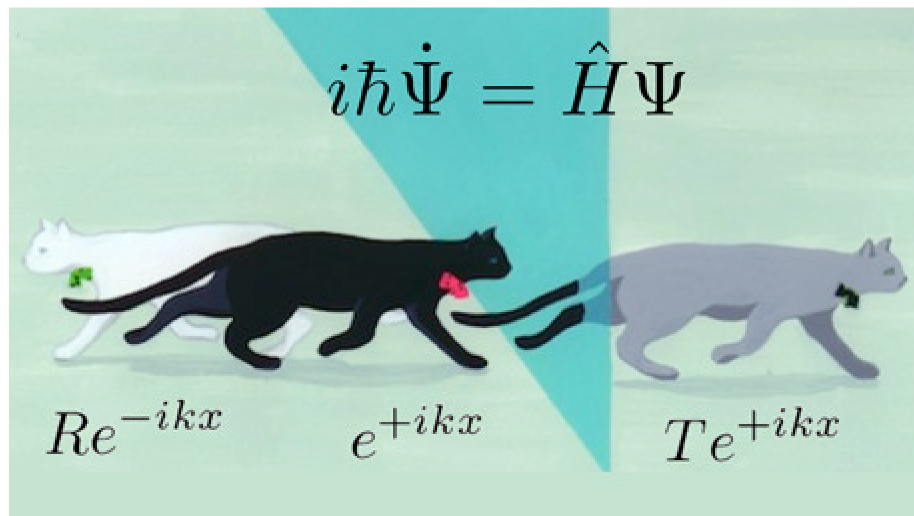
Exploring Quantum Physics

Coursera, Spring 2013 Instructors: Charles W. Clark and Victor Galitski

Guest Lecture: Electron Spin

Part I: Zeeman effect



Guest lecturer:
Prof. Ian Appelbaum, U. Maryland Physics Dept.
http://appelbaum.physics.umd.edu

