3.012 Fund of Mat Sci: Bonding – Lecture 7

ALPHABET SOUP

Photograph of a bowl of alphabet soup removed for copyright reasons.

Homework for Wed Oct 5

- Study: 21.5, 21.6
- Read: 17.2 (Stern-Gerlach)
- Non-graded PS3 will be posted today

Last time:

1. Hamiltonian in a spherical potential:

CENTRAL

$$\hat{H} = -\frac{\hbar^2}{2m_e}\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d}{dr}\right) + \frac{L^2}{2m_e r^2} + V(r)$$

2. $\hat{H}$, $\hat{L}^2$, and $\hat{L}_z$ all commute with each other
3. We can find common eigenfunctions

$$\psi_{nlm}(\vec{r}) = R_{nl}(r) Y_{lm}(\vartheta, \varphi)$$

labeled with the 3 quantum numbers ***n, l, m***

Three Quantum Numbers

- $\hat{H} \leftrightarrow$ Principal quantum number **n** (energy, accidental degeneracy)

$$E_n = -\frac{e^2}{8\pi\varepsilon_0}\frac{Z^2}{a_0 n^2} = -\left(13.6058 \text{ eV}\right)\frac{Z^2}{n^2} = -\left(1 \text{ Ry}\right)\frac{Z^2}{n^2}$$

BOHR RADIUS = 0.527 Å = 0.527 10^{-10} m

- $\hat{L}^2 \leftrightarrow$ Angular momentum quantum number ***l***

l = 0,1,…,n-1   (a.k.a. s, p, d… orbitals) $\hbar^2 l(l+1)$

- $\hat{L}_z \leftrightarrow$ Magnetic quantum number ***m***

m = -l,-l+1,…,l-1,l

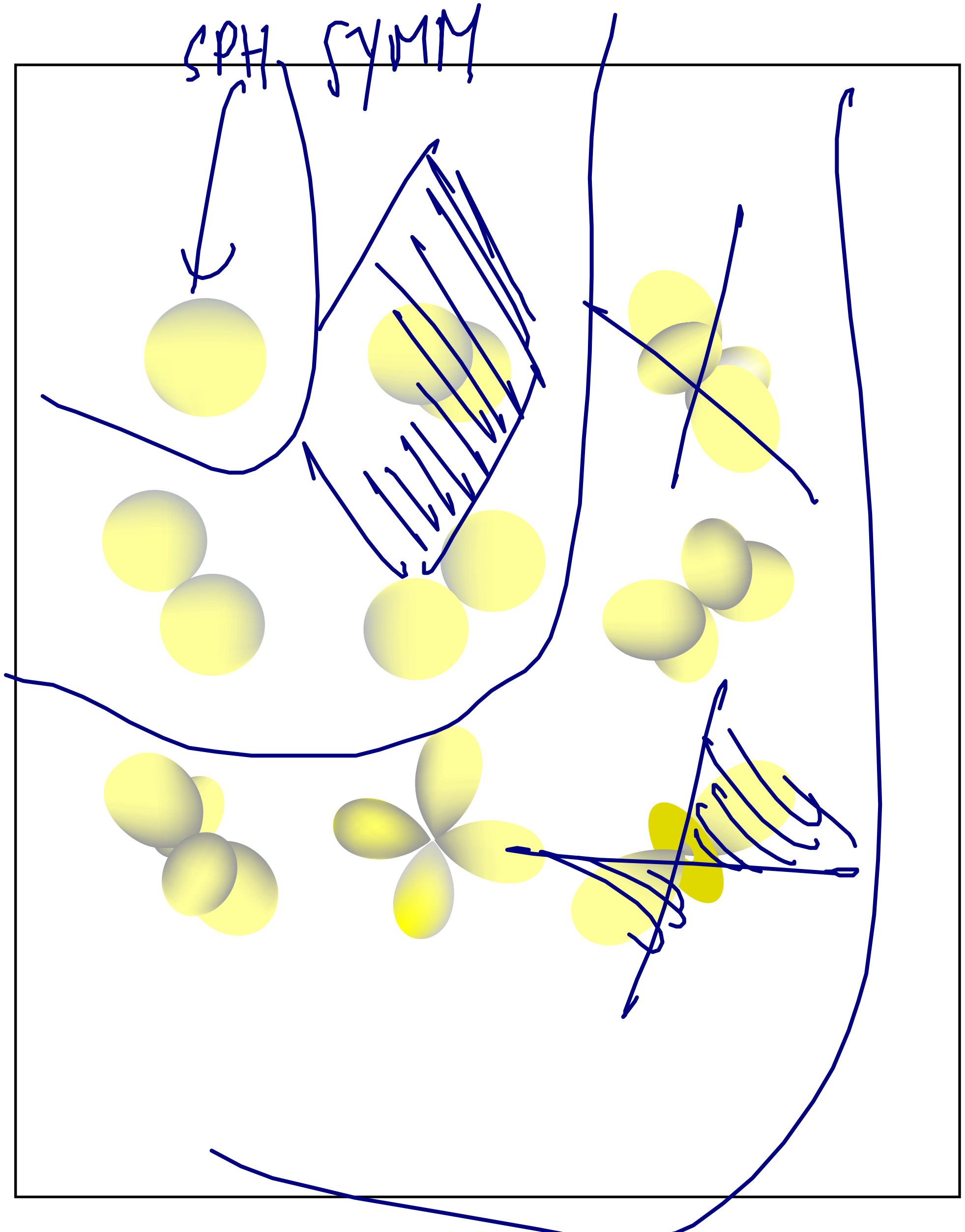
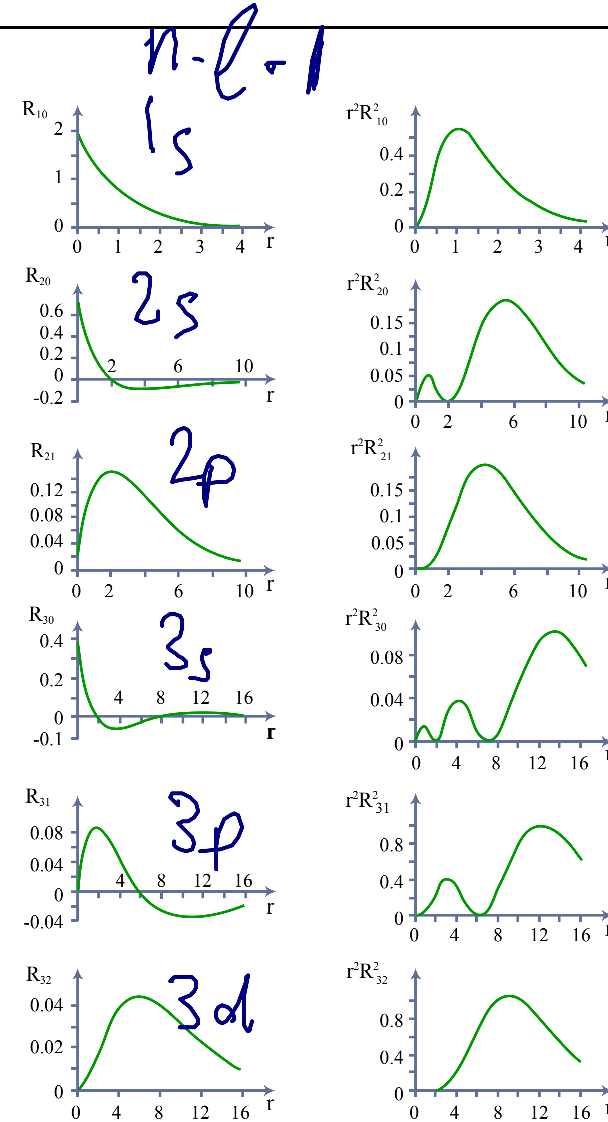


