of the atom. ***This led to the foundations of quantum mechanics***.

Properties of waves: Addition for reinforcement or cancellation



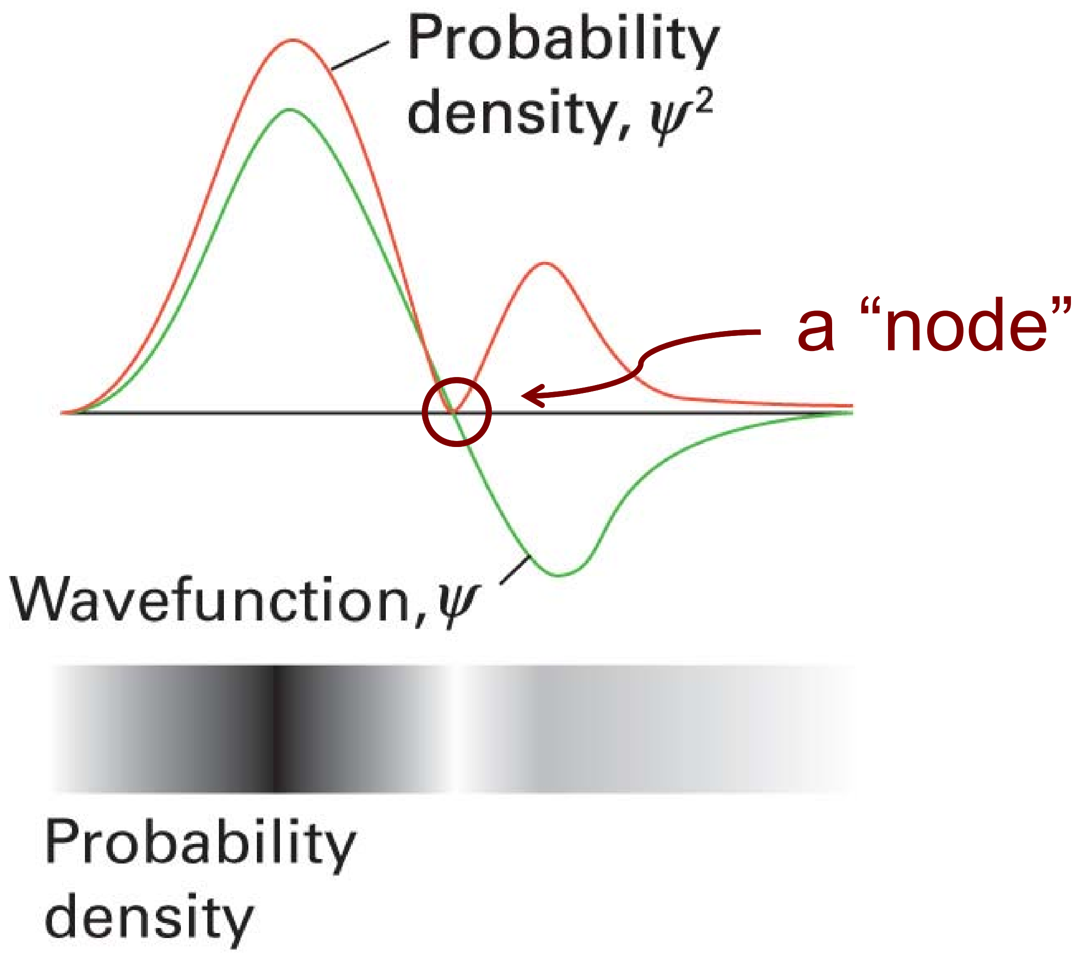
Properties of waves: Squared = amplitude
Boundaries => Restrictions on values