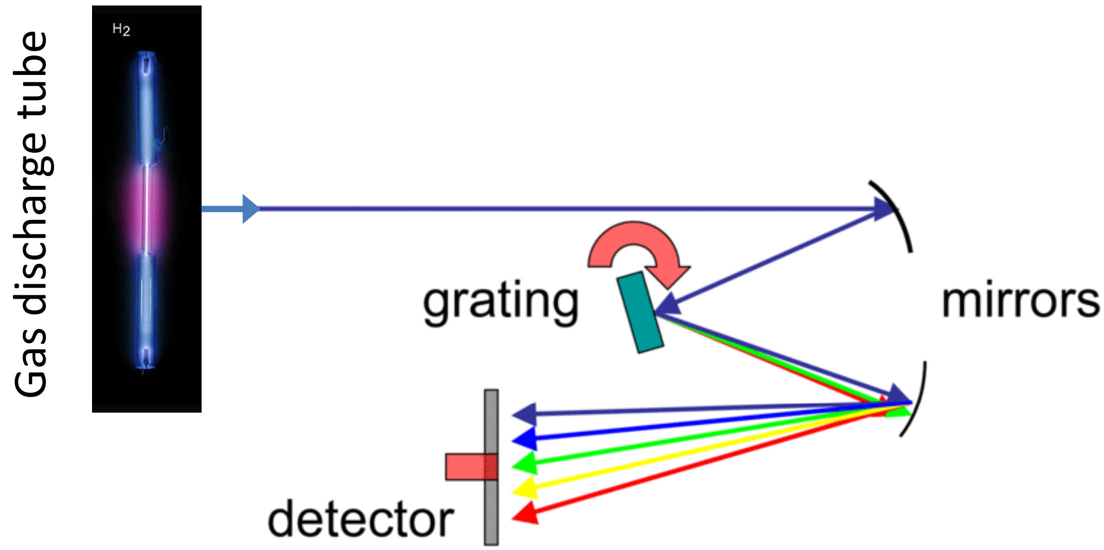
Photon emission spectrum of Hydrogen

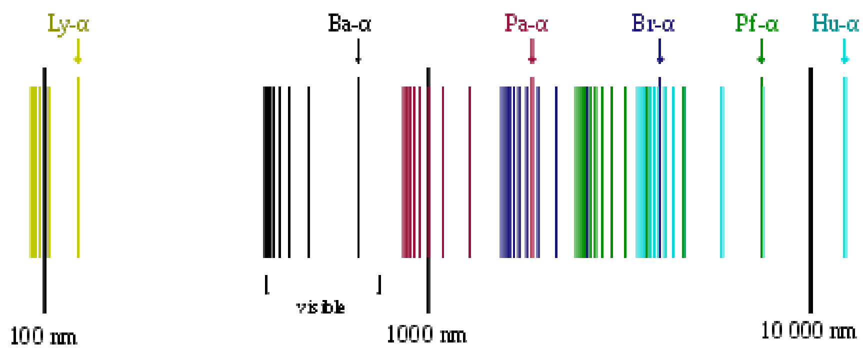
Johannes Rydberg

$$\frac{1}{\lambda} = R_\infty \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$

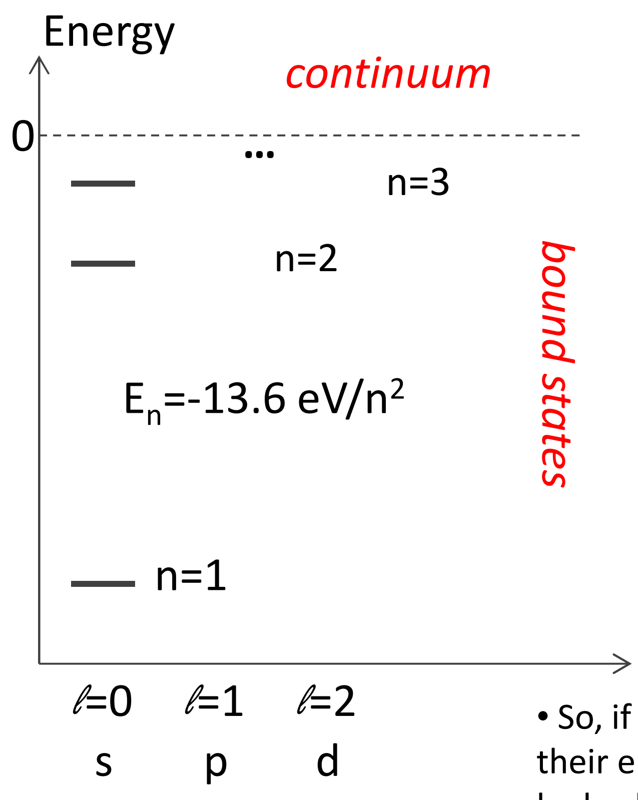
Niels Bohr

$$E_n \approx -\frac{13.6}{n^2} eV$$





Degeneracy of spherically symmetric eigenstates



•Imagine we have a *classical* electron orbit with total angular momentum

$$|\hat{L}| = \sqrt{l(l+1)}\hbar$$

•This circulating charged particle comprises a current and so the orbit has a magnetic moment

$$|\vec{\mu}| = I \cdot Area = -ef \cdot \pi r^2 = -\frac{ev}{2\pi r} \cdot \pi r^2$$

$$= -\frac{evr}{2} = -\frac{e\hbar}{2m}\frac{mvr}{\hbar} = -\mu_B \frac{|\vec{L}|}{\hbar}$$

μ_B: “Bohr magneton”

• Therefore, the electron has additional energy in magnetic field:

$$E = -\vec{\mu} \cdot \vec{B} \qquad\qquad E = -\mu_z B_z \quad (\text{for } \vec{B}=B_z\hat{z})$$

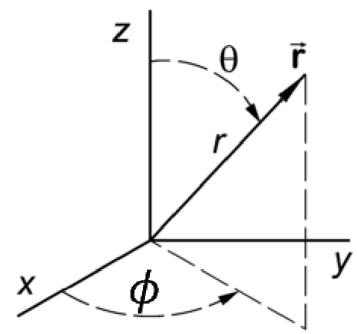
• So, if different states with the same principle quantum number n have different $\langle\mu_z\rangle$, their energy eigenvalues will shift differently in a magnetic field and the degeneracy will be broken!