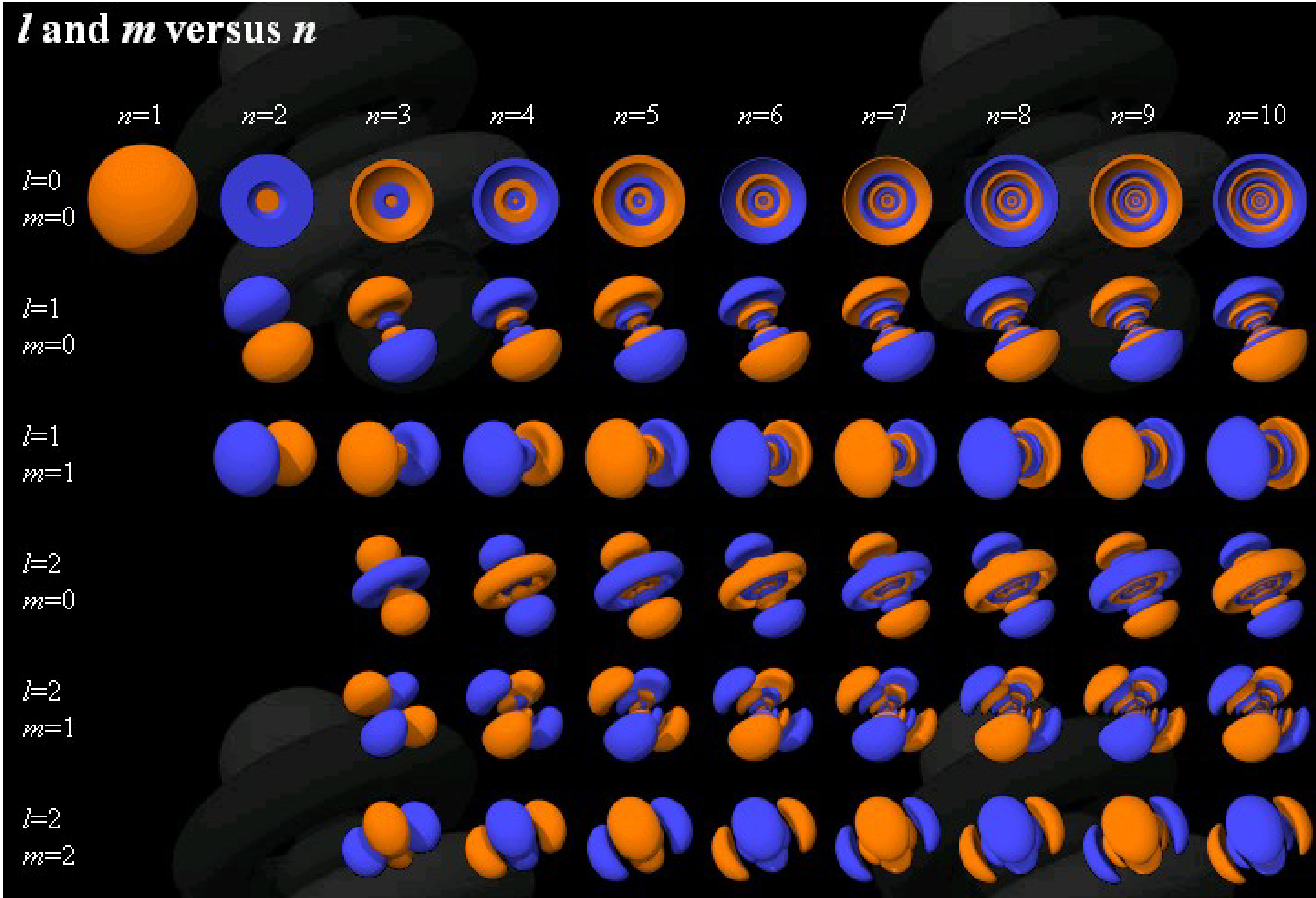
Figure by MIT OCW.



