11. Considere a transição $E_2 \rightarrow E_1$ para o átomo de hidrogénio. Por razões ainda não consideradas, o estado 2s não contribui para esta transição. Portanto, apenas os três estados 2p são relevantes. O comprimento de onda desta transição é igual a 122 nanometros.
Num campo magnético as energias ligantes do electrão nos estados 2p, alteram-se de forma diferente para cada estado.

a Mostre que no modelo semi-clássico o momento magnético $\vec{\mu}_{\text{mag}}$ do electrão (aqui representado pela sua massa reduzida μ_{e} e pela sua carga eléctrica $-e$) na sua órbita (representada pelo momento angular orbital $\vec{L}_{\text{int}}$), é igual a

$$\vec{\mu}_{\text{mag}} = -\frac{e}{2\mu_{\text{e}}}\vec{L}_{\text{int}} \quad .$$

A quantidade $-e/(2m_{\text{e}})$, que apenas envolve a carga eléctrica e a massa do electrão, chama-se *razão giromagnética* do electrão.

b Suponhamos que a mudança de energia ligante do electrão ΔE devida a um campo magnético fraco de intensidade B é caracterizada por

$$\Delta E = m\frac{e\hbar}{2\mu_{\text{e}}}B \quad ,$$

onde m representa o número quântico magnético do estado.
Calcula as mudanças dos comprimentos de onda (o efeito de Zeeman, 1896, prémio Nobel 1902) das três transições $E_2 \rightarrow E_1$ num campo magnético com intensidade de 1000 T (Tesla).
A quantidade $e\hbar/(2m_{\text{e}})$ chama-se *magnetão de Bohr* e tem um valor igual a 9.27×10^{-24} J/T = 5.79 $\times10^{-5}$ eV/T.

Solution:

a. The magnetic moment of a planar loop of electric current is defined as

$$\vec{\mu} = I\vec{a} \quad .$$

where $\vec{\mu}$ is the magnetic moment, a vector measured in joules per tesla, $\vec{a}$ is the vector area of the current loop, and I is the current in the loop (assumed to be constant).
By convention, the direction of the vector area is given by the right hand grip rule: curling the fingers of one's right hand in the direction of the current around the loop, when the palm of the hand is "touching" the loop's outer edge, and the straight thumb indicates the direction of the vector area and thus of the magnetic moment.

The current I equals the amount of charge that passes per second at any point of the electron's orbit. If the electron has velocity v (in distance per second) and the circular orbit has radius r, then the electron passes $v/2\pi r$ times per second at any point of the orbit. The electron carries charge $-e$. Consequently, at any point of the orbit passes $-ev/2\pi r$ charge:

$$I = \frac{-ev}{2\pi r} \quad .$$

The area which is enclosed by the circular orbit is given by πr^2. Hence, the orbital magnetic moment of the electron equals

$$\mu_{\text{mag}} = I \times \text{area} = \frac{-ev}{2\pi r} \times \pi r^2 = -\frac{1}{2}\,evr \quad .$$

The angular momentum of the electron with respect to the center of the orbit equals $L_{\text{int}} = \mu_{\text{e}} rv$ and points in the direction of the area vector $\vec{a}$. Hence,

$$\vec{\mu}_{\text{mag}} \;=\; -\frac{e}{2\mu_{\text{e}}}\vec{L}_{\text{int}} \quad .$$

b. For $B = 1000$ T, we must determine

$$\frac{e\hbar}{2\mu_{\text{e}}}B = \left(5.79 \times 10^{-5}\ \text{ eV/T}\right) \times \left(10^3\ \text{ T}\right) = 5.79 \times 10^{-2}\ \text{ eV} \quad .$$

Moreover, we need to know

$$hc = \left(4.1356673 \times 10^{-15}\ \text{ eVs}\right) \times \left(2.99792458 \times 10^{17}\ \text{ nm/s}\right) = 1.239841874 \times 10^3\ \text{ eV nm} \quad .$$

Furthermore, 122 nm corresponds to

$$E_2 - E_1 = hf = \frac{hc}{\lambda} = \frac{1.239841874 \times 10^3\ \text{ eV nm}}{122\ \text{ nm}} = 10.16\ \text{ eV} \quad .$$

Hence, the contribution of the interaction with the magnetic field yields 5.79/10.16%= 0.57% difference per unit magnetic quantum number.
For $m = 1$ the available energy is 0.57% more, hence, since energy and wave length are inversely proportional, the wave length 0.57% of 122 nm less, *i.e.* 0.7 nm less.
For $m = -1$ the available energy is 0.57% less, hence the wave length 0.57% of 122 nm more, *i.e.* 0.7 nm more.
For $m = 0$ the contribution of the interaction with the magnetic field equals zero. Consequently, the available energy is the same, hence the wave length equals 122 nm.

