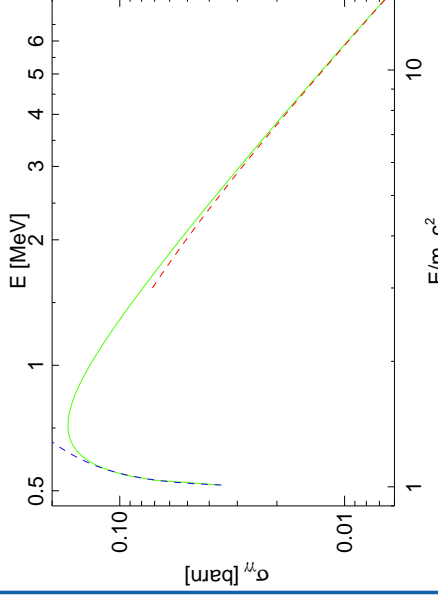




Photon-Photon Pair Production



Photon Photon Pair Production



Pair production is the reaction:



In center of mass system for $\epsilon = E/m_e c^2 > 1$:

$$\sigma_{\gamma\gamma} = \frac{\pi r_0^2}{\epsilon^2} \left(\left(2 + \frac{2}{\epsilon^2} - \frac{1}{\epsilon^4} \right) \ln \left(\epsilon + \sqrt{\epsilon^2 - 1} \right) - \sqrt{1 - \frac{1}{\epsilon^2}} \left(1 + \frac{1}{\epsilon^2} \right) \right) \quad (8.1)$$

Low energy cut-off due to large annihilation probability of created pairs.

Physical Foundations



Introduction

Pair production:

Generation of electron positron pairs in environments with very high radiation energy density.

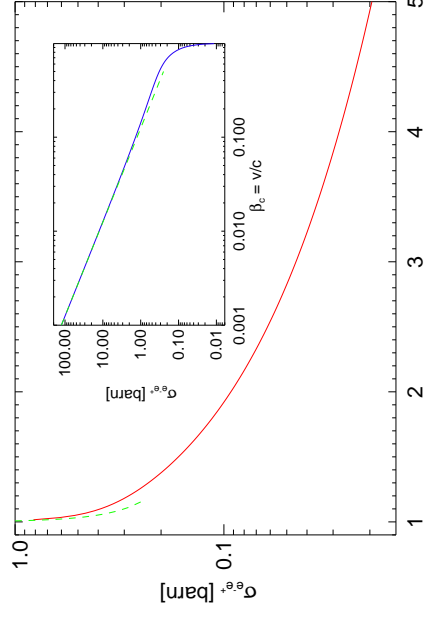
References:

Longair, Volume I
Svensson, R. 1982, ApJ 258, 321
Zdziarski, A. 1980, Acta Astron. 30, 371

Introduction



Annihilation



Annihilation is the inverse of photon-photon pair production.

In center of mass system, with $\beta_c = v_{\text{CM}}/c$

$$\sigma_{e^+e^-} = \pi r_0^2 \left(\frac{1 - \beta_c^2}{4\beta_c} \right) \left\{ \frac{3 - \beta_c^4}{\beta_c} \ln \left(\frac{1 + \beta_c}{1 - \beta_c} \right) + 2 (\beta_c^2 - 2) \right\} \quad (8.2)$$

For low energies $\sigma_{e^+e^-} \propto 1/\beta_c$ (dashed line in the figure)

Physical Foundations



Compactness Parameter

Pair production occurs for photon energies $E_{\text{ph}} \gtrsim m_e c^2$. These energies can be reached, e.g., by Comptonized soft photons.

Optical depth for photon-photon interactions in source of size R :

$$\tau_{\gamma\gamma} = n_{\gamma} \sigma_{\gamma\gamma} R \sim n_{\gamma} \sigma_T R \quad (8.3)$$

since $\max\{\sigma_{\gamma\gamma}\} \approx \sigma_T$.