Radial functions $R_{nl}(r)$ and radial distribution functions $r^2R^2_{nl}(r)$ for atomic hydrogen. The unit of length is $a_\mu = (m/_\mu)\ a_0$, where a_0 is the first Bohr radius.

Figure by MIT OCW.

The Full Alphabet Soup $(\psi_{1s}|\psi_{2s})$



Courtesy of David Manthey. Used with permission. Source: http://www.orbitals.com/orb/orbtable.htm

Orbital levels in hydrogenoid atoms

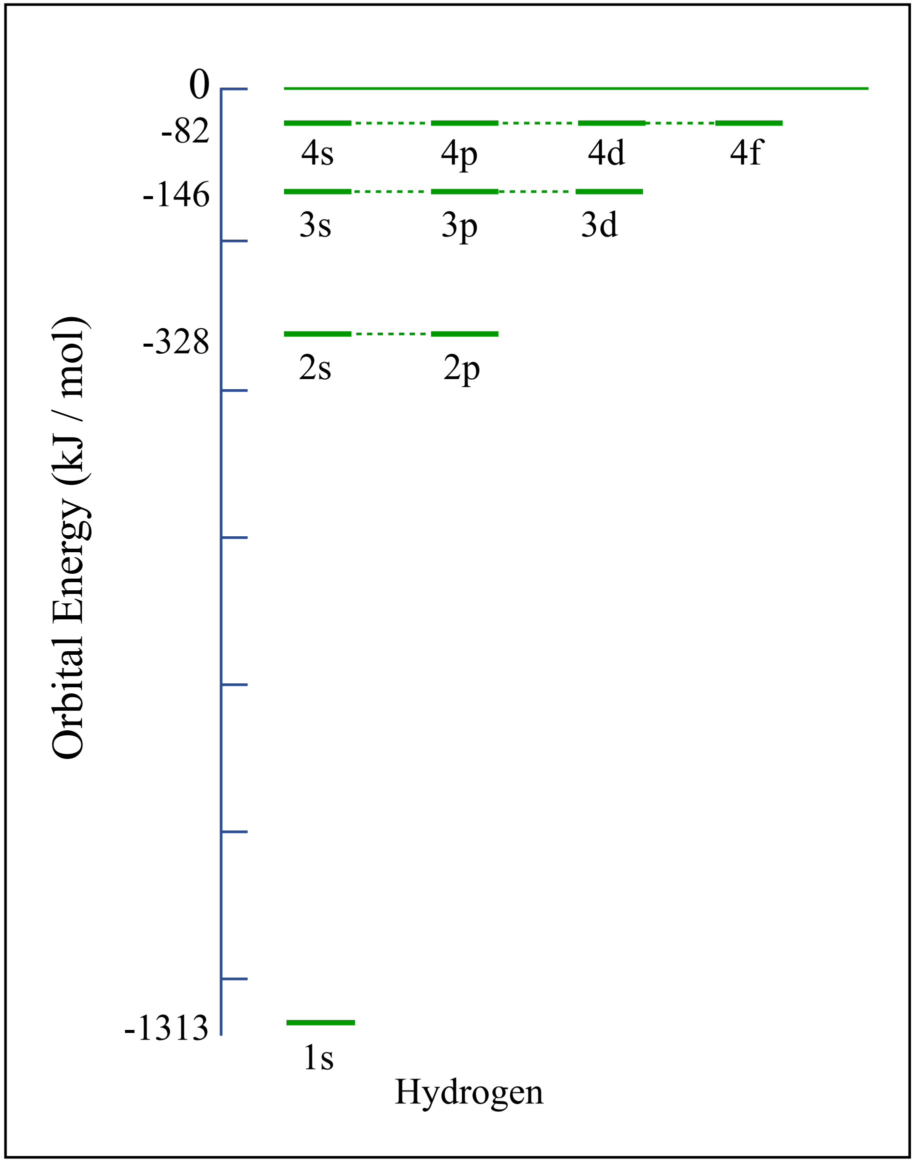


Figure by MIT OCW.

