

Physics 531, Problem Set #6

Solutions

Problem 1: Perturbation calculation

We consider a configuration  $(1s)(2p)$  of a Helium-like atom of nuclear charge  $Zc$ , approximating each orbital as hydrogenic  $(1s)$  with nucleus  $Zc$ ,  $(2p)$  with nucleus  $(Z-1)e$ .

(a) We consider the matrix element

$$\langle \phi_A(1) \phi_B(2) | \frac{1}{r_{12}} | \phi_C(1) \phi_D(2) \rangle$$

where the  $\phi$ 's are:  $\phi_{nlm}(\vec{r}) = \frac{u_{nl}(r)}{r} Y_{lm}(\theta, \phi)$

with  $u_{nl}(r)$  the (reduced) radial wave function of a Hydrogen state with some nuclear charge

We use the "addition theorem"

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \frac{(r_<)^l}{(r_>^{l+1})} \frac{4\pi}{2l+1} \sum_{m=-l}^l Y_{l,m}^*(\theta_1, \phi_1) Y_{l,m}(\theta_2, \phi_2)$$

where  $r_<(r_>)$  is the lesser (greater) of

$r_1$  or  $r_2$

$$\rightarrow \langle \phi_A(\omega) \phi_B(\omega) | \frac{1}{r_{12}} | \phi_C(\omega) \phi_D(\omega) \rangle$$

$$= \sum_l \frac{4\pi}{2l+1} \int_0^\infty dr_1 \int_0^\infty dr_2 \frac{(r_2)^l}{(r_1)^{2l+1}} u_A(\omega) u_C(\omega) u_B(\omega) u_D(\omega)$$

$$\sum_m \int d\Omega_1 Y_{l,m}^*(\theta_1, \phi_1) Y_{l,m}^*(\theta_2, \phi_2) Y_{l,m}(\theta_1, \phi_1)$$

$$\int d\Omega_2 Y_{l,m}^*(\theta_2, \phi_2) Y_{l,m}(\theta_2, \phi_2) Y_{l,m}(\theta_1, \phi_1)$$

By the rules of the integrals of 3  $Y_{l,m}$ 's the two integrals vanish, unless

$$m_B = m + m_D$$

$$m_C = m + m_A$$

$$\Rightarrow m_B - m_D = m_C - m_A \Rightarrow \boxed{m_A + m_B = m_C + m_D}$$

thus

$$\langle \phi_A(\omega) \phi_B(\omega) | \frac{1}{r_{12}} | \phi_C(\omega) \phi_D(\omega) \rangle$$

$$= \sum_{m_A + m_B = m_C + m_D} \sum_l \frac{4\pi}{2l+1} F^{(l)}(AB, CD)$$

$$F^{(l)}(AB, CD)$$

where  $C_{l'm, l'm'}^{(k)} \equiv \int d\Omega Y_{lm}^*(\theta, \phi) Y_{l'm-m'}(\theta, \phi) Y_{l', m'}$   
 $= C_{l'm, l'm'}^{(k)*}$  (real)

$$F^{(k)}(A, B, C, D) \equiv \int dr_1 dr_2 \frac{r_1^k}{r_1^{k+1}} \mathcal{Y}_A^{(k)}(r_1, \theta_1) \mathcal{Y}_B^{(k)}(r_2, \theta_2) \mathcal{Y}_C^{(k)}(r_2, \theta_2)$$

(b) The two terms arising from the (1s)(1p) config

$$1P_{(1s)} = \frac{1}{\sqrt{2}} \left\{ \phi_{1s}^{(2)}(1) \phi_{2p, m_z}^{(2-1)}(2) + \phi_{2p, m_z}^{(2-1)}(1) \phi_{1s}^{(2)}(2) \right\} \chi_{m_s}^{\text{singlet}}$$

$$3P_{(m_1, m_2)} = \frac{1}{\sqrt{2}} \left\{ \phi_{1s}^{(2)}(1) \phi_{2p, m_z}^{(2-1)}(2) - \phi_{2p, m_z}^{(2-1)}(1) \phi_{1s}^{(2)}(2) \right\} \chi_{m_s}^{\text{triplet}}$$

Note: I have denoted these states with  $m_1, m_2$  quantum numbers, though in the absence of external fields the energy does not depend on them, and they may be chosen arbitrarily.