Here photon density, n_{γ} :

$$n_{\gamma} \approx \frac{U_{\text{rad}}}{m_e c^2} = \frac{L_{\gamma}}{4\pi R^2} \cdot \frac{1}{c} \cdot \frac{1}{m_e c^2} = \frac{L_{\gamma}}{4\pi R^2 m_e c^3} \quad (8.4)$$

for typical photon energies of $E \sim m_e c^2$

$\Rightarrow \tau_{\gamma\gamma} \gtrsim 1$ for

$$\ell = \frac{L_{\gamma}}{R} \frac{\sigma_T}{m_e c^3} \gtrsim 4\pi \quad (8.5)$$

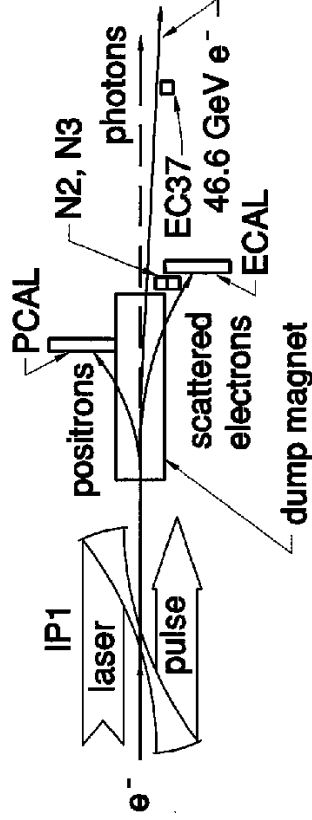
where ℓ is called the compactness parameter (Guilbert et al., 1983, MNRAS 205, 593).

Astrophysical Context

1



Laboratory Experiments



Experimental realization: 527 nm (2.35 eV) Laser photons Compton upscattered off 46.6 GeV electrons in Stanford Linear Accelerator Center (SLAC) (Burke et al., 1997, Phys. Rev. Let. 79, 1626).

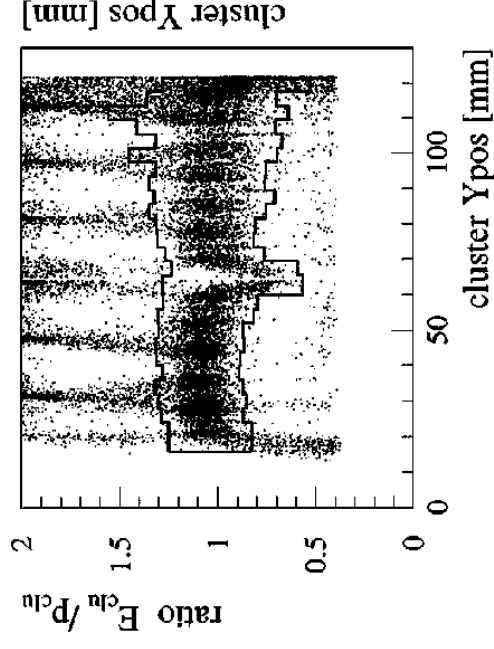
Only multi-photon pair-production possible since 511 keV threshold for two-photon pair production not reached in beam.

Laboratory Experiments

1



Laboratory Experiments



Possible positrons are located within solid line.

Subtract measurements without laser photons to obtain number of pairs.

Result: pair production raises as 5th power of laser intensity, in agreement with theory. See Burke et al. (1997) for details.

Laboratory Experiments

2



Atomic Physics



Introduction

Most important radiation process in IR, optical, and UV:

Line emission and absorption from atoms and ions

⇒ Will give quick review of atomic physics necessary to understand line emission, focusing on atomic structure.