1-el atoms

H $Z=1$

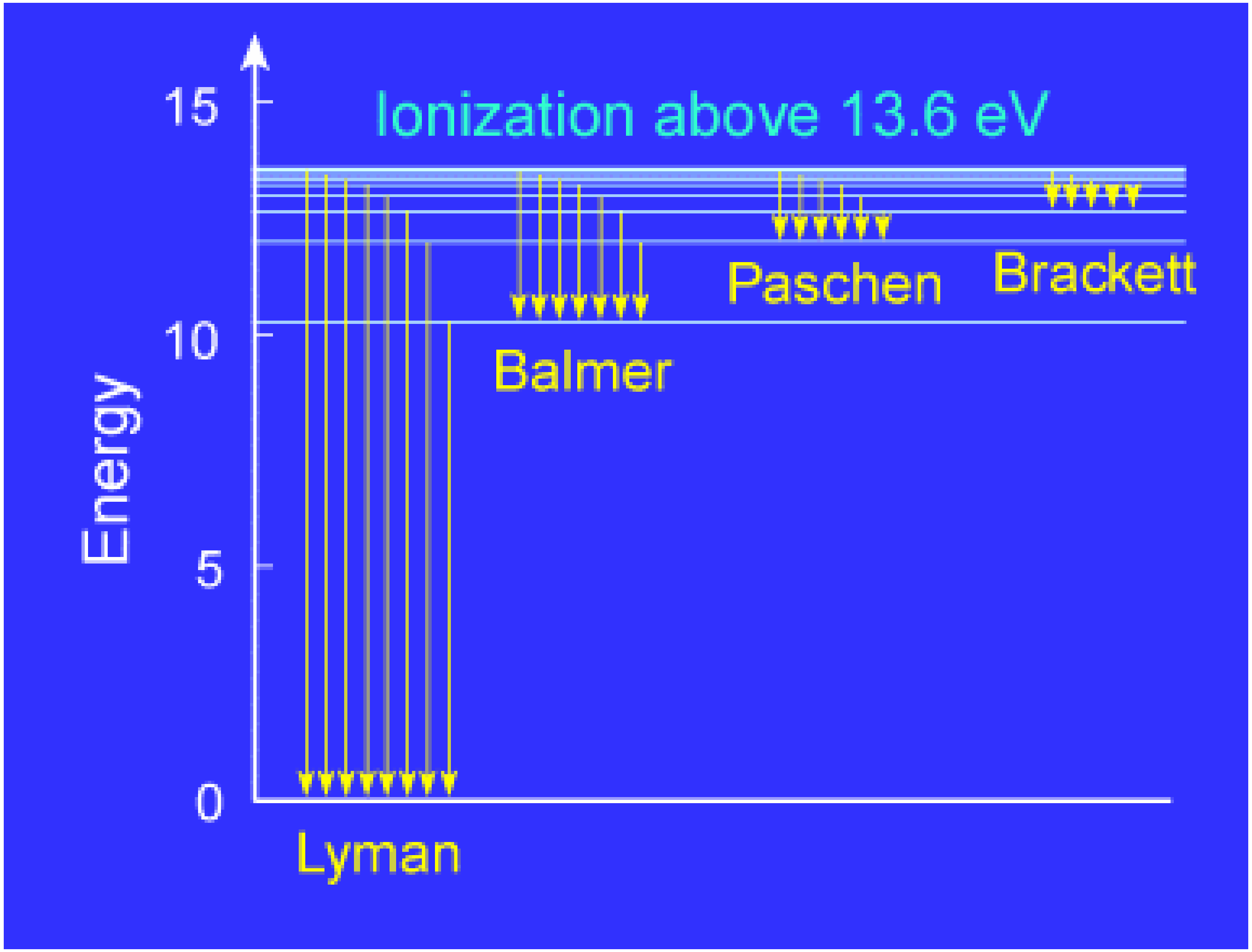
He^{+} $Z=2$

Li^{++} $Z=3$

⋮

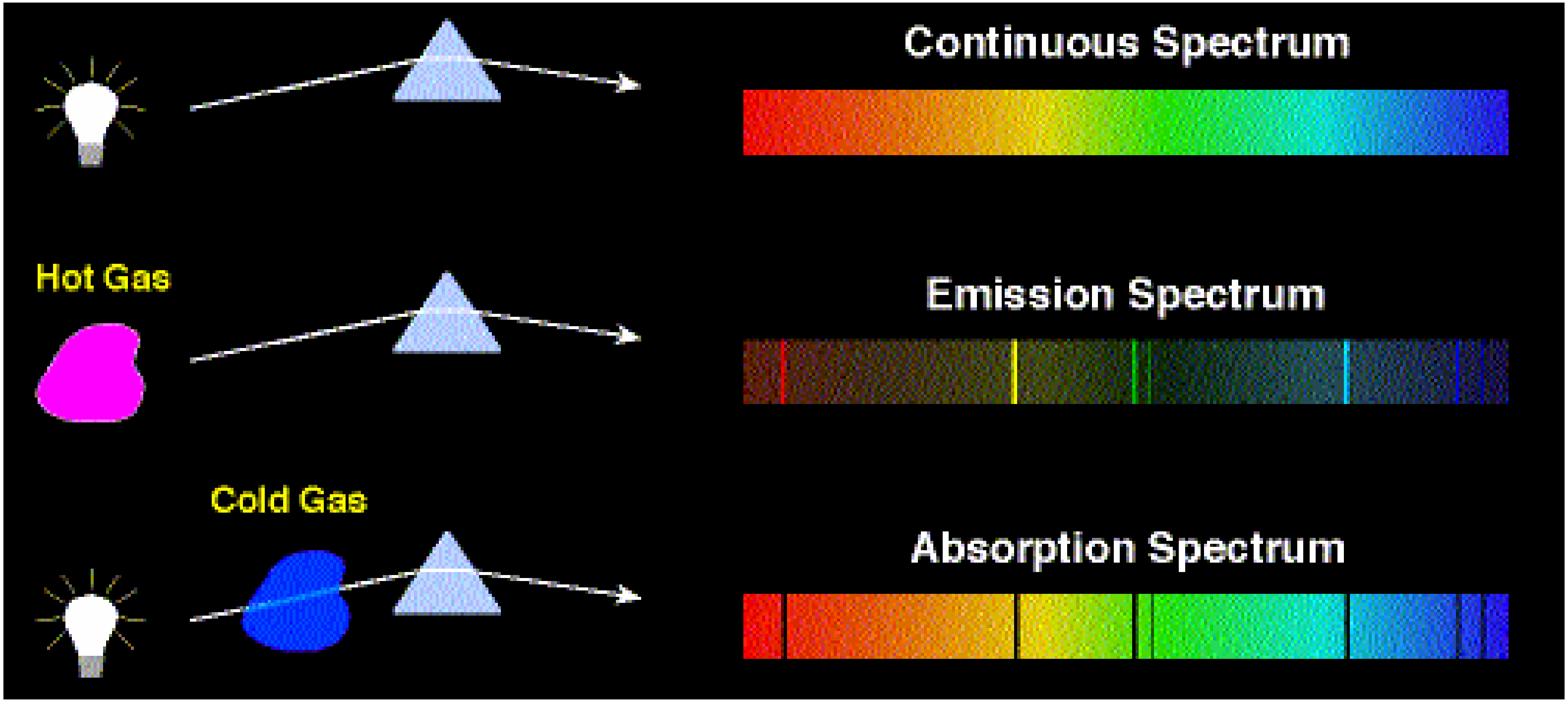
$$E_n = -\frac{Z^2}{n^2} \text{ (Ry)}$$

Balmer lines in a hot star



Courtesy of the Department of Physics and Astronomy at the University of Tennessee. Used with permission.