Orbital angular momentum in z-direction

$$\vec{\mu} = -\mu_B \frac{\vec{L}}{\hbar} \qquad \text{So:} \quad \mu_z = -\mu_B \frac{L_z}{\hbar}$$

• What is $\langle L_Z \rangle$?

• We know: $\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$ $\quad \hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}$ $\quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z}$



• By analogy, $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi}$

$$\langle L_z \rangle = \left\langle \psi_{nlm} \middle| \frac{\hbar}{i}\frac{\partial}{\partial \phi} \middle| \psi_{nlm} \right\rangle = \frac{\hbar}{i}\left\langle e^{im\phi}\varphi(\theta, r) \middle| \frac{\partial}{\partial \phi} \middle| e^{im\phi}\varphi(\theta, r) \right\rangle$$

$$= \frac{\hbar}{i} im \langle \psi_{nlm} | \psi_{nlm} \rangle = \hbar m$$

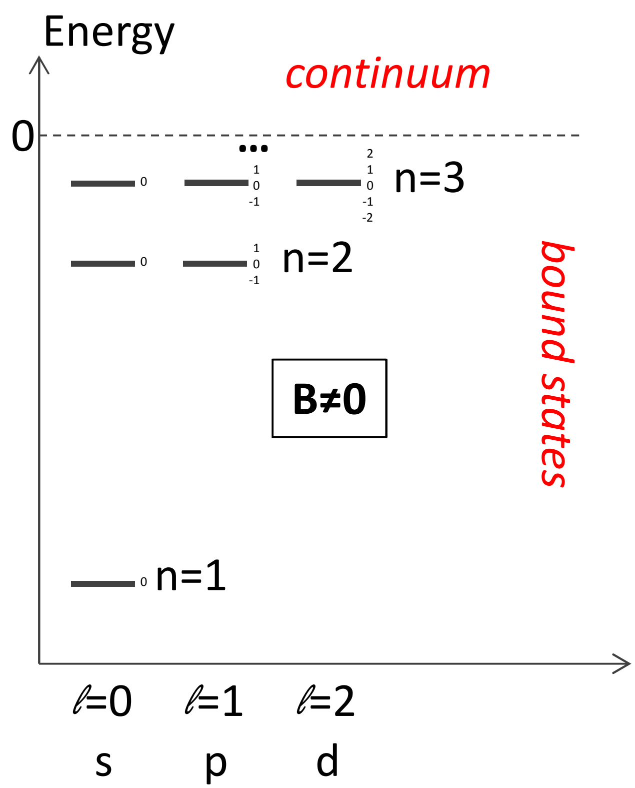
(*m*: "magnetic quantum number")

• So the energy added to each state due to the magnetic field is

$$E = -\langle \mu_z \rangle B_z = \mu_B \frac{\langle L_z \rangle}{\hbar} B_z = \mu_B m B_z \qquad (\text{for } \vec{B} = B_z \hat{z})$$

• Note that $\mu_B = 5.8 \times 10^{-5}$ eV/T (small in comparison to electronic transitions even for large magnetic fields)

“Normal” Zeeman effect



- In a magnetic field, the otherwise degenerate $l \neq 0$ levels split into “multiplets” separated by “Zeeman” energy

- What effect does this have on the observed optical spectra? i.e. what did Zeeman see?

- Not all transitions are allowed!