Literature

- Rybicki & Lightman
- Dopita & Sutherland, *Astrophysics of the Diffuse Universe*, Springer
- Lecture notes from Ernie Seaquist (University of Toronto;
<http://www.astro.utoronto.ca/~seaquist/radiation/index.html>)
- Lang, *Astrophysical Formulae*, Vol. 1

Introduction

1



Bohr-Sommerfeld Theory

Most of the properties of atoms can be understood in terms of “classical quantum mechanics”, which is based on the following postulates:

1. Action is quantized (Sommerfeld):

$$\text{Action} = \oint p_i dq_i = n_i h \quad (9.1)$$

Integral is performed over one period of electron motion, p_i, q_i : generalized momentum and coordinate

2. Heisenberg's uncertainty principle: States for which $\Delta p_i \Delta q_i < h$ cannot be distinguished
3. Pauli Exclusion Principle: Two particles with half-integer spin cannot occupy same cell in phase space (i.e., cannot have same position, momentum, and spin direction)

Bohr-Sommerfeld Theory

1



Bohr-Sommerfeld Theory

Quantization of action leads to Bohr-Sommerfeld theory of hydrogen atom:

Motion of electron in Coulomb field of nucleus (charge Ze) on circular orbits:

$$\frac{Ze^2}{r^2} = \frac{mv^2}{r} \implies r = \frac{Ze^2}{mv^2} \quad (9.2)$$

Quantization of action (Eq. 9.1) gives:

$$\oint p dq = \oint mvr d\phi = 2\pi mvr = n h \quad (9.3)$$

such that

$$v = \frac{nh}{2\pi mr} = \frac{nh}{mr} \quad (9.4)$$

where $\hbar = h/2\pi$.

Therefore

$$r_n = \frac{n^2 \hbar^2}{Zm_e e^2} \sim 0.5 \text{ \AA} \cdot \frac{n^2}{Z} \quad (n = 1, 2, \dots) \quad (9.5)$$

Bohr-Sommerfeld Theory

2



Bohr-Sommerfeld Theory

To get better approximation to reality, refine theory slightly:

1. Take into account finite mass of nucleus, in effect, this means to use reduced mass $\mu = m_e M / (m_e + M)$ where M is mass of nucleus, instead of m (e.g., radii in Deuterium slightly smaller than in normal H).

2. Elliptical orbits are also possible ⇒ need to compute action for radial and azimuthal momenta:

$$\oint p_r dr = n_r h \quad \text{and} \quad \oint p_\phi d\phi = n_\phi h =: (\ell + 1) h \quad (9.6)$$

Principal quantum number is $n = n_r + n_\phi = n_r + \ell + 1$, ℓ : orbital angular momentum quantum number, $\ell = 0, 1, \dots, n - 1$.

Further refinements (e.g., relativistic treatment...) in principle possible.

With n and ℓ , semi-major axis a , and semi-minor axis b of orbit is given by

$$a = n^2 \frac{\hbar^2}{Z\mu e^2} \quad \text{and} \quad b = n(\ell + 1) \frac{\hbar^2}{Z\mu e^2} \quad (9.7)$$

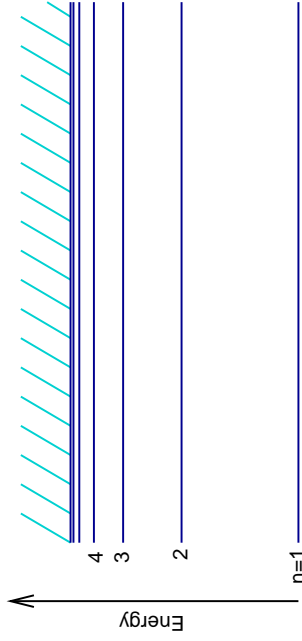
(i.e., $\ell = n - 1 \implies$ circular orbit)

Bohr-Sommerfeld Theory

3



Bohr-Sommerfeld Theory



Ground state (-13.6eV)