Emission and absorption lines



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XPS in Condensed Matter

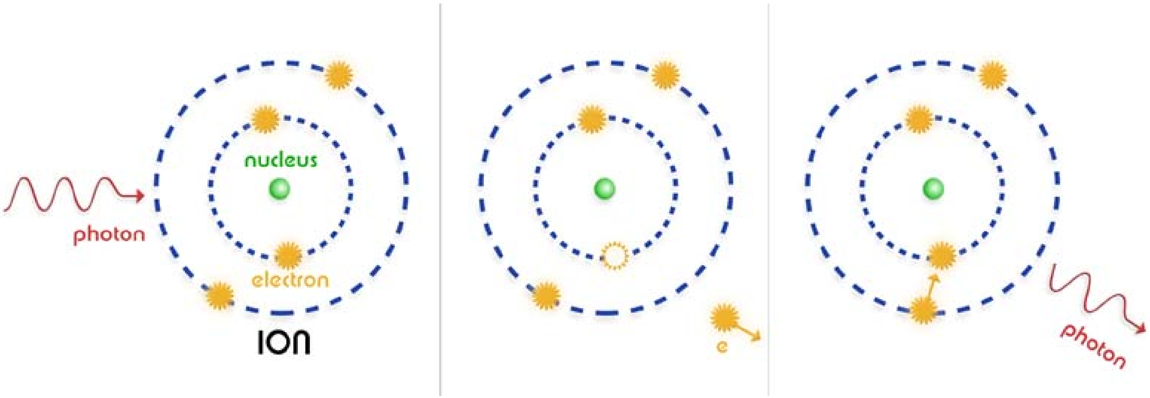


Diagram of Moon composition as seen in X-rays removed for copyright reasons.