I will pick  $m_2 = 0$

$$\Rightarrow \phi_{1s}^{(2)}(r) = \frac{2Z^{3/2}}{\sqrt{4\pi}} e^{-2r}$$

$$\phi_{2p, 0}^{(2-1)}(r, \theta) = \frac{(2-1)^{5/2}}{2\sqrt{6}} r e^{-\frac{(2-1)}{2}r} \underbrace{\sqrt{\frac{3}{4\pi}} \cos\theta}_{Y_{10}^{(0)}(\theta)}$$

$$R_{2p}^{(2-1)}(r)$$

$$Y_{10}^{(0)}(\theta)$$

The total Hamiltonian is (in atomic units)

$$H = -\frac{1}{2} \nabla_1^2 - \frac{Z}{r_1} - \frac{1}{2} \nabla_2^2 - \frac{Z}{r_2} + \frac{1}{r_{12}}$$

The energy to first order is the expectation value

$$E = \langle \psi_{\pm} | H | \psi_{\pm} \rangle = \langle \psi_{\pm} | H_0^{(1)} | \psi_{\pm} \rangle + \langle \psi_{\pm} | H_0^{(2)} | \psi_{\pm} \rangle + \langle \psi_{\pm} | \frac{1}{r_{12}} | \psi_{\pm} \rangle$$

where  $|\psi_{\pm}\rangle \stackrel{\text{singlet}}{\underset{\text{triplet}}{=}} \frac{1}{\sqrt{2}} (\phi_{1s}^{(2)}(1) \phi_{2p,0}^{(2-1)}(2) \pm \phi_{2p,0}^{(2)}(1) \phi_{2s}^{(1)}(2))$

(Where  $H_0^{(2)}(i) = \frac{1}{2} \nabla_i^2 - \frac{Z}{r_i}$   
is the Hydrogenic Hamiltonian)

Following Lect. 11 notes

$$\begin{aligned} \langle \psi_{\pm} | H_0 | \psi_{\pm} \rangle &= \frac{1}{2} \left( \langle \phi_{1s}^{(2)}(1) | H_0^{(2)}(1) | \phi_{1s}^{(2)}(1) \rangle + \langle \phi_{1s}^{(2)}(2) | H_0^{(2)}(2) | \phi_{1s}^{(2)}(2) \rangle \right) \\ &\quad + \frac{1}{2} \left( \langle \phi_{2p}^{(2-1)}(1) | H_0^{(2)}(1) | \phi_{2p}^{(2-1)}(1) \rangle + \langle \phi_{2p}^{(2-1)}(2) | H_0^{(2)}(2) | \phi_{2p}^{(2-1)}(2) \rangle \right) \\ &= \underbrace{\langle \phi_{1s}^{(2)} | H_0^{(2)} | \phi_{1s}^{(2)} \rangle}_{E_0^{(2)}(1s, Z)} + \underbrace{\langle \phi_{2p}^{(2-1)} | H_0^{(2)} | \phi_{2p}^{(2-1)} \rangle}_{E_0^{(2)}(2p, Z-1)} \end{aligned}$$

The first term is just the Hydrogenic energy for one electron in a nucleus of charge  $Z$

$$E_0^{(2)}(1s, Z) = -\frac{Z^2}{2}$$

To calculate  $E_0^{(2)}(2p, Z-1)$  we use the Virial theorem as in Lecture 11

$$\langle \phi_{2p}^{(Z-1)} | H_0^{(2)} | \phi_{2p}^{(Z-1)} \rangle = \langle \phi_{2p}^{(Z-1)} | \frac{1}{2} \nabla^2 | \phi_{2p}^{(Z-1)} \rangle + \langle \phi_{2p}^{(Z-1)} | \frac{Z}{r} | \phi_{2p}^{(Z-1)} \rangle$$