12. As soluções próprias $|n,\ell,m\rangle$ do Hamiltoniano com o potencial Coulombiano, dado por

$$H \;=\; \frac{p^2}{2\mu_e} \;+\; V_C(r) \quad ,$$

são simultaneamente as funções próprias do quadrado e da componente zz do momento angular orbital:

$$L^2|n,\ell,m\rangle \;=\; \hbar^2\ell(\ell+1)|n,\ell,m\rangle \quad \text{e} \quad L_z|n,\ell,m\rangle \;=\; \hbar m|n,\ell,m\rangle \quad .$$

Isto é uma consequência da seguinte propriedade

$$\left[H \;,\; \vec{L}\right] \;=\; H\,\vec{L} - \vec{L}\,H \;=\; 0 \quad . \tag{1}$$

O momento linear $\vec{p}$ representa-se pelo operador

$$\vec{p} \;=\; (p_x,\, p_y,\, p_z) \;=\; -i\hbar\left(\frac{\partial}{\partial x},\, \frac{\partial}{\partial y},\, \frac{\partial}{\partial z}\right) \quad ,$$

o momento angular orbital $\vec{L}$ pelo operador $\vec{r}\times\vec{p}$, enquanto $r = \sqrt{x^2+y^2+z^2}$ representa a distância relativa entre o protão e o electrão.
Mostra que:

a

$$[p_x \;,\; L_z] \;=\; -i\hbar p_y \quad , \quad [p_y \;,\; L_z] \;=\; i\hbar p_x \quad \text{e} \quad [p_z \;,\; L_z] \;=\; 0 \quad .$$

b

$$\left[p_x^2 \;,\; L_z\right] \;=\; -2i\hbar p_x p_y \quad , \quad \left[p_y^2 \;,\; L_z\right] \;=\; 2i\hbar p_x p_y \quad \text{e} \quad \left[p_z^2 \;,\; L_z\right] \;=\; 0 \quad .$$

c

$$\left[p^2 \;,\; L_z\right] \;=\; 0 \quad \text{e} \quad [V_C(r) \;,\; L_z] \;=\; 0 \quad .$$

Portanto, verifica-se a relação (1) para a componente L_z.

Solution:

We use $[p_x \;,\; x] = -i\hbar$, $[p_y \;,\; y] = -i\hbar$, $[p_z \;,\; z] = -i\hbar$, $[p_x \;,\; y] = 0$, $[p_x \;,\; z] = 0$, $[p_y \;,\; x] = 0$, $[p_y \;,\; z] = 0$, $[p_z \;,\; x] = 0$ and $[p_z \;,\; y] = 0$. This is summarised in the following table.

$[\vec{p} \;,\; \vec{r}]$	x	y	z
p_x	$-i\hbar$	0	0
p_y	0	$-i\hbar$	0
p_z	0	0	$-i\hbar$

Furthermore,

$$L_z \; = \; [\vec{r} \times \vec{p}]_z \; = \; x p_y - y p_x$$

a.

$$[p_x \; , \; L_z] \; = \; [p_x \; , \; x p_y - y p_x] \; =$$

$$= \; [p_x \; , \; x p_y] - [p_x \; , \; y p_x] = x \, [p_x \; , \; p_y] + [p_x \; , \; x] \, p_y - y \, [p_x \; , \; p_x] - [p_x \; , \; y] \, p_x$$

$$= \; 0 - i\hbar p_y + 0 + 0 = -i\hbar p_y \quad ,$$

$$[p_y \; , \; L_z] \; = \; [p_y \; , \; x p_y - y p_x] \; =$$

$$= \; [p_y \; , \; x p_y] - [p_y \; , \; y p_x] = x \, [p_y \; , \; p_y] + [p_y \; , \; x] \, p_y - y \, [p_y \; , \; p_x] - [p_y \; , \; y] \, p_x$$

$$= \; 0 + 0 + 0 + i\hbar p_x = i\hbar p_x \quad ,$$

and

$$[p_z \; , \; L_z] \; = \; [p_z \; , \; x p_y - y p_x] \; =$$

$$= \; [p_z \; , \; x p_y] - [p_z \; , \; y p_x] = x \, [p_z \; , \; p_y] + [p_z \; , \; x] \, p_y - y \, [p_z \; , \; p_x] - [p_z \; , \; y] \, p_x$$

$$= \; 0 + 0 + 0 + 0 = 0 \quad .$$

b.