- We must derive “selection rules”

Pieter Zeeman
Nobel Prize, 1902

Electronic Dipole Transitions

$$\psi_{nlm} \rightarrow \psi_{n'l'm'}$$

initial → final

- During transition, electron is in a superposition state

$$\Psi \sim \psi_{nlm} e^{-i\frac{E_n}{\hbar}t} + \psi_{n'l'm'} e^{-i\frac{E_{n'}}{\hbar}t}$$

- This charged electron “cloud” has a dipole moment

$$\text{-}e\langle \vec{r} \rangle = -e\langle \Psi | \vec{r} | \Psi \rangle$$

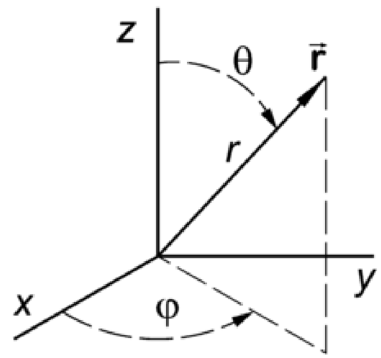
$$\omega = \frac{E_n - E_{n'}}{\hbar}$$

$$= -e \int \vec{r} \left\{ |\psi_{nlm}|^2 + |\psi_{nlm}|^2 + \psi^*_{n'l'm'} \psi_{nlm} e^{-i\omega t} + \psi^*_{nlm} \psi_{n'l'm'} e^{+i\omega t} \right\} d^3 r$$

$$= -e \int \vec{r} \left\{ \psi^*_{n'l'm'} \psi_{nlm} e^{-i\omega t} + \psi^*_{nlm} \psi_{n'l'm'} e^{+i\omega t} \right\} d^3 r$$

Selection Rules

$$\vec{r} = \begin{cases} |r| \sin\theta \cos\phi \, \hat{x} \\ |r| \sin\theta \sin\phi \, \hat{y} \\ |r| \cos\theta \, \hat{z} \end{cases}$$



- Vector components of ϕ integral:

$$\boxed{\sin\phi = \frac{e^{i\phi} - e^{-i\phi}}{2i}}$$

$$\boxed{\cos\phi = \frac{e^{i\phi} + e^{-i\phi}}{2}}$$

$$\hat{x}, \hat{y} \propto \int_0^{2\pi} e^{-im'\phi} (\sin\phi, \cos\phi) e^{im\phi} d\phi$$

$$= \int_0^{2\pi} e^{i(-m' \pm 1 + m)\phi} \, d\phi = 0$$ UNLESS m-m'= ±1

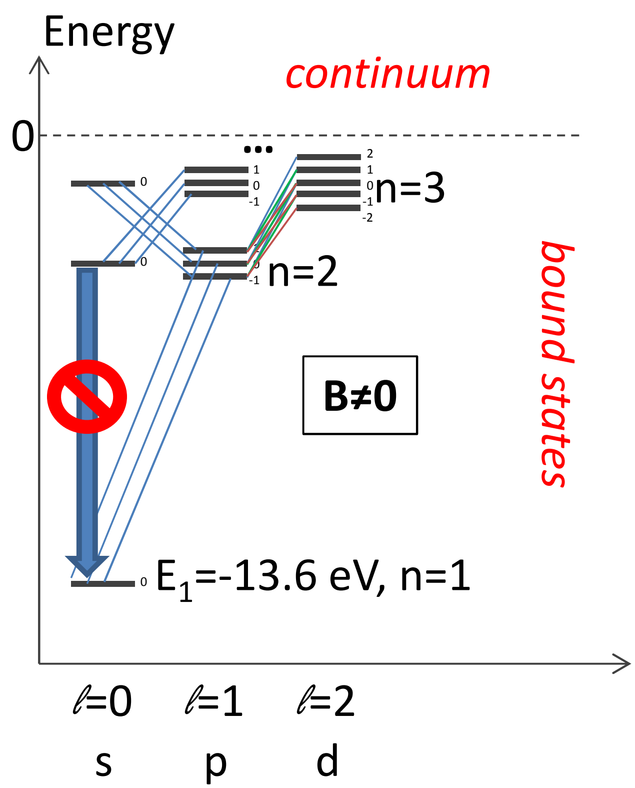
$$\hat{z} \propto \int_0^{2\pi} e^{-im'\phi} e^{im\phi} d\phi = 0$$ UNLESS m-m'= 0

- So the only transitions allowed have Δm=0,+1, or -1. This is our "selection rule"

- Also, from the symmetry of the polar angle θ integral, we have another selection rule $\Delta\ell$ =+1 or -1 (without proof)

“Normal” Zeeman selection rules

$\Delta\ell$=+1 or -1 and Δm=0,+1, or -1.