Energy only depends on semi-major axis a , i.e., in Bohr-Sommerfeld theory orbits with the same n and different ℓ have the same energy:

$$E = -\frac{Ze^2}{r} + \frac{mv^2}{2} = -\frac{Ze^2}{r} + \frac{Ze^2}{2r} = -\frac{Ze^2}{2r} \quad (9.8)$$

insert $a (= r_n$ from Eq. 9.5):

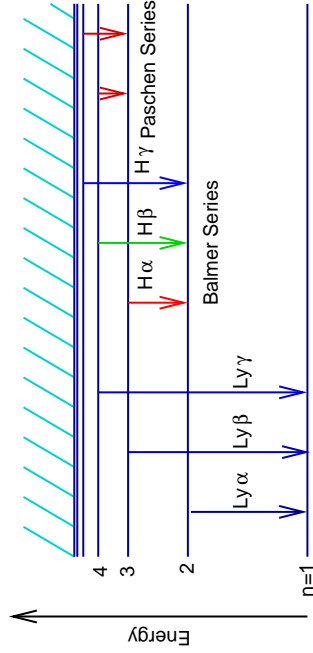
$$E_n = -\frac{2\pi^2\mu e^4}{\hbar^2} \cdot \frac{Z^2}{n^2} \quad (9.9)$$

Bohr-Sommerfeld Theory

4



Bohr-Sommerfeld Theory



Lyman Series Ground state (-13.6eV)

Line emission through transitions between orbits with different n . Photon energy:

$$h\nu_{21} = \frac{2\pi^2\mu e^4 Z^2}{\hbar^2} \left(\frac{1}{n_2^2} - \frac{1}{n_1^2} \right) \quad (9.10)$$

where the constant is called 1 Rydberg:

$$1 \text{ Ry} := \frac{2\pi^2\mu e^4}{\hbar^2} \sim 13.6 \text{ eV} \quad (9.11)$$

Bohr-Sommerfeld Theory

5



Schrödinger Equation

To obtain exact solutions, use quantum mechanics, where behavior of wave function, Ψ , is obtained from solving the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi \quad (9.12)$$

where H is the Hamiltonian of the system. For our case, neglecting spin, relativistic and nuclear effects:

$$H = -\frac{\hbar^2}{2m_e} \sum_j \nabla_j^2 - Ze^2 \sum_j \frac{1}{r_j} + \sum_{i>j} \frac{e^2}{r_{ij}} \quad (9.13)$$

Often, need only stationary solutions, i.e., Energy eigenstates \implies Make ansatz

$$\Psi(\mathbf{r}, t) = \psi(\mathbf{r}) e^{-iEt/\hbar} \quad (9.14)$$

to obtain time independent Schrödinger equation

$$E\psi = H\psi \quad (9.15)$$

Schrödinger Equation

1



Motivation

Typical atom has $N > 1$ electrons \implies complicated to solve.

Assumption to make solution practical: Electron moves in field of nucleus plus averaged potential of $N - 1$ electrons \implies self-consistent field approximation.

Assume averaged potential to be spherically symmetric \implies central field approximation.

Form of potential:

- Large r : Nucleus shielded
- Small r : Nucleus dominates

Therefore, potential has form

$$V(r) \sim \begin{cases} \frac{Z-N+1}{r} & \text{for } r \rightarrow \infty \\ \frac{Z}{r} & \text{for } r \rightarrow 0 \end{cases} \quad (9.16)$$

Central field approximation

1



Wave Functions

If $H = H(r)$, then the Schrödinger equation separates:

$$\psi(r, \theta, \phi) = \frac{1}{r} R_{nl}(r) Y_{lm}(\theta, \phi) \quad (9.17)$$

where the quantum numbers n , l , and m are integers and where the spherical harmonics are

$$Y_{lm}(\theta, \phi) = \left(\frac{(l-|m|)! 2l+1}{(l+|m|)! 4\pi} \right)^{1/2} \cdot (-1)^{(m+|m|)/2} P_l^{(|m|)}(\cos \theta) e^{im\phi} \quad (9.18)$$

where P_l^m is an associated Legendre function.