$$\left[p_x^2 \; , \; L_z\right] = p_x \, [p_x \; , \; L_z] + [p_x \; , \; L_z] \, p_x = p_x \, (-i\hbar p_y) + (-i\hbar p_y) \, p_x = -2i\hbar p_x p_y \quad ,$$

$$\left[p_y^2 \; , \; L_z\right] = p_y \, [p_y \; , \; L_z] + [p_y \; , \; L_z] \, p_y = p_y \, (i\hbar p_x) + (i\hbar p_x) \, p_y = 2i\hbar p_x p_y \quad ,$$

and

$$\left[p_z^2 \; , \; L_z\right] = p_z \, [p_z \; , \; L_z] + [p_z \; , \; L_z] \, p_z = p_z \, (0) + (0) \, p_z = 0 \quad .$$

c.

$$\left[p^2 \; , \; L_z\right] \; = \; \left[p_x^2 + p_y^2 + p_z^2 \; , \; L_z\right] =$$

$$= \; \left[p_x^2 \; , \; L_z\right] + \left[p_y^2 \; , \; L_z\right] + \left[p_z^2 \; , \; L_z\right] = -2i\hbar p_x p_y + 2i\hbar p_x p_y + 0 = 0 \quad .$$

Furthermore, in polar coordinates $L_z = -i\hbar\partial/\partial\varphi$. Hence, any function which does not depend on φ commutes with L_z.
But, it can also be shown in a straightforward manner that L_z commutes with $V_C(r)$ as we will see below.
First regard the following.

$$\frac{\partial V_C(r)}{\partial x} = \frac{\partial r}{\partial x} \, \frac{dV_C(r)}{dr} = \frac{x}{r} \, \frac{dV_C(r)}{dr} \quad .$$

We find then

$$[V_C(r)\ ,\ p_x] = \left[V_C(r)\ ,\ -i\hbar\frac{\partial}{\partial x}\right] =$$

$$= -i\hbar V_C(r)\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}V_C(r) = -i\hbar V_C(r)\frac{\partial}{\partial x} + i\hbar\frac{\partial V_C(r)}{\partial x} + i\hbar V_C(r)\frac{\partial}{\partial x}$$

$$= i\hbar\frac{\partial V_C(r)}{\partial x} = i\hbar\frac{x}{r}\ \frac{dV_C(r)}{dr} \quad .$$

Similarly

$$[V_C(r)\ ,\ p_y] = i\hbar\frac{y}{r}\ \frac{dV_C(r)}{dr} \quad .$$

We obtain then

$$[V_C(r)\ ,\ L_z] \;=\; [V_C(r)\ ,\ xp_y - yp_x] =$$

$$= [V_C(r)\ ,\ xp_y] - [V_C(r)\ ,\ yp_x]$$

$$= x\,[V_C(r)\ ,\ p_y] + [V_C(r)\ ,\ x]\,p_y - y\,[V_C(r)\ ,\ p_x] - [V_C(r)\ ,\ y]\,p_x$$

$$= xi\hbar\frac{y}{r}\ \frac{dV_C(r)}{dr} + 0 - yi\hbar\frac{x}{r}\ \frac{dV_C(r)}{dr} + 0 = 0 \quad .$$

We may thus conclude

$$[H\ ,\ L_z] = \left[\frac{p^2}{2\mu_e} + V_C(r)\ ,\ L_z\right] = \frac{1}{2\mu_e}\left[p^2\ ,\ L_z\right] + [V_C(r)\ ,\ L_z] = 0 \quad .$$

We may repeat all steps for L_x and L_y to find that they also commute with H.

