Overview continued

How atomic/molecular structure ⇝ what you see in e.m. spectrum.

1st approximation to atomic structure = H-like ions, non-relativistic, no spin
(H-like means?)

H itself is of special importance because

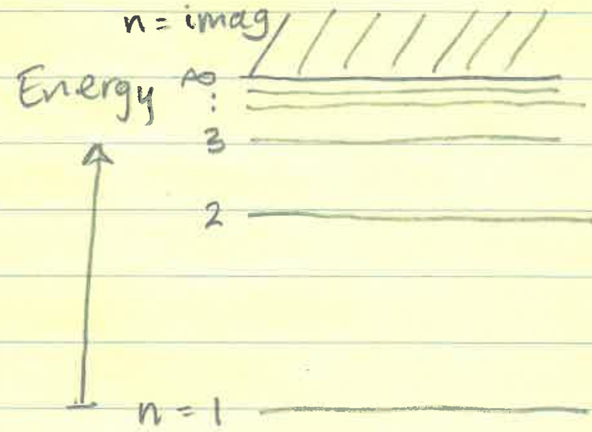
- H is most abundant element in Universe, 75% by mass, 90% by number of nuclei (But atomic matter makes up only 4% of total mass-energy of Universe. How do we know?)
- H lines prominent in astron spectra.
- H plays major role in ionization/thermal equilibrium
  - Sun & stars
  - Gas planets
  - Interplanetary / interstellar / intergalactic medium
  - Star formation
  - Cosmic Microwave Background

Atomic physics of H-like ions is well understood theoretically, as is He-like ions.
Atom physics of multi-electron ions is in progressively worse theoretical shape – rely more on experimental data, especially for neutrals, which are easiest to prepare in lab.

Energy levels of H

$$E_n = -\frac{1}{2n^2} \quad \text{a.u}$$

$$= -\frac{1}{n^2} \quad \text{Rydberg}$$



Each energy level is $2\,n^2$ - fold degenerate

2 electron spin states ↗ (2); various angular momentum states ↖ (n^2)

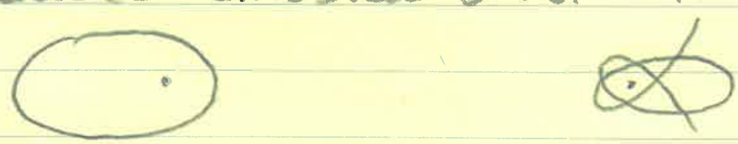
This ignores nuclear spin (depends on nucleus).

Each individual state is an eigenstate of mutually commuting operators:

Quantity	Operator	Quantum number	Values
Energy	Hamiltonian H	n	$1, 2, \ldots \infty$, imag
$\lvert\text{Ang mom}\rvert^2$	L^2	ℓ	$0, 1, \ldots, n-1$
Ang. mom z-cpt	L_z	m	$-\ell, \ldots, \ell$

m (magnetic) states degenerate because of isotropy. (what?)
(why?)

ℓ states degenerate because of accidental symmetry in 2-body Coulomb problem that causes classical orbit to close



closed orbit — general non-closed orbit.

Relativity splits ℓ-state degeneracy.

Perturbations from H-like approx in multi-electron atoms

(a) Electrostatic interactions between electrons.

$\Delta E \sim 1$ a.u.

Splits some but not all energy levels.

(b) Spin-orbit, spin-spin interactions

(Spin = elec spin; orbit = elec orb. ang mom; spin-spin ↑↑ = elec spins)

Spin absent from non-rel Schrödinger eq, but arises in relativistic Dirac* eq.

Energy (Hamiltonian) contains piece

$\sigma \cdot B$

(σ = elec spin; B = atomic mag field)

*Rel Schrod, with elec spin = 0, gives wrong fine-structure.

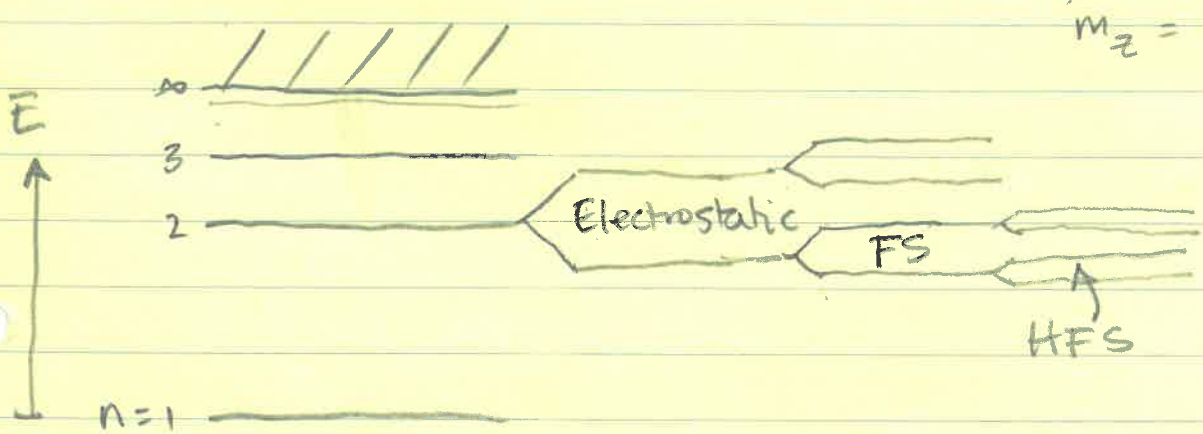
$$\Delta E \sim \frac{v^2}{c^2} \text{ a.u.} \sim \left(\frac{1}{137}\right)^2 \text{ a.u.}$$

= "Fine structure".