Y_{lm} is associated with orbital angular momentum, $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and obeys

$$\mathbf{L}^2 Y_{lm} = l(l+1) Y_{lm} \quad \text{and} \quad L_z Y_{lm} = m Y_{lm} \quad (9.19)$$

Here, $m = -l, -l+1, \dots, +l$.

More precisely, should write m_l for m , however, the l is often omitted. . .

$l = 0, 1, 2, 3, \dots$ is denoted s, p, d, f, g, \dots

Note that the Y_{lm} form an orthonormal system,

$$\int Y_{lm}^*(\theta, \phi) Y_{l'm'\theta, \phi} d\Omega = \delta_{l,l'} \delta_{m,m'} \quad (9.20)$$

Central field approximation

2



Wave Functions

The radial wave function $R_{nl}(r)$ is solution of

$$\frac{1}{2} \frac{dR_{nl}^2}{dr^2} + \left(E - V(r) - \frac{l(l+1)}{2r^2} \right) R_{nl} = 0 \quad (9.21)$$

where energy is labeled with integer n for discrete [bound] states:

$$n = l + 1, l + 2, l + 2, \dots$$

R is also normalized

$$\int_0^\infty R_{nl}(r) R_{n'l'}(r) dr = \delta_{n,n'} \quad (9.22)$$

and $R_{nl}(r)^2$ gives probability that electron is between r and $r + dr$.

For the pure Coulomb case,

$$V(r) = -\frac{Z}{r} \quad (9.23)$$

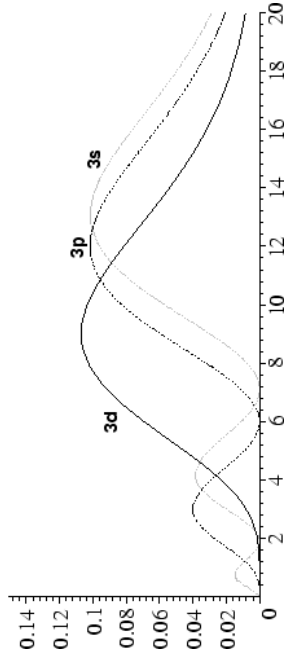
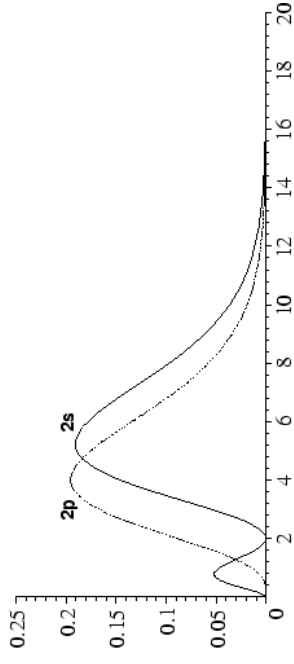
one finds with $\rho = 2Zr/n$:

$$R_{nl}(\rho) = - \left(\frac{Z(n-l-1)!}{n^2[(n+l)!]^3} \right)^{1/2} e^{-\rho/2} \rho^{l+1} L_{n+l}^{2l+1}(\rho) \quad \text{and} \quad E_n = -\frac{Z^2}{2n^2} \quad (9.24)$$

where $L_{n+l}^{2l+1}(x)$: associated Laguerre polynomials.

Central field approximation

3



courtesy D. Finley



Many Electron Systems, I

To summarize the previous slides: central field approximation specifies each state ("orbital") with quantum numbers:

n : principal quantum number,

$$n = l + 1, l + 2, \dots$$

l : angular momentum quantum number,

$$l = 0, 1, 2, \dots$$

m : magnetic quantum number,

$$m = -l, -l+1, \dots, l-1, l$$

m_s : spin quantum number,

$$m_s = \pm 1/2$$

The wave function of N electrons is then a combination of products

$$u_a(1) u_b(2) \cdots u_k(N) \quad (9.25)$$

where $a = (n, l, m, m_s)$ for first electron and so on.