In problem (14) we show that $[L_x\ ,\ L_y] = i\hbar L_z$, $[L_y\ ,\ L_z] = i\hbar L_x$ and $[L_z\ ,\ L_x] = i\hbar L_y$. This gives

$$\left[L_x^2\ ,\ L_z\right] = L_x\,[L_x\ ,\ L_z] + [L_x\ ,\ L_z]\,L_x = -i\hbar L_xL_y - i\hbar L_yL_x \quad .$$

$$\left[L_y^2\ ,\ L_z\right] = L_y\,[L_y\ ,\ L_z] + [L_y\ ,\ L_z]\,L_y = i\hbar L_yL_x + i\hbar L_xL_y \quad .$$

$$\left[L_z^2\ ,\ L_z\right] = L_z\,[L_z\ ,\ L_z] + [L_z\ ,\ L_z]\,L_z = 0 + 0 = 0 \quad .$$

Hence,

$$\left[L^2\ ,\ L_z\right] = \left[L_x^2 + L_y^2 + L_z^2\ ,\ L_z\right] =$$

$$= \left[L_x^2\ ,\ L_z\right] + \left[L_y^2\ ,\ L_z\right] + \left[L_z^2\ ,\ L_z\right]$$

$$= -i\hbar L_xL_y - i\hbar L_yL_x + i\hbar L_yL_x + i\hbar L_xL_y + 0 = 0 \quad .$$

Thus, if we consider the operators H, L_x, L_y, L_z and L^2, then we found in the above that the maximum sets of commuting operators are given by $\{H, L^2, L_z\}$, or also $\{H, L^2, L_x\}$ or $\{H, L^2, L_y\}$. It is common practice to select the first of those sets to classify the solutions for hydrogen. They are then simultaneously eigenstates of H, with eigenvalue E_n, of L^2, with eigenvalue $\hbar^2\ell(\ell+1)$, and of L_z, with eigenvalue $\hbar m$.
This is denoted by $|n, \ell, m\rangle$.

13. Além da sua posição, indicada por $\vec{r} = (r, \vartheta, \varphi)$, um electrão tem outro grau de liberdade: o seu *spin*. Num campo magnético há duas orientações diferentes possíveis para o spin do electrão. Se o campo magnético é orientado ao longo do eixo dos zz, os dois possíveis estados do electrão são indicados por

$$\left|+\tfrac{1}{2}\right\rangle = \left|s_z = +\tfrac{1}{2}\right\rangle \quad \text{e} \quad \left|-\tfrac{1}{2}\right\rangle = \left|s_z = -\tfrac{1}{2}\right\rangle \quad .$$

Os operadores associados com os observaveis do spin do electrão são designados por $\vec{S} = (S_x, S_y, S_z)$, com as seguintes propriedades.

$$\begin{aligned} S_x\left|+\tfrac{1}{2}\right\rangle &= \frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle \quad , \quad S_x\left|-\tfrac{1}{2}\right\rangle = \frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle \\ S_y\left|+\tfrac{1}{2}\right\rangle &= i\frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle \quad , \quad S_y\left|-\tfrac{1}{2}\right\rangle = -i\frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle \\ S_z\left|+\tfrac{1}{2}\right\rangle &= \frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle \quad , \quad S_z\left|-\tfrac{1}{2}\right\rangle = -\frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle \quad . \end{aligned}$$

a Numa representação matricial, onde os dois estados do spin do electrão são representados pelos vectores

$$\left|+\tfrac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{e} \quad \left|-\tfrac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad ,$$

determina as matrizes que representam os operadores S_x, S_y e S_z (*as matrizes de Pauli*, inventadas por Wolfgang Pauli).

b Determina a matriz que representa $S^2 = S_x^2 + S_y^2 + S_z^2$.

c Determina como actuam os operadores de *subida*, $S_+ = S_x + iS_y$, e de *descida*, $S_- = S_x - iS_y$, nos dois estados do spin do electrão.

d Determina os comutadores $[S_x\ ,\ S_y]$, $[S_y\ ,\ S_z]$ e $[S_z\ ,\ S_x]$.

Solution:

a. S_x, S_y, S_z, must here be represented by 2×2 matrices, say

$$S_x = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \quad , \quad S_y = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix} \quad , \quad S_z = \begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix} \quad .$$