(c) Nuclear spin - elec spin interaction

$$\Delta E \sim \frac{v^2}{c^2}\frac{m_e}{m_Z} \text{ a.u.} \sim \left(\frac{1}{137}\right)^2 \frac{1}{2000} \text{ a.u}$$

for H itself, $m_Z = m_p$



(d) Zeeman effect.

Selection rules - Allowed transitions

Not all radiative transitions between energy levels are equally fast.

Fastest are those involving emission / absorption of photon with

(i) unit ang. mom $\hbar$ = "dipole" photon

(ii) odd parity

= "allowed" or "permitted" transition.

Parity = behavior of wavefunction under coordinate inversion

$$P\psi(\vec{x}) = \psi(-\vec{x}) = \pm\,\psi(\vec{x})$$

$+$ = even parity

$-$ = odd parity.

Total parity is rigorously conserved in any reaction, eg

$$X^* \longrightarrow X + y$$

X^*	X	y	
even	odd	odd	OK
even	even	odd	not OK

Almost absorption lines in stellar spectra are from allowed transitions

BUT in astronomy Forbidden (= not allowed) lines are important in low density (means?) environments

such as interstellar / interplanetary space.

Ex 1/ [O III] 5007 Å "nebulium" green line

brackets denotes "forbidden"

O III or O^{++}

$Z = 8$, 6 electrons

has 2 valence electrons with $\ell = 1$.

Ground electronic configuration
split into 3 ($L = 0, 1, 2$)
by electrostatic interaction

$$\text{Parity} = (-)^{\sum_{\text{elecs}} \ell}$$

= same for all levels of ground elec config

⇒ transitions between levels of ground elec config are <u>all</u> parity forbidden.

Such transitions don't happen in lab, Why not?

Ex 2/ [OI] 6300, 5577 auroral lines
pink green
1000s 1s
decay decay

Prob set.

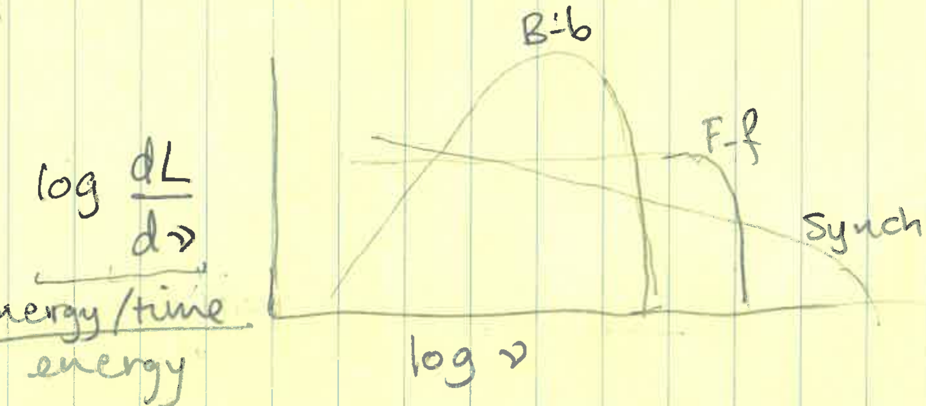
<u>Molecular structure overview</u>
3 ~ independent modes
(a) electronic ≈ like atoms
$\Delta E_{elec} \sim$ a.u.
(b) vibrational ≈ simple harmonic oscillator
$\Delta E_{vib} \sim \left(\frac{m_e}{m_x}\right)^{1/2}$ a.u.
(c) rotational ≈ solution of rotator
$\Delta E_{rot} \sim \left(\frac{m_e}{m_x}\right)$ a.u.

	Radio	Microwave	Infrared	Visible	Ultraviolet	X-ray	γ-ray
Lines							
Atomic	Hyperfine	Fine structure		Elec split forbidden	Allowed	High-Z allowed	(nuclear)
	Radio rec.	recomb		Balmer H	Lyman H	High-Z H-like	
Molecular	Rotational		Vibrational		Electronic	— (molecules dead)	
Continuum							
Blackbody = Planck		CMB 2.7K	Dust 20-40K	Planets 300K	Stars 3000-10,000 K	Hot WDs 10^5K	Neutron stars 10^6K

Free-free = Bremstrahlung = "Thermal" ⟶ extending up to $h\nu \approx kT$

Synchrotron = "Non-thermal" ⟶ extending up to $h\nu \approx h\nu_{gyro}\gamma_A^3$

γ = Lorentz factor



why?