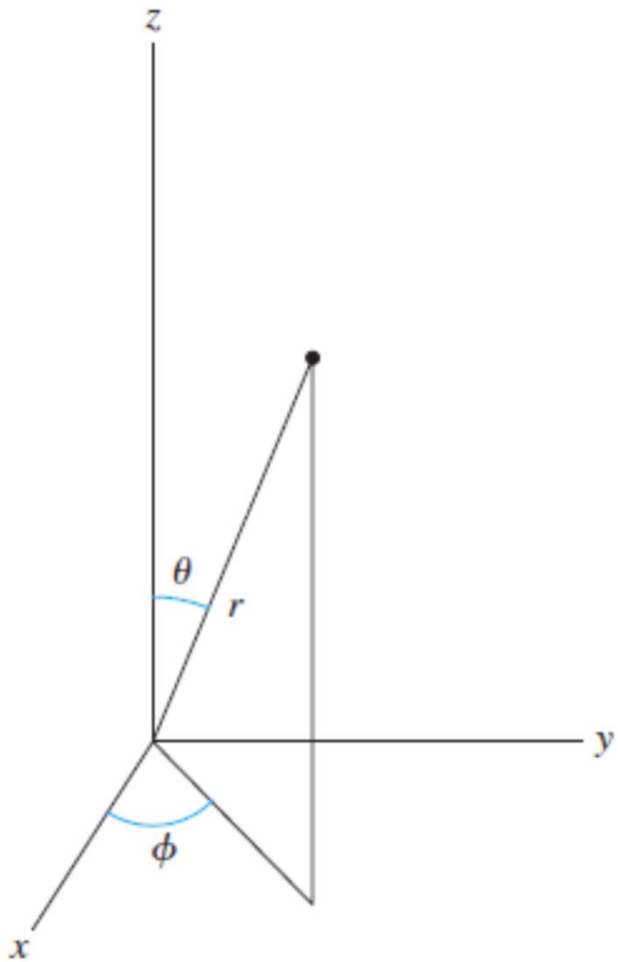
W. H. FREEMAN

Time-independent Schrödinger equation
(general—one dimension)