We obtain then

$$\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle = S_x\left|+\tfrac{1}{2}\right\rangle = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} x_{11} \\ x_{21} \end{pmatrix} \quad ,$$

from which we may conclude

$$x_{11} = 0 \quad \text{and} \quad x_{21} = \frac{\hbar}{2} \quad .$$

Similarly

$$\frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle = S_x\left|-\tfrac{1}{2}\right\rangle = \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} x_{12} \\ x_{22} \end{pmatrix} \quad ,$$

from which we may conclude

$$x_{12} = \frac{\hbar}{2} \quad \text{and} \quad x_{22} = 0 \quad .$$

Also

$$i\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = i\frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle = S_y\left|+\tfrac{1}{2}\right\rangle = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} y_{11} \\ y_{21} \end{pmatrix} \quad ,$$

from which we may conclude

$$y_{11} = 0 \quad \text{and} \quad y_{21} = i\frac{\hbar}{2} \quad .$$

Moreover,

$$-i\frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -i\frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle = S_y\left|-\tfrac{1}{2}\right\rangle = \begin{pmatrix} y_{11} & y_{12} \\ y_{21} & y_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} y_{12} \\ y_{22} \end{pmatrix} \quad ,$$

from which we may conclude

$$y_{12} = -i\frac{\hbar}{2} \quad \text{and} \quad y_{22} = 0 \quad .$$

Finally,

$$\frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\left|+\tfrac{1}{2}\right\rangle = S_z\left|+\tfrac{1}{2}\right\rangle = \begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} z_{11} \\ z_{21} \end{pmatrix} \quad ,$$

from which we may conclude

$$z_{11} = \frac{\hbar}{2} \quad \text{and} \quad z_{21} = 0 \quad ,$$

and

$$-\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\left|-\tfrac{1}{2}\right\rangle = S_z\left|-\tfrac{1}{2}\right\rangle = \begin{pmatrix} z_{11} & z_{12} \\ z_{21} & z_{22} \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} z_{12} \\ z_{22} \end{pmatrix} \quad ,$$

from which we may conclude

$$z_{12} = 0 \quad \text{and} \quad z_{22} = -\frac{\hbar}{2} \quad .$$

Hence, the Pauli matrices are given by

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad , \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad .$$

Note that $\left|+\tfrac{1}{2}\right\rangle$ and $\left|-\tfrac{1}{2}\right\rangle$ are eigenstates of S_z with eigenvalues $\hbar/2$ and $-\hbar/2$ respectively.

b.

$$S_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad S_y^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad S_z^2 = \frac{\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad .$$

Hence,

$$S^2 = S_x^2 + S_y^2 + S_z^2 = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad .$$

Note that $\frac{3}{4} = s(s+1)$ with $s = \frac{1}{2}$.

c. The raising S_+ and lowering S_- operators are defined by

$$S_+ = S_x + iS_y = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + i\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad ,$$

and

$$S_- = S_x - iS_y = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - i\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad .$$

Hence,

$$S_+\left|+\tfrac{1}{2}\right\rangle = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0 \quad ,$$

$$S_+\left|-\tfrac{1}{2}\right\rangle = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\left|+\tfrac{1}{2}\right\rangle \quad ,$$

$$S_-\left|+\tfrac{1}{2}\right\rangle = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\left|-\tfrac{1}{2}\right\rangle \quad \text{and}$$

$$S_-\left|-\tfrac{1}{2}\right\rangle = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0 \quad .$$

Note that this is very much the same as the operation of the raising L_+ and lowering L_- operators on the sperical harmonics (see problem 7). Here we have

$\lvert m_s\rangle$	s	m_s	raising S_+	lowering S_-
$\left\lvert+\frac{1}{2}\right\rangle$	$\frac{1}{2}$	$+\frac{1}{2}$	0	$\hbar\left\lvert-\frac{1}{2}\right\rangle$
$\left\lvert-\frac{1}{2}\right\rangle$	$\frac{1}{2}$	$-\frac{1}{2}$	$\hbar\left\lvert+\frac{1}{2}\right\rangle$	0

d.

$$[S_x\ ,\ S_y] = S_xS_y - S_yS_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} =$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = i\frac{\hbar^2}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i\hbar S_z \quad .$$

$$[S_y\ ,\ S_z] = S_yS_z - S_zS_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} =$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 0 & 2i \\ 2i & 0 \end{pmatrix} = i\frac{\hbar^2}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = i\hbar S_x \quad .$$

$$[S_z\ ,\ S_x] = S_zS_x - S_xS_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} =$$

$$= \frac{\hbar^2}{4}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} - \frac{\hbar^2}{4}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} = i\frac{\hbar^2}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = i\hbar S_y \quad .$$

Note that the above relations are exactly the same as for the three components of the angular momentum operator $\vec{L}$ (see Problem 14a).

