

PHYS2581 Foundations2A: QM 8

The unperturbed wavefunctions of Hydrogen including spin are  $\psi_{n,l,m,m_s}^0 = R_{nl}Y_{lm}X_{\pm}$  where  $X_+$  (spin up) and  $X_-$  (spin down) are the common eigenfunctions of the spin operators  $S^2$  and  $S_z$  with eigenvalues  $s(s+1)\hbar^2 = \frac{3}{4}\hbar^2$  and  $m_s\hbar$  for  $m_s = \pm\frac{1}{2}$ . Similarly,  $Y_{lm}$  are the common eigenfunctions of  $L^2$  and  $L_z$  with eigenvalues  $l(l+1)\hbar^2$  and  $m\hbar$ , and  $\psi_{n,l,m,m_s}^0$  are the eigenfunctions of  $H^0$  with eigenvalues  $E_n$ .

Spin-orbit coupling in Hydrogen gives rise to a perturbation of  $H' \propto \underline{L} \cdot \underline{S}$  where  $\underline{L}$  and  $\underline{S}$  are the orbital and electron spin angular momentum operators, respectively.  $H^0$ ,  $L^2$ ,  $L_z$ ,  $S^2$  and  $S_z$  all commute with each other.

- (a)  $\underline{L} \cdot \underline{S} = L_x S_x + L_y S_y + L_z S_z$ . Show that this can be rewritten using the ladder operators  $L_{\pm} = L_x \pm iL_y$  and  $S_{\pm} = S_x \pm iS_y$  as  $\underline{L} \cdot \underline{S} = \frac{1}{2}(L_+ S_- + L_- S_+) + L_z S_z$  [2 marks]
- (b) Ladder operators raise and lower their associated angular momentum quantum number by unity, so  $S_- X_+ = a X_-$  and  $S_+ X_- = a X_+$  where  $a = \hbar/\sqrt{2}$ , and  $L_{\pm} Y_{lm} = A_{lm\pm} Y_{l,m\pm 1}$  where  $A_{lm\pm} = \hbar\sqrt{l(l+1) - m(m\pm 1)}$ . All angular momenta have a maximum value beyond which the upwards ladder operator gives zero, and a minimum below which the downwards ladder operator gives zero.

Use this together with the definition of  $\underline{L} \cdot \underline{S}$  in terms of ladder operators in (b) above to show that

$$\underline{L} \cdot \underline{S} \psi_{2,1,-1,1/2}^0 = \frac{\hbar^2}{2} (\psi_{2,1,0,-1/2}^0 - \psi_{2,1,-1,1/2}^0)$$

Are the unperturbed energy eigenfunctions of Hydrogen also eigenfunctions of  $\underline{L} \cdot \underline{S}$ ? [5 marks]

- (c) Use  $\underline{L} \cdot \underline{S} = L_x S_x + L_y S_y + L_z S_z$ , together with the the standard commutation relations for any general angular momenta  $[J_x, J_y] = i\hbar J_z$ ,  $[J_y, J_z] = i\hbar J_x$ ,  $[J_z, J_x] = i\hbar J_y$ , (i.e. these relations hold for the components of  $\underline{L}$  and  $\underline{S}$  as well as  $\underline{J}$ ) to show that  $[\underline{L} \cdot \underline{S}, L_z] \neq 0$  and  $[\underline{L} \cdot \underline{S}, S_z] \neq 0$  but that  $[\underline{L} \cdot \underline{S}, J_z] = [\underline{L} \cdot \underline{S}, L_z + S_z] = 0$ .

Which set of quantum numbers allow the effect of the perturbation to be calculated using non-degenerate perturbation theory? [3 marks]