By Virial  $\langle KE \rangle = -E_{2p}^{(Z-1)} = \frac{+(Z-1)^2}{8}$

$$\langle PE \rangle = \frac{+Z}{(Z-1)} \langle \phi_{2p}^{(Z-1)} | \frac{(Z-1)}{r} | \phi_{2p}^{(Z-1)} \rangle = \frac{Z(Z-1)}{4}$$

$$ZE_{2p}^{(Z-1)} = Z \frac{(Z-1)^2}{2(Z)^2}$$

Thus,

$$\langle H \rangle_{\pm} = -\frac{Z^2}{2} + \frac{(Z-1)^2}{8} - \frac{Z(Z-1)}{4} + \left\langle \frac{1}{r_{12}} \right\rangle_{\pm}$$

The first term is the  $\text{He}^+(1s)$  binding energy. The energy of the state relative to the first ionization threshold is

$$E_{\pm} = \frac{(Z-1)^2}{8} - \frac{Z(Z-1)}{4} + \left\langle \frac{1}{r_{12}} \right\rangle_{\pm} \quad (\text{au})$$

$$\text{Now } \left\langle \frac{1}{r_{12}} \right\rangle_{\pm} = \underbrace{\left\langle \phi_{1s}^{(1)} \phi_{2p}^{(2)} \left| \frac{1}{r_{12}} \right| \phi_{1s}^{(1)} \phi_{2p}^{(2)} \right\rangle}_{\equiv F \text{ (direct)}} + \underbrace{\left\langle \phi_{1s}^{(2)} \phi_{2p}^{(1)} \left| \frac{1}{r_{12}} \right| \phi_{1s}^{(1)} \phi_{2p}^{(2)} \right\rangle}_{\equiv G \text{ (exchange)}}$$

From Part (a)

$$F = \sum_k \frac{4\pi}{2k+1} \int dr_1 dr_2 \frac{r_2^k}{r_1^{k+1}} |u_{1s}^{(2)}(r_1)|^2 |u_{2p}^{(2)}(r_2)|^2 \int d\Omega Y_{00}^* Y_{k0} Y_{k0} Y_{00}$$

$$\int d\Omega Y_{10}^* Y_{k0} Y_{k0} Y_{10}$$

Only one  $k$  value satisfies the triangle inequality,  $k=0$   
 $Y_{00} = \frac{1}{\sqrt{4\pi}}$

$$\Rightarrow F = \int dr_1 dr_2 \frac{1}{r_1} |u_{1s}^{(2)}(r_1)|^2 |u_{2p}^{(2)}(r_2)|^2$$

$$= \frac{Z^3 (Z-1)^5}{6} \int dr_1 \int dr_2 \frac{1}{r_1} r_1^2 e^{-2Zr_1} r_2^4 e^{-(Z-1)r_2}$$

$$= \frac{Z^3 (Z-1)^5}{6} \int_0^{\infty} dr_2 r_2^4 e^{-(Z-1)r_2} \left\{ \frac{1}{r_1} \int_0^{r_2} dr_1 r_1^2 e^{-2Zr_1} + \int_{r_2}^{\infty} dr_1 r_1 e^{-2Zr_1} \right\}$$

$$\left\{ \frac{1}{4Z^3} r_2 (1 - e^{-2Zr_2}) - \frac{1}{4Z^2} e^{-2Zr_2} \right\}$$

$$= \frac{(Z-1)^5}{24} \int_0^{\infty} dr_2 \left( r_2^3 (e^{-(Z-1)r_2} - e^{-(3Z-1)r_2}) - Z r_2^4 e^{-(3Z-1)r_2} \right)$$

$$\Rightarrow F = \frac{Z-1}{4} - \frac{(Z-1)^5}{4(3Z-1)^4} - \frac{Z(Z-1)^5}{(3Z-1)^5} = \frac{Z-1}{4} - \frac{(Z-1)^5(7Z-1)}{4(3Z-1)^5}$$