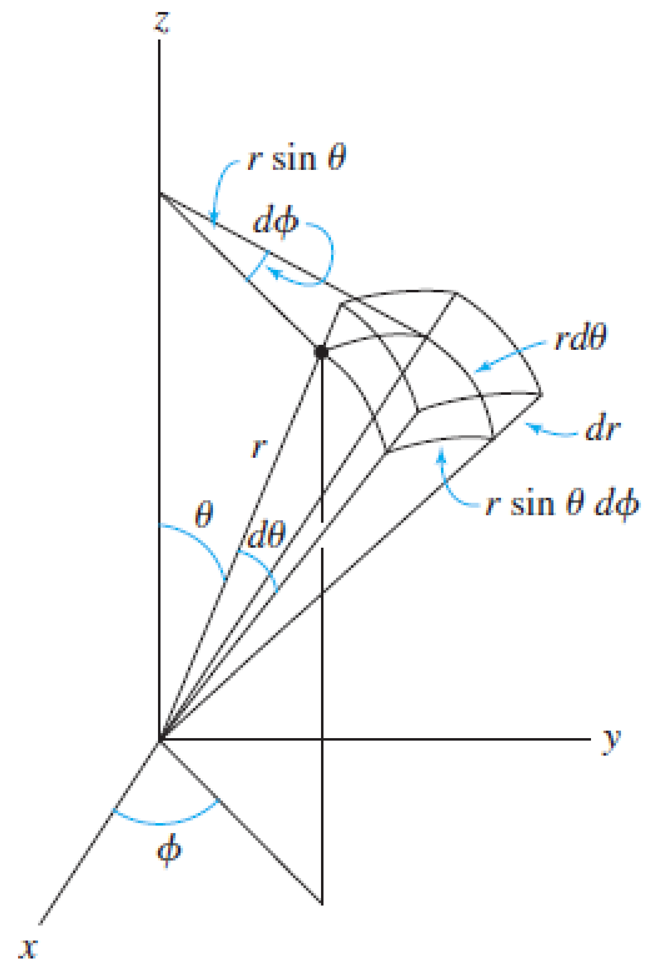
E ψ = H ψ



Need for Spherical Coordinates and Volume Elements



Spherical coordinates



Volume element

Need both radial and angular functions

1.4

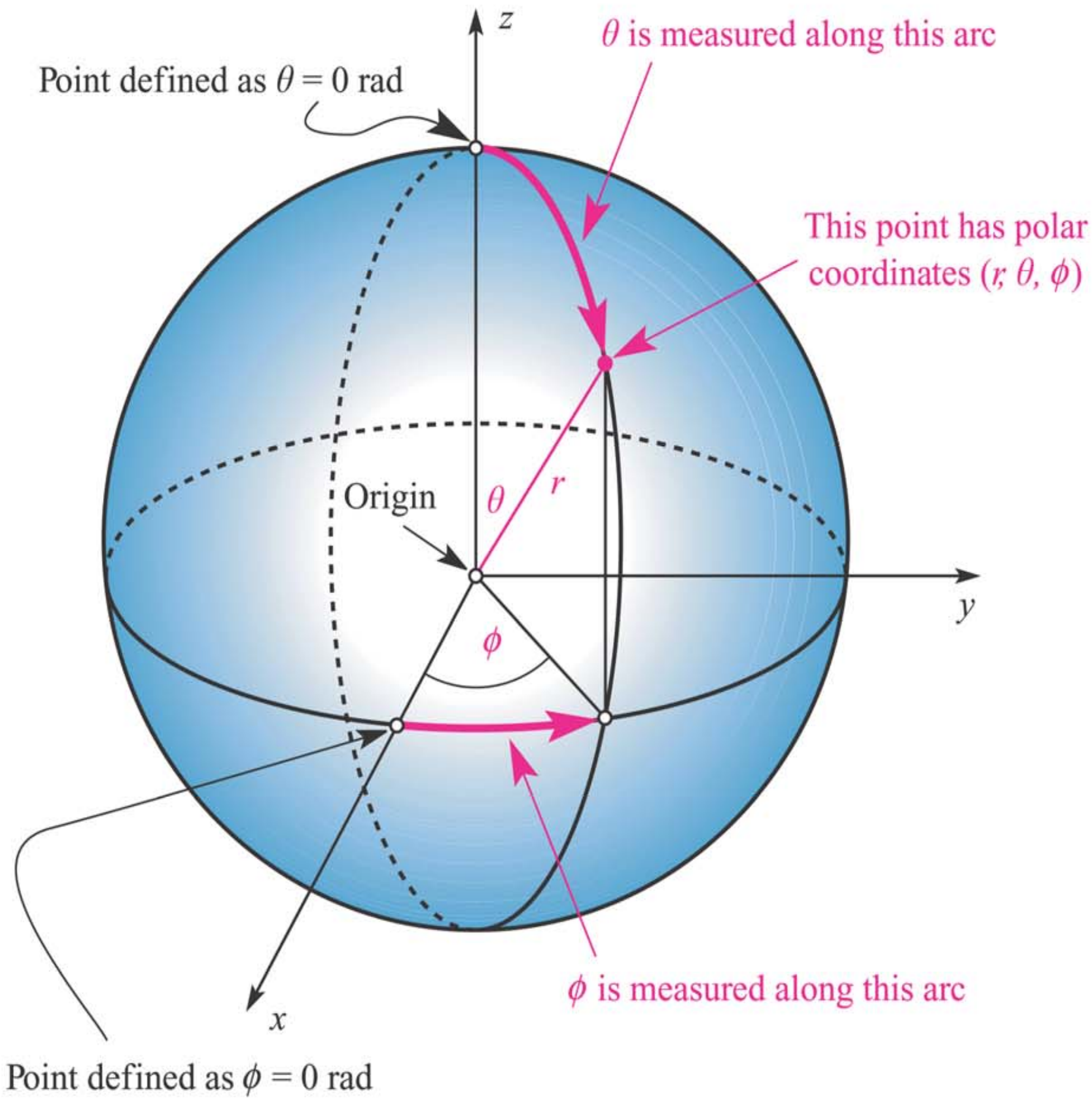


Fig. 1.4 Definition of the polar coordinates (r, θ, ϕ) for a point shown here in pink; r is the radial coordinate and θ and ϕ are angular coordinates. θ and ϕ are measured in radians (rad). Cartesian axes (x, y and z) are also shown.

1.18

Summarizing: Solutions Required Quantum Numbers

Quantum Numbers

Atomic orbital	n	l	m_l	Radial part of the wavefunction, $R(r)^{\dagger}$	Angular part of wavefunction, $A(\theta, \phi)$
$1s$	1	0	0	$2e^{-r}$	$\frac{1}{2\sqrt{\pi}}$
$2s$	2	0	0	$\frac{1}{2\sqrt{2}}(2-r)\,e^{-r/2}$	$\frac{1}{2\sqrt{\pi}}$
$2p_x$	2	1	+1	$\frac{1}{2\sqrt{6}}r\,e^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\cos\phi)}{2\sqrt{\pi}}$
$2p_z$	2	1	0	$\frac{1}{2\sqrt{6}}r\,e^{-r/2}$	$\frac{\sqrt{3}(\cos\theta)}{2\sqrt{\pi}}$
$2p_y$	2	1	−1	$\frac{1}{2\sqrt{6}}r\,e^{-r/2}$	$\frac{\sqrt{3}(\sin\theta\sin\phi)}{2\sqrt{\pi}}$

† For the $1s$ atomic orbital, the formula for $R(r)$ is actually $2(\frac{Z}{a_0})^{\frac{3}{2}}\,e^{-Zr/a_0}$ but for the hydrogen atom, $Z = 1$ and $a_0 = 1$ atomic unit. Other functions are similarly simplified.

Table 1.2 Solutions of the Schrödinger equation for the hydrogen atom which define the $1s$, $2s$ and $2p$ atomic orbitals. For these forms of the solutions, the distance r from the nucleus is measured in atomic units.

Lecture 3 362 January 18, 2019

Quantum Numbers
Effective Nuclear Charge
Slater's Rules

Lecture 2 362 January 16, 2019

Paradigm Shift:
Development of Current
Atomic Theory—
Spectroscopy and Energy
Levels in Atoms

OR,
"Show me the Electrons!"