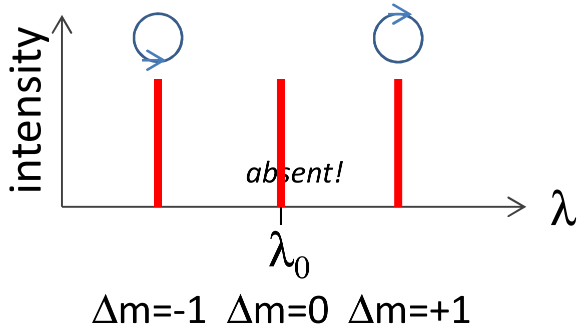
- Each spectral line splits into a triplet

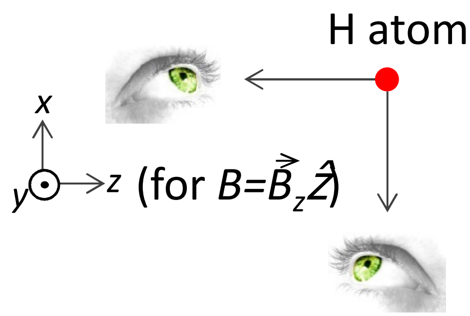
- By the uncertainty principle $\Delta t \Delta E$~h, ΔE (spectral linewidth) is inversely proportional to excited state lifetime Δt

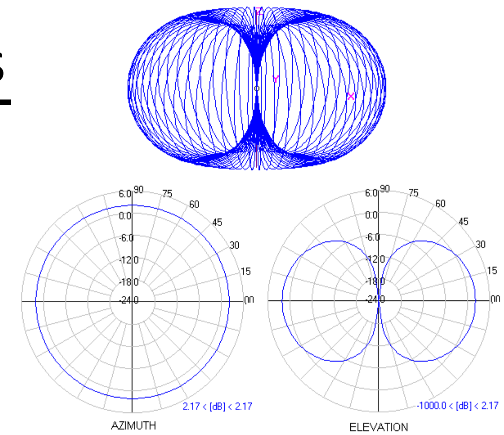
- Note that 2s-1s is forbidden by dipole selection rules. Since the 2s lifetime Δt is large, the spectral linewidth ΔE is (very) small! This enables precision measurements at 1 part in 10^{15} such as the “Lamb shift”: experimental verification of quantum electrodynamical effects

Willis Lamb
Nobel Prize, 1955

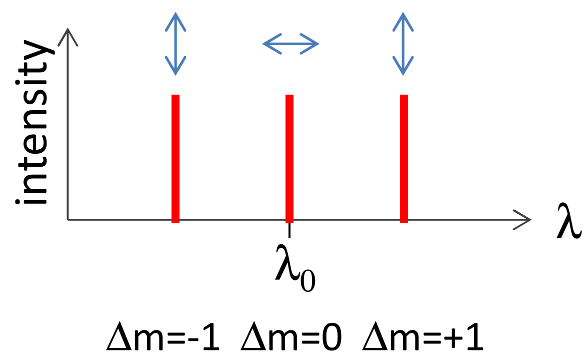
Polarization of radiative transitions





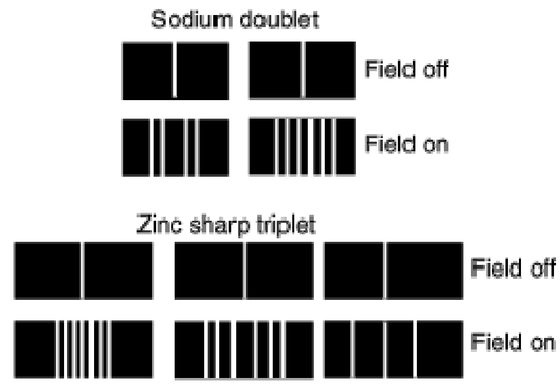


- Polarizations can be derived from the electric dipole vector components



Hendrik Lorentz
Nobel Prize, 1902

"Anomalous" Zeeman effect



- More commonly we see multiplet splitting other than 3!
- What are we forgetting?
- Go back to assumptions:

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = i\hbar\frac{\partial}{\partial t}\Psi \quad \text{(free particle)}$$

- This uses the nonrelativistic kinetic energy $E=1/2mv^2=p^2/2m$
- Note this equation does not treat time and space on an equal footing: 1st derivative for time and 2nd derivative for space

- More correctly we should use the relativistic expression for kinetic energy

$$E = \sqrt{(mc^2)^2 + (pc)^2}$$

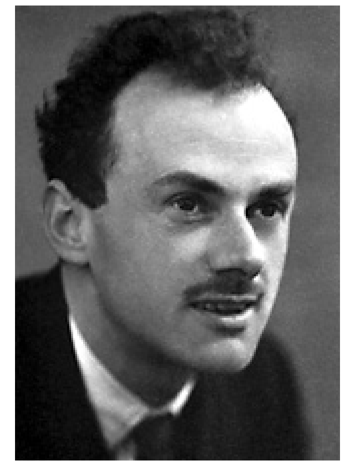
- Note that this is asymptotically equivalent to classical expression:

$$E = mc^2\sqrt{1 + \left(\frac{pc}{mc^2}\right)^2} \approx mc^2\left(1+\frac{1}{2}\left(\frac{pc}{mc^2}\right)^2 + \cdots\right) \quad = mc^2 + \frac{p^2}{2m} \text{ + small relativistic corrections}$$

Relativistic Quantum Mechanics

• Interpret total energy expression as an operator to construct wave equation

$$\sqrt{(mc^2)^2 + (pc)^2}\Psi = i\hbar\frac{\partial}{\partial t}\Psi \quad \text{(free particle)}$$



Paul Dirac
Nobel Prize, 1932

• But how to interpret the action of an operator from within a square root??

• This problem disappears if the expression inside is a perfect square… is it??

$$(mc^2)^2 + (pc)^2 = (\alpha_0 mc^2 + \alpha_1 p_1 c + \alpha_2 p_2 c + \alpha_3 p_3 c)^2$$

$$= \left(\alpha_0 mc^2 + \textstyle\sum_{j=1}^{3} \alpha_j p_j c\right)^2$$

Only if $\alpha_i^2=1$ and $\alpha_i\alpha_j+\alpha_j\alpha_i=\{\alpha_i,\alpha_j\}=0$ for $i\neq j$: This defines a "Clifford algebra"

$$\left(\alpha_0 mc^2 + \sum_{j=1}^{3} \alpha_j p_j c\right)\Psi = i\hbar\frac{\partial}{\partial t}\Psi \qquad \text{"Dirac Equation"}$$

• Note that this puts space and time on equal footing as required by relativity (only first derivatives)

"Irreducible representation" of Clifford Algebra

- Must use matrices – but how big?
- smallest which satisfy algebra are 4x4:

$$\alpha_0 = \begin{bmatrix} I_2 & 0_2 \\ 0_2 & -I_2 \end{bmatrix} \qquad \alpha_j = \begin{bmatrix} 0_2 & \sigma_j \\ \sigma_j & 0_2 \end{bmatrix} \qquad j = 1,2,3$$

•Pauli matrices

$$\sigma_1 = \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \qquad \sigma_2 = \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \qquad \sigma_3 = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\begin{bmatrix} mc^2 I_2 & \vec{\sigma}\cdot\vec{p}c \\ \vec{\sigma}\cdot\vec{p}c & -mc^2 I_2 \end{bmatrix}\Psi = i\hbar\frac{\partial}{\partial t}\Psi \qquad (\vec{\sigma} = \sigma_x\hat{x} + \sigma_y\hat{y} + \sigma_z\hat{z})$$

- Note that when p=0, eigenvalues are $+mc^2$ and $-mc^2$ (twofold degenerate)

- Degeneracies are a signature of symmetry… but which one? What degree of freedom do these two values correspond to? Look to experiment for a clue…