Composition Analysis

Images of X-Ray element maps of mine waste soil particles removed for copyright reasons.

Orbital levels in multi-electron atoms

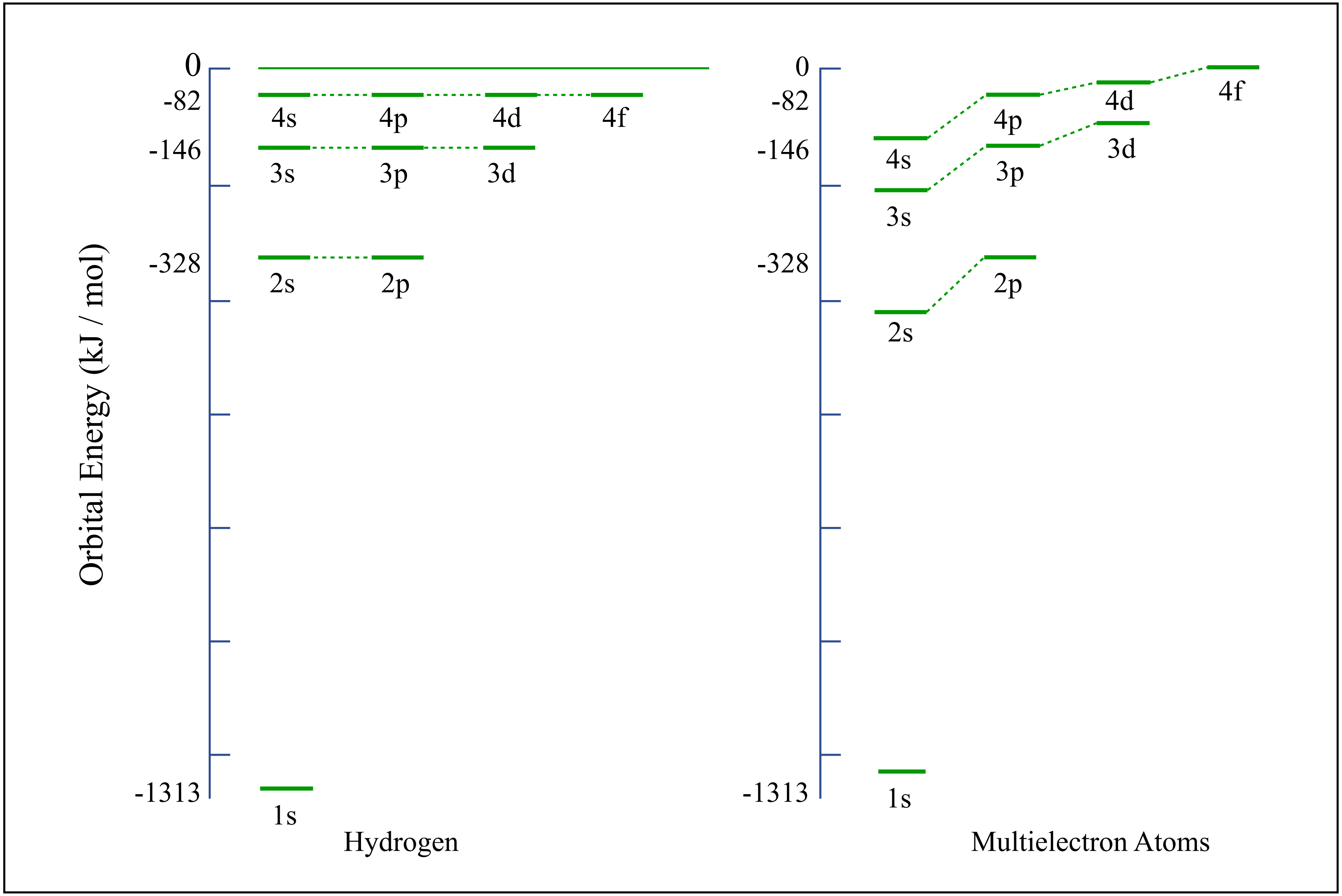


Figure by MIT OCW.