Products (9.25) form a complete set, which allows to describe any state of atom.

Many Electron Systems

1



Many Electron Systems, II

Problem: Eq. (9.25) does not take into account quantum nature
 \Rightarrow Electrons are identical
 \Rightarrow Cannot determine *which* electron in what state
 \Rightarrow Base state is sum of all linear combinations of Eq. (9.25):

$$\frac{1}{\sqrt{N!}} \sim_p \epsilon_p P(u_a(1)u_b(2) \cdots u_k(N)) \quad (9.26)$$

where sum goes over all $N!$ permutations $P(x, y, z, \dots)$ of the u_i .
 To obey Pauli exclusion principle, choose

$$\epsilon_p = \begin{cases} +1 & \text{if } p \text{ is even permutation} \\ -1 & \text{if } p \text{ is odd permutation} \end{cases} \quad (9.27)$$

i.e., if two electrons in same orbital \Rightarrow subtracts out.

Permutations can be conveniently written as Slater determinant

$$\psi \propto \frac{1}{\sqrt{N!}} \begin{vmatrix} u_a(1) & u_a(2) & \cdots & u_a(N) \\ u_b(1) & u_b(2) & \cdots & u_b(N) \\ \cdots & \cdots & \cdots & \cdots \\ u_k(1) & u_k(2) & \cdots & u_k(N) \end{vmatrix} \quad (9.28)$$

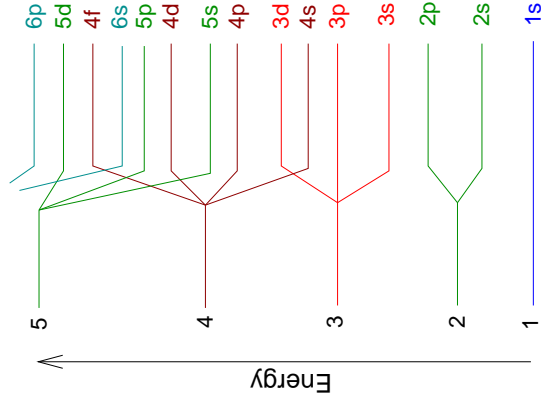
Result of calculations with such wave functions: atomic structure

Many Electron Systems

2



Atomic Structure, I



Will now look at Atomic Structure.

Typical notation:

$$l = \begin{array}{cccc} 0 & 1 & 2 & 3 \\ s & p & d & f \end{array}$$

$$n = \begin{array}{cccc} 0 & 1 & 2 & 3 \\ K & L & M & N \end{array}$$

Calculations show that the order of filling is as follows:

1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5p, 6p, 7s, 6d, ...

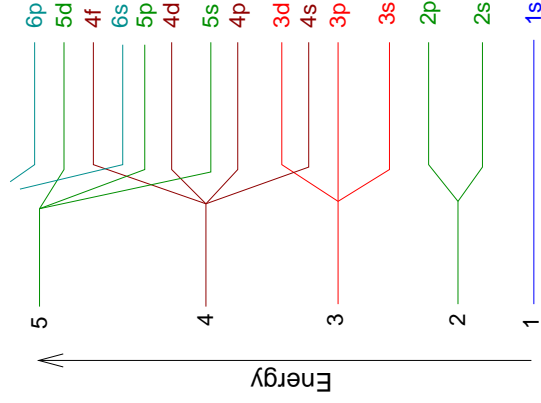
Note that 4s, 5s, ... out of order \Rightarrow s-subshell closer to nucleus, effective potential gives more binding energy to electrons close to nucleus!

Many Electron Systems

3



Atomic Structure, II



For example, Sodium ($Z = 11$) ground state configuration

$$\text{Na: } 1s^2 2s^2 2p^6 3s^1$$

(upper indices denote number of electrons).