The exchange term

$$G = \left\langle \phi_{1s}^{(1)} \phi_{2p}^{(2)} \left| \frac{1}{r_{12}} \right| \phi_{2p}^{(1)} \phi_{1s}^{(2)} \right\rangle$$

$$= \sum_k \frac{4\pi}{2k+1} \int dr_1 dr_2 u_{1s}(r_1) u_{2p}^{(2)}(r_2) u_{2p}^{(1)}(r_1) u_{1s}(r_2)$$

$$\int d\Omega_1 Y_{00}^*(1) Y_{k0}(1) Y_{l0}(1)$$

$$\int d\Omega_2 Y_{00}^*(2) Y_{k0}(2) Y_{l0}(2)$$

Here only  $k=1$ , each angular integral =  $\frac{1}{4\pi}$

$$\Rightarrow G = \frac{2Z^3(Z-1)^5}{18} \int_0^\infty dr_1 r_1^3 e^{-(3Z-1)r_1/2} \int_0^\infty dr_2 \frac{r_1}{r_2^2} r_2^3 e^{-(3Z-1)r_2/2}$$

by symmetry =  $\frac{2Z^3(Z-1)^5}{18} \int_0^\infty dr r^4 e^{-(3Z-1)r/2} \int_{r'}^\infty dr' r' e^{-(3Z-1)r'/2}$

$$= \frac{2Z^3(Z-1)^5}{18} \int_0^\infty dr r^4 e^{-(3Z-1)r/2} \left( \frac{2r}{3Z-1} + \frac{4}{(3Z-1)^2} \right) e^{-(3Z-1)r/2}$$

$$\Rightarrow G = \frac{112}{3} \frac{Z^3(Z-1)^5}{(3Z-1)^7}$$

$$E_{\pm} = -\frac{(Z-1)^2}{8} - \frac{(Z-1)^5}{4(3Z-1)^3} (7Z-1) \pm \frac{112}{3} \frac{Z^3(Z-1)^5}{(3Z-1)^7}$$

For He  $Z=2$ ,  $1 \text{ Hartree} = 2.1947 \times 10^5 \text{ cm}^{-1}$

$$E_+ = E_{2p} = -0.1222 \text{ au} = -26,819 \text{ cm}^{-1} \text{ for } 1p$$

$$E_- = E_{3p} = -0.1299 \text{ au} = -28,509 \text{ cm}^{-1} \text{ for } 3p$$

OK agreement  $\sim 1\% - 2\%$  of level energies  
 $10 - 20\%$  of splitting

(c) The splitting is twice the exchange interaction

$$1s 2p \xrightarrow{\downarrow \uparrow} \boxed{-26}$$

$$\Delta E = 26 = \frac{224}{3} \frac{Z^3}{(3Z-1)^2} * 2.195 \times 10^5 \text{ cm}^{-1}/\text{au}$$

Atom	$1p$ ( $\text{cm}^{-1}$ )	$\langle 3p \rangle$ ( $\text{cm}^{-1}$ )	$\Delta E_{\text{expt}}$ ( $\text{cm}^{-1}$ )	$\Delta E_{\text{theory}}$ ( $\text{cm}^{-1}$ )
H I	171,135	169,086	2047	1,690
Li II	501,809	499,266	7542	6,752
Be III	997,454	983,366	14,089	13,071
B IV	1,657,480	1,636,438	21,042	19,901
C V	2,483,372	2,455,169	28,203	26,960
N VI	3,473,790	3,438,320	35,470	34,151
O VII	4,629,201	4,585,680	43,521	41,921
F VIII	5,949,900	5,900,750	49,150	48,745

Better agreement as  $Z \rightarrow \infty$

Error due to single particle orbital choice



## Problem 2: Russell-Saunders Coupling of 3 equivalent p-electrons

Consider a configuration  $(np)^3$  as in Nitrogen

(a) For three equivalent p-electrons, there are

$$\frac{6 \cdot 5 \cdot 4}{3!} = 20 \text{ sublevels, consistent with the Pauli-exclusion principle}$$

We use the Slater technique of enumerating the possible  $M_L$  and  $M_S$  values, and then assigning to "Terms"