14. O momento linear $\vec{p}$ representa-se pelo operador

$$\vec{p} = (p_x, p_y, p_z) = -i\hbar \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \quad ,$$

o momento angular orbital $\vec{L}$ pelo operador $\vec{r} \times \vec{p}$, enquanto $r = \sqrt{x^2 + y^2 + z^2}$ representa a distância relativa entre o protão e o electrão.
O operador $\vec{S}$ (definido no problema 13) está relacionado com a rotação interna do electrão e consequentemente é independente do movimento orbital do electrão. Portanto, considera-se que (observáveis independentes)

$$\left[\vec{L} \ , \ \vec{S} \right] = 0 \quad .$$

a Determina os comutadores $[L_x \ , \ L_y]$, $[L_y \ , \ L_z]$ e $[L_z \ , \ L_x]$.

b Para $\vec{L} \cdot \vec{S} = L_x S_x + L_y S_y + L_z S_z$, determina os comutadores $\left[\vec{L} \cdot \vec{S} \ , \ L_x \right]$, $\left[\vec{L} \cdot \vec{S} \ , \ L_y \right]$, $\left[\vec{L} \cdot \vec{S} \ , \ L_z \right]$, $\left[\vec{L} \cdot \vec{S} \ , \ S_x \right]$, $\left[\vec{L} \cdot \vec{S} \ , \ S_y \right]$ e $\left[\vec{L} \cdot \vec{S} \ , \ S_z \right]$.

c Determina os comutadores $\left[\vec{L} \cdot \vec{S} \ , \ L^2 \right]$ e $\left[\vec{L} \cdot \vec{S} \ , \ S^2 \right]$.

Solution:

We use $[p_x \ , \ x] = -i\hbar$, $[p_y \ , \ y] = -i\hbar$, $[p_z \ , \ z] = -i\hbar$, $[p_x \ , \ y] = 0$, $[p_x \ , \ z] = 0$, $[p_y \ , \ x] = 0$, $[p_y \ , \ z] = 0$, $[p_z \ , \ x] = 0$ and $[p_z \ , \ y] = 0$.

a:

$$\begin{aligned} L_x &= [\vec{r} \times \vec{p}]_x = yp_z - zp_y \\ L_y &= [\vec{r} \times \vec{p}]_y = zp_x - xp_z \\ L_z &= [\vec{r} \times \vec{p}]_z = xp_y - yp_x \end{aligned}$$

Hence,

$[L_x \ , \ L_y] = [yp_z - zp_y \ , \ zp_x - xp_z] =$

$$= (yp_z - zp_y)(zp_x - xp_z) - (zp_x - xp_z)(yp_z - zp_y)$$

$$= yp_z zp_x - yp_z xp_z - zp_y zp_x + zp_y xp_z - zp_x yp_z + zp_x zp_y + xp_z yp_z - xp_z zp_y$$

$$= y(-i\hbar + zp_z)p_x - yxp_z p_z - z^2 p_y p_x + zxp_y p_z - zyp_x p_z + z^2 p_x p_y + xyp_z p_z - x(-i\hbar + zp_z)p_y$$

$$= -i\hbar(yp_x - xp_y) = i\hbar L_z$$

$[L_y \ , \ L_z] = [zp_x - xp_z \ , \ xp_y - yp_x] =$

$$= \; (zp_x - xp_z)\,(xp_y - yp_x) \; - \; (xp_y - yp_x)\,(zp_x - xp_z)$$

$$= \; zp_x xp_y - zp_x yp_x - xp_z xp_y + xp_z yp_x - xp_y zp_x + xp_y xp_z + yp_x zp_x - yp_x xp_z$$

$$= \; z(-i\hbar + xp_x)p_y - zyp_xp_x - x^2p_zp_y + xyp_zp_x - xzp_yp_x + x^2p_yp_z + yzp_xp_x - y(-i\hbar + xp_x)p_z$$

$$= \; i\hbar(yp_z - zp_y) = i\hbar L_x$$

$$[L_z\ ,\ L_x] = [xp_y - yp_x\ ,\ yp_z - zp_y] \; =$$

$$= \; (xp_y - yp_x)\,(yp_z - zp_y) \; - \; (yp_z - zp_y)\,(xp_y - yp_x)$$

$$= \; xp_y yp_z - xp_y zp_y - yp_x yp_z + yp_x zp_y - yp_z xp_y + yp_z yp_x + zp_y xp_y - zp_y yp_x$$

