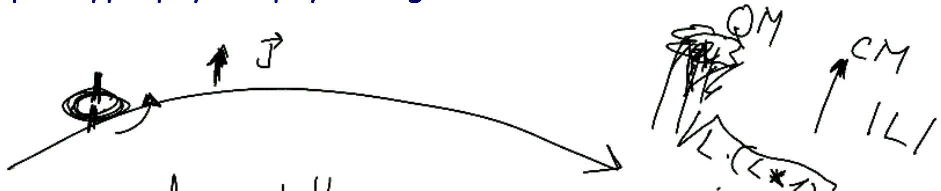
Lecture Thursday 30 August 2007 (Revised Sept. 5^{th}, 2007)

Topics Helium atom part 2 Repulsion is smaller for triplet states

Conservation of angular momentum; Angular momentum and spin angular momentum
Spin degrees of freedom + Something on Dirac Equation
It might be useful to read about spin in textbooks on Quantum Theory, as well as many different entries on Wikipedia and Hyperphysics
(http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html See a discussion below.....)



$\sqrt{L(L+1)}\,\hbar$

integer L

half integer for σ

$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}a\\b\end{pmatrix}$ described by Pauli Spinor

$\begin{pmatrix}b\\a\end{pmatrix}$ $\begin{bmatrix}a\\b\end{bmatrix}$ up down $\left.\begin{matrix}|a|^2\\|b|^2\end{matrix}\right\}$ Probability

L_x L_y L_z ψ

σ_z $\begin{pmatrix}1&0\\0&-1\end{pmatrix}$ $-i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$ L_z

σ_x $\begin{pmatrix}0&1\\1&0\end{pmatrix}$ $-i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$ L_x

σ_y $\begin{pmatrix}0&-i\\i&0\end{pmatrix}$ $\frac{1}{2}\hbar\sigma_x$ $\frac{1}{2}\hbar\sigma_y$ $\frac{1}{2}\hbar\sigma_z$ $\boxed{e^{i\alpha\sigma_x}}$

.... When you throw a spinning object, its L keeps the direction. The Earth keeps its L and therefore we have springs, summers, winters ... Discuss that .. (J and L are both used for angular momentum)

Pauli Matrices

$$e^{i\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}} = I\cos\alpha + i\sin\alpha\begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix} = \begin{pmatrix}1&0\\0&1\end{pmatrix} \qquad I = 1 = \begin{pmatrix}1&0\\0&1\end{pmatrix}$$

$$\sigma_1 = \sigma_x = \begin{pmatrix}0&1\\1&0\end{pmatrix}$$

$$\sigma_2 = \sigma_y = \begin{pmatrix}0&-i\\i&0\end{pmatrix}$$

$$\sigma_3 = \sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

REMEMBER BICYCLE WHEEL !!!!

Spin ANTISYMMETRIC and Spin SYMMETRIC

$\begin{bmatrix}1\\0\end{bmatrix} \uparrow +$ $\begin{bmatrix}0\\1\end{bmatrix} \downarrow -$ $\uparrow$ $\downarrow$

$\uparrow(1)\uparrow(2)$ sym. $\uparrow(1)\downarrow(2)$

$\downarrow(1)\downarrow(2)$ sym $\downarrow(1)\uparrow(2)$ no symmetry

$\frac{1}{\sqrt{2}}\left(\uparrow(1)\downarrow(2) + \downarrow(1)\uparrow(2)\right)$ SYM.

$\frac{1}{\sqrt{2}}\left(\uparrow(1)\downarrow(2) - \downarrow(1)\uparrow(2)\right)$ 0 — because $\frac{1}{2}+(-\frac{1}{2})$ Antisymmetric

4 possible $\longrightarrow$ 3 symmetric triplet $S=1$

1 antisymmetric singlet $S=0$

$(2S+1)$ / 3, 1

$\vec{s}_1$ $\vec{s}_2$ $\vec{S} = \vec{s}_1 + \vec{s}_2$ .... Eigenvalues and vectors of $\vec{S}\cdot\vec{S} \equiv S^2$

QUALITATIVE "PROOF"

space SYMMETRIC - Spin ANTISYMMETRIC (spin SINGLET)

space ANTISYMMETRIC - Spin SYMMETRIC (spin TRIPLET)

$$\Psi_A(1,2) = \phi_A(1,2)\,\Xi_S(1,2)$$

$$\Psi_A(1,2) = \phi_S(1,2)\,\Xi_A(1,2)$$

$$\left[\phi_a(r_1)\chi_a(1)\,\phi_b(r_2)\chi_b(2) - \phi_b(r_1)\chi_b(1)\,\phi_a(r_2)\chi_a(2)\right]$$

$$\left[\phi_a(r_1)\phi_b(r_2) \pm \phi_b(r_1)\phi_a(r_2)\right]\left[\chi_a(1)\chi_b(2) \mp \chi_b(1)\chi_a(2)\right]$$

SPACE symmetric	SPIN antisymmetric
SPACE antisymmetric	SPIN symmetric

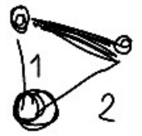
The reason is simple to see now: repulsion is reduced for space asymmetric function
Space asymmetric vanishes (-> 0) when r1 -> r2

Space symmetric → Spin singlet

Space antisymmetric → spin triplet

$$T_1+T_2+V_1+V_2+V_{12}$$

$$+\frac{e^2}{|\vec{r}_1-\vec{r}_2|}$$



Space symmetric $\quad \varphi_a(r_1)\,\varphi_b(r_2)$

$\vec{r}_1=\vec{r}_2 \quad \varphi_a(r)\varphi_b(r)+\varphi_a(r)\varphi_b(r)$

BIG REPULSION

space antisymmetric → SMALL REPULSION

zero

$\vec{r}_1=\vec{r}_2 \quad \varphi_a(r)\varphi_b(r)-\varphi_a(r)\varphi_b(r)$

The story you should learn to perform:

Here starting:
The two electron atoms have the spin symmetry feature. You can make the total wavefunction antisymmetric by taking symmetric spin and space function antisymmetric. Or you can take antisymmetric spin and then this aplies space function is symmetric. Symmetric spins are called triplet, because there are 3 of them, antisymmetric is a singlet.