	$m_{l_1}$	$m_{l_2}$	$m_{l_3}$	$m_{s_1}$	$m_{s_2}$	$m_{s_3}$	$M_L$	$M_S$
1)	1	1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	2	$\frac{1}{2}$
2)	1	1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	2	$-\frac{1}{2}$
3)	1	1	-1	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	1	$\frac{1}{2}$
4)	1	1	-1	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$
5)	1	0	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	1	$\frac{1}{2}$
6)	1	0	0	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	1	$-\frac{1}{2}$
7)	1	0	-1	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{3}{2}$
8)	1	0	-1	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$\frac{1}{2}$
9)	1	0	-1	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$
10)	1	0	-1	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{1}{2}$
11)	1	0	-1	$-\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$
12)	1	0	-1	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{1}{2}$
13)	1	0	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$
14)	1	0	-1	$-\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	0	$-\frac{3}{2}$
15)	0	-1	0	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	-1	$\frac{1}{2}$
16)	0	-1	0	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	-1	$-\frac{1}{2}$
17)	-1	-1	+1	$\frac{1}{2}$	$-\frac{1}{2}$	$\frac{1}{2}$	-1	$\frac{1}{2}$
18)	-1	-1	+1	$\frac{1}{2}$	$-\frac{1}{2}$	$-\frac{1}{2}$	-1	$-\frac{1}{2}$
19)	0	-1	-1	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	-2	$\frac{1}{2}$
20)	0	-1	-1	$-\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{2}$	-2	$-\frac{1}{2}$

We now tabulate the number of possible sub-levels with total  $M_L$  and  $M_S$ , assign them to Terms, remove them, repeat, until all are assigned

$M_S \backslash M_L$	2	1	0		$M_S \backslash M_L$	1	0
$\frac{3}{2}$			1	$\Rightarrow$ $2D$ $(L=2)$ $S=\frac{1}{2}$	$\frac{3}{2}$		1
$\frac{1}{2}$	1	2	3		$\frac{1}{2}$	1	2

$\Rightarrow$	$M_S \backslash M_L$	1	0	$\Rightarrow$	No level left
$2P$			1	$4S$	
$(L=1)$			1	$(L=0)$	
$(S=\frac{1}{2})$				$(S=\frac{3}{2})$	

Thus the possible terms,  $2P, 2D, 4S$

The multiplets:  $2P_{1/2, 3/2}, 2D_{5/2, 3/2}, 4S_{3/2}$

(b) The  $4S_{3/2}$  state is one in which the spin is totally symmetric under exchange, whereas the spatial state is totally antisymmetric (lowest energy). To examine the nature of the wavefunction consider the sublevel with  $M_S = \frac{3}{2}$ . In this case all three electrons must have different  $m_l = 0, -1$  (case (7) in the Slater table)

We thus have as our orbital  $R_{n,2}(r) Y_{2,m}(\theta, \phi)$   $m = (0, -1)$

Recall  $Y_{1,0} \sim \frac{z}{r}$      $Y_{1,\pm 1} \sim \mp \frac{(x \pm iy)}{r}$

⇒ The spatial wave function is described by the Slater determinant

$$\bar{\Psi}(\vec{r}_1, \vec{r}_2, \vec{r}_3) = f(r_1)f(r_2)f(r_3) \begin{vmatrix} z_1 & -(x_1 + iy_1) & x_1 - iy_1 \\ z_2 & -(x_2 + iy_2) & x_2 - iy_2 \\ z_3 & -(x_3 + iy_3) & x_3 - iy_3 \end{vmatrix}$$

$$= f(r_1)f(r_2)f(r_3) \left[ z_1 (i x_2 y_3 - i x_3 y_2) + (x_1 + iy_1) \left( \begin{matrix} z_2 x_3 - z_3 x_2 \\ -i(z_2 y_3 - z_3 y_2) \end{matrix} \right) \right. \\ \left. - (x_1 - iy_1) (z_3 x_2 - z_2 x_3 - i(z_2 y_3 - z_3 y_2)) \right]$$

$$= -2i f(r_1)f(r_2)f(r_3) \left[ x_1 (y_2 z_3 - z_2 y_3) \right. \\ \left. + y_1 (z_2 x_3 - x_2 z_3) \right. \\ \left. + z_1 (x_2 y_3 - y_2 x_3) \right]$$

$$= \boxed{-2i f(r_1)f(r_2)f(r_3) \vec{r}_1 \cdot (\vec{r}_2 \times \vec{r}_3)}$$

The vector  $\vec{r}_1 \cdot (\vec{r}_2 \times \vec{r}_3)$  is a scalar under rotation of all vector ⇒  $L=0$ , and totally antisymmetric

Note: The sublevels of  ${}^4S_{3/2}$  with  $M_J = \pm 3/2$  are separable in orbit and spin.