We will see later that filled shells do generally not participate in producing lines \Rightarrow only give valence electrons, e.g., by writing [Ne] 3s¹ for the above configuration. Furthermore, the "1" is often omitted: [Ne] 3s.

Many Electron Systems

4



LS coupling

Configuration not sufficient to specify state of ion

\Rightarrow need to take into account electrostatic interaction between electrons and spin orbit interaction.

QM perturbation theory shows: Total state of ion determined from combining spin and orbital angular momenta:

$$S = \sum_i s_i \quad \text{and} \quad L = \sum_i l_i \quad (9.29)$$

and then forming total angular momentum

$$J = L + S \quad (9.30)$$

following quantum mechanical combination rules. This is called LS-coupling or Russell-Saunders coupling. A combination of S and L is called a "term" or "multiplet".

Result for energy: Hund's rules:

1. Terms with larger S have lower energy

Larger $S \Rightarrow$ spins coaligned \Rightarrow Pauli: larger separation of electrons.

2. For same S , terms with largest L are lower in energy

Large $L \Rightarrow$ similar $l_i \Rightarrow$ electrons go around nucleus in similar directional sense \Rightarrow have to be farther separated because of Pauli.

Many Electron Systems

5

**LS coupling**

Once a term with S , L is known, energy can split further due to spin-orbit interaction. QM shows that this split ("Thomas precession") is related to

$$J = \mathbf{L} + \mathbf{S} \quad (9.31)$$

and that individual shift is proportional to $J(J+1)$. Therefore, energy splitting

$$E_{J+1} - E_J \propto C((J+1)(J+2) - J(J+1)) = 2C(J+1) \quad (9.32)$$

where

$$C \begin{cases} > 0 & \text{if shell less than half-full (normal term)} \\ < 0 & \text{if shell more than half-full (inverted term)} \end{cases}$$

Full state then denoted as follows

$$2S+1 L_J \quad (9.33)$$

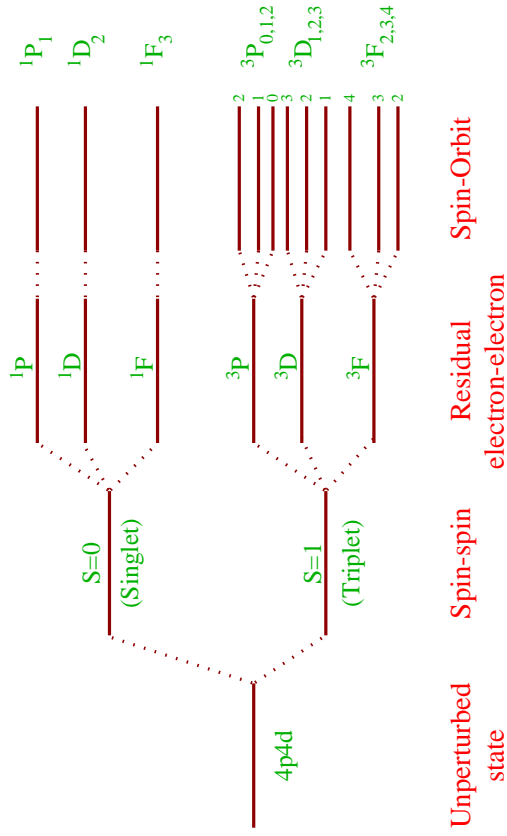
where $L = S, P, \dots$ for $L = 1, 2, \dots$

Examples: $^2P_{1/2}, ^3D_{2, \dots}$

When constructing states, need to look whether n, l of two electrons to be combined are identical (nonequivalent electrons) or not (equivalent electrons).

For equivalent electrons, some possible terms are unavailable because of Pauli.

Many Electron Systems

**LS coupling**

Example: $4p4d$ configuration in LS Coupling (R&L, Fig. 9.2a)

Many Electron Systems