Two electrons repel each other. The repulsion adds energy, positive potential.

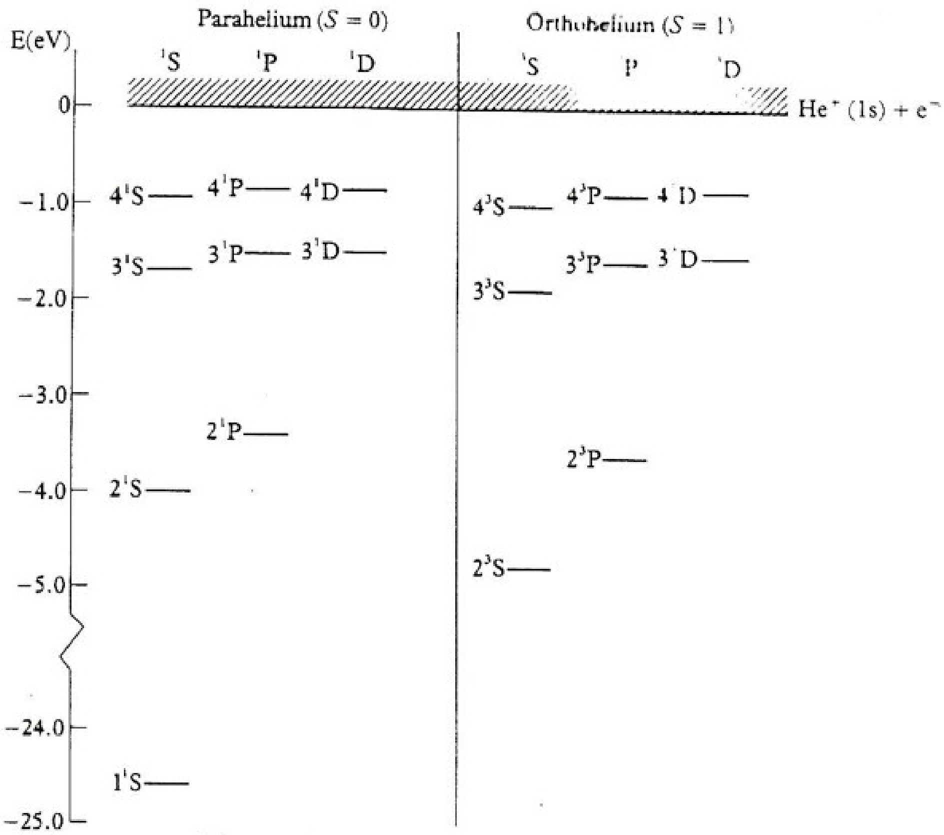
It is now possible to see that the repulsion is larger for singlets than for corresponding triplet. Think e.g. about 1s 2p orbitals, as states a and b. Then schematically

Psi(antisym) -> a(1) b(2) – b(1) a(2) Psi(sym) -> a(1) b(2) + b(1) a(2)

when the repulsion is greatest? It is when r1->r2 - and then Psi(sym) is BIG,
Psi(antisym) is very small ...

So if you manage to follow:
triplet -> spin SYM -> space ASYM -> for r1->r2 Psi(antisym) is very small the repulsion is very small .
singlet -> spin ASYM -> space SYM -> for r1->r2 Psi(sym) is BIG, the repulsion is BIG,

Experiment – Level scheme for Helium



The experimental values of the lowest energy levels of helium.
$E = 0$ corresponds to the ionisation threshold.

Spin degrees of freedom + Something on Dirac Equation

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(http://hyperphysics.phy-astr.gsu.edu/hbase/hframe.html to get there -just google it instead of copying this long link). Both of these sources should be taken as orientation, i.e. not too seriously – i.e. not as «authoritative».

Dirac equation: The story is fascinating. Originally intended to repair the inconsistencies of relativistic Schrödinger euation:
obtained by replacing T+V=E by $p^2 + m^2c^4 = E^2$

from Hyperphysics:
$$E = mc^2 = \sqrt{p^2c^2 + m_0^2c^4}$$

just according to the above. E was taken as in non-rel Schrödinger euation, but the square root was «linearized» using unknown objects, now known as Dirac Matrices:

$$E\,\psi = c(\ \alpha_x p_x + \alpha_y p_y + \alpha_z p_z + \beta\ m c^2\ )\,\psi$$

(here E and p_i are the usual operators), but are new type of objects, Dirac spinors.
It lead later to explanation of antiparticles etc etc.

P.A.M. Dirac is one of the most important contributors to modern physics (read about him)

Explanation of Spectra – repeat your SELECTION RULES – then you can understand how the spectrum is related to the Level scheme