For  $\{M_J = 3/2, \text{ the spin state is } |\uparrow\uparrow\uparrow\rangle\}$

$\{M_J = -3/2, \text{ the spin state is } |\downarrow\downarrow\downarrow\rangle\}$

The  $M_J = \pm 1/2$ , do not have unique spin states. They are entangled in space and spin.

(c) The term  ${}^2P_{3/2}$  has sublevels  $M_J = 3/2, 1/2, -1/2, -3/2$ .

The sublevel  $M_J = 3/2$  follows from the addition of angular momenta and exchange symmetry. From the Slater table, there are two sets of orbitals with  $M_L = 1, M_S = 1/2 \rightarrow M_J = 3/2$ , these are (3) + (5). From the table constructed in part (a)

$$P_{3/2, M_J = 3/2} = R_{np}(r_1) R_{np}(r_2) R_{np}(r_3)$$

$$+ C_1 \begin{bmatrix} Y_{10}(1) |\uparrow\rangle_1 & Y_{11}(1) |\downarrow\rangle_1 & Y_{1-1}(1) |\uparrow\rangle_1 \\ Y_{10}(2) |\uparrow\rangle_2 & Y_{11}(2) |\downarrow\rangle_2 & Y_{1-1}(2) |\uparrow\rangle_2 \\ Y_{10}(3) |\uparrow\rangle_3 & Y_{11}(3) |\downarrow\rangle_3 & Y_{1-1}(3) |\uparrow\rangle_3 \end{bmatrix}$$

$$+ C_2 \begin{bmatrix} Y_{11}(1) |\uparrow\rangle_1 & Y_{10}(1) |\uparrow\rangle_1 & Y_{10}(1) |\downarrow\rangle_1 \\ Y_{11}(2) |\uparrow\rangle_2 & Y_{10}(2) |\uparrow\rangle_2 & Y_{10}(2) |\downarrow\rangle_2 \\ Y_{11}(3) |\uparrow\rangle_3 & Y_{10}(3) |\uparrow\rangle_3 & Y_{10}(3) |\downarrow\rangle_3 \end{bmatrix}$$

To find the coefficients, let us first ignore exchange symmetry and construct a wave function from these orbitals with  $M_L = 1$ ,  $M_S = 1/2$ ,  $\Rightarrow M_J = 3/2$ .

We can do this by first adding together the orbital angular momentum of two p-electrons to get  $M_{L,2} = 0$  and then adding  $m_{l,3} = 1$ . This is the spatial wave function

$$\underbrace{f(r_1)f(r_2)f(r_3)}_{\text{radial wave function and factors}} \times \underbrace{(\vec{r}_1 \cdot \vec{r}_2)}_{\text{}} \times \underbrace{(x_3 + iy_3)}_{Y_{11}(3)}$$

$$\left[ \sum_{m=-1}^1 (-1)^m Y_{1,1}(1) Y_{1,m}(2) \right] Y_{11}(3)$$

A  $m_J = 1/2$  spin-state is obtained by adding two spins to form a singlet and then tensoring in a third

$$(|\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2) |\uparrow\rangle_3$$

The total wave function is then a product of space and spin, the anti-symmetrized over perturbations

$$\Psi(1,2,3) = \sum_P (-1)^P f(r_1)f(r_2)f(r_3) (\vec{r}_1 \cdot \vec{r}_2) (x_3 + iy_3) (|\uparrow_1 \downarrow_2 \uparrow_3\rangle - |\downarrow_1 \uparrow_2 \uparrow_3\rangle)$$

We see this as arising from the superposition of the two Slater determinants on the previous page with  $C_1 = 1$   $C_2 = -1$