(I) "Centripetal" repulsion

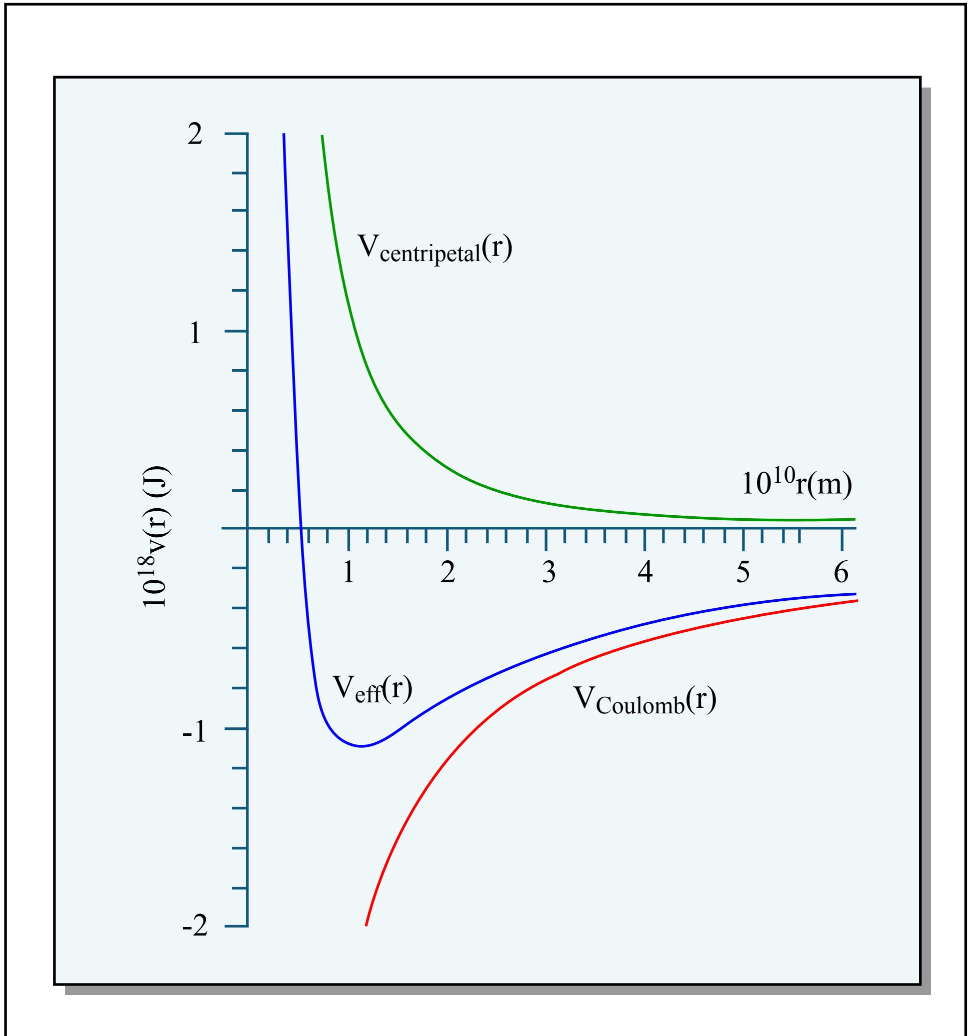


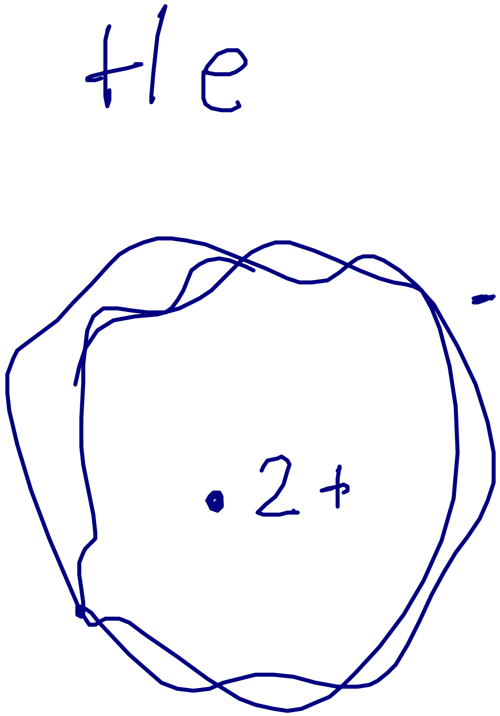
Figure by MIT OCW.

$\hbar^2 l(l+1)$

$$H = -\frac{\hbar^2}{2m}\nabla_r^2 + \frac{\hat{L}^2}{2mr^2} + V(r)$$

$$\left(\frac{1}{r^2}\nabla \frac{1}{r}\nabla\right)$$

(II) Screening



$$E^{FIRST} = -\frac{Z^2}{n^2} = -4\ Ry$$

$$E^{SECOND} = \begin{cases} \text{NON-INT} = -4\ Ry \\ \text{FAR AWAY} = -1\ Ry \end{cases}$$

$$-8\ Ry \qquad -5.804\ Ry \qquad -5\ Ry$$

ELECTRON 1

(III) Screening

$$\rho_2 = \|\psi_2\|^2$$

$$\underbrace{-\frac{\hbar^2}{2m}\nabla_r^2 + \frac{l^2}{2m_e r^2} + \left(-\frac{Z}{4\pi\varepsilon_0 r} + \int \frac{\rho_2(r')}{|r'-r|}\,dr'\right)}$$

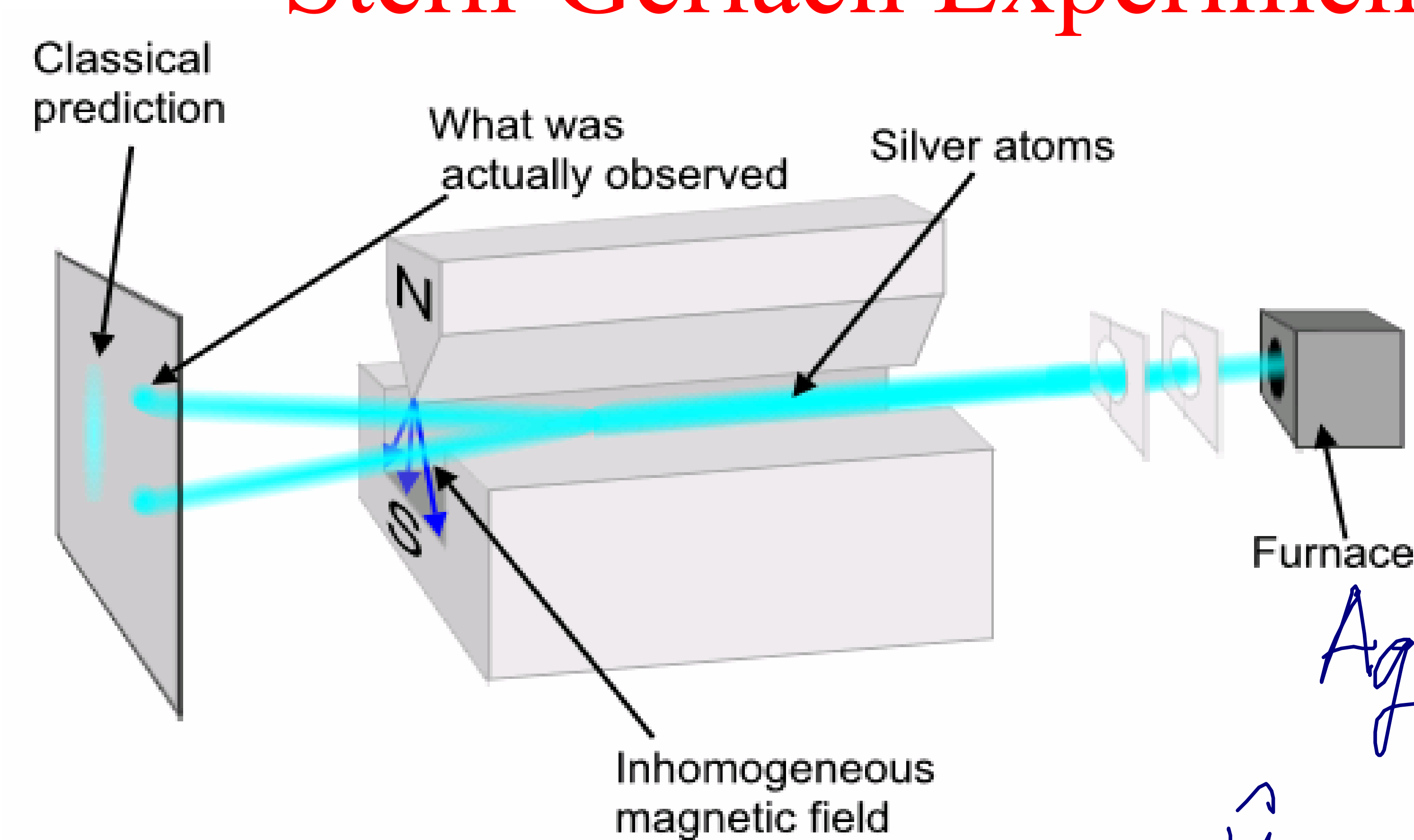
$$H\psi_1 = E_1\psi_1$$

ELECTRON 2

$$-\frac{\hbar^2}{2m}\nabla_r^2 + \frac{l^2}{2m_e r^2} + \left(-\frac{Z}{4\pi\varepsilon_0 r} + \int \frac{\rho_1(r')}{|r'-r|}\,dr'\right)$$

$$\rho_1 = \|\psi_1\|^2$$

Stern-Gerlach Experiment



Ag

$\hat{H} \mapsto \hat{H} + \hat{L} \cdot \hat{B}$

$$\hat{H} \rightarrow \hat{H} + \frac{\mu_B}{\hbar}(\hat{L} + 2\hat{S}) \cdot \vec{B} = \hat{H} + \frac{\mu_B}{\hbar}(\hat{L}_z + 2\hat{S}_z)B_z$$

Image courtesy of Theresa Knott.

Goudsmit and Uhlenbeck

Spin

- Dirac derived the relativistic extension of Schrödinger's equation; for a free particle he found two independent solutions for a given energy
- There is an operator (spin S) that commutes with the Hamiltonian and that can only have two eigenvalues
- In a magnetic field, the spin combines with the angular momentum, and they couple via

$$\hat{H} \rightarrow \hat{H} + \frac{\mu_B}{\hbar}(\hat{L} + 2\hat{S}) \cdot \vec{B}$$

Spin Eigenvalues/Eigenfunctions

- Norm (s integer → bosons, half-integer → fermions)

$$\hat{S}^2 \Psi_{spin} = \hbar^2 s(s+1) \Psi_{spin}$$

- Z-axis projection (electron is a fermion with s=1/2)

$$\hat{S}_z \Psi_{spin} = \pm \frac{\hbar}{2} \Psi_{spin}$$

- Spin-orbital: product of the "space" wavefunction and the "spin" wavefunction