$$= \; x(-i\hbar + yp_y)p_z - xzp_yp_y - y^2p_xp_z + yzp_xp_y - yxp_zp_y + y^2p_zp_x + zxp_yp_y - z(-i\hbar + yp_y)p_x$$

$$= \; i\hbar(zp_x - xp_z) = i\hbar L_y$$

b:

$$\left[\vec{L}\cdot\vec{S}\ ,\ L_x\right] = [L_xS_x + L_yS_y + L_zS_z\ ,\ L_x] \; =$$

$$= \; [L_xS_x\ ,\ L_x] + [L_yS_y\ ,\ L_x] + [L_zS_z\ ,\ L_x]$$

$$= \; L_x\,[S_x\ ,\ L_x] + [L_x\ ,\ L_x]\,S_x + L_y\,[S_y\ ,\ L_x] + [L_y\ ,\ L_x]\,S_y + L_z\,[S_z\ ,\ L_x] + [L_z\ ,\ L_x]\,S_z$$

$$= \; 0 + 0 + 0 - i\hbar L_zS_y + 0 + i\hbar L_yS_z \; = \; i\hbar\left[\vec{L}\times\vec{S}\right]_x$$

$$\left[\vec{L}\cdot\vec{S}\ ,\ L_y\right] = [L_xS_x + L_yS_y + L_zS_z\ ,\ L_y] \; =$$

$$= \; [L_xS_x\ ,\ L_y] + [L_yS_y\ ,\ L_y] + [L_zS_z\ ,\ L_y]$$

$$= \; L_x\,[S_x\ ,\ L_y] + [L_x\ ,\ L_y]\,S_x + L_y\,[S_y\ ,\ L_y] + [L_y\ ,\ L_y]\,S_y + L_z\,[S_z\ ,\ L_y] + [L_z\ ,\ L_y]\,S_z$$

$$= \; 0 + i\hbar L_zS_x + 0 + 0 + 0 - i\hbar L_xS_z \; = \; i\hbar\left[\vec{L}\times\vec{S}\right]_y$$

$$\left[\vec{L}\cdot\vec{S}\ ,\ L_z\right] = [L_xS_x + L_yS_y + L_zS_z\ ,\ L_z] \; =$$

$$= \; [L_xS_x\ ,\ L_z] + [L_yS_y\ ,\ L_z] + [L_zS_z\ ,\ L_z]$$

$$= \; L_x\,[S_x\ ,\ L_z] + [L_x\ ,\ L_z]\,S_x + L_y\,[S_y\ ,\ L_z] + [L_y\ ,\ L_z]\,S_y + L_z\,[S_z\ ,\ L_z] + [L_z\ ,\ L_z]\,S_z$$

$$= \; 0 - i\hbar L_yS_x + 0 + i\hbar L_xS_z + 0 + 0 \; = \; i\hbar\left[\vec{L}\times\vec{S}\right]_z$$

Consequently

$$\left[\vec{L}\cdot\vec{S}\ ,\ \vec{L}\right] \; = \; i\hbar\vec{L}\times\vec{S} \quad .$$

Furthermore

$$\left[\vec{L}\cdot\vec{S}\ ,\ S_x\right] = \left[L_xS_x + L_yS_y + L_zS_z\ ,\ S_x\right]\ =$$

$$=\ \left[L_xS_x\ ,\ S_x\right] + \left[L_yS_y\ ,\ S_x\right] + \left[L_zS_z\ ,\ S_x\right]$$

$$=\ L_x\left[S_x\ ,\ S_x\right] + \left[L_x\ ,\ S_x\right]S_x + L_y\left[S_y\ ,\ S_x\right] + \left[L_y\ ,\ S_x\right]S_y + L_z\left[S_z\ ,\ S_x\right] + \left[L_z\ ,\ S_x\right]S_z$$

$$=\ 0 + 0 - i\hbar L_yS_z + 0 + i\hbar L_zS_y + 0\ =\ -i\hbar\left[\vec{L}\times\vec{S}\right]_x$$

$$\left[\vec{L}\cdot\vec{S}\ ,\ S_y\right] = \left[L_xS_x + L_yS_y + L_zS_z\ ,\ S_y\right]\ =$$

$$=\ \left[L_xS_x\ ,\ S_y\right] + \left[L_yS_y\ ,\ S_y\right] + \left[L_zS_z\ ,\ S_y\right]$$

$$=\ L_x\left[S_x\ ,\ S_y\right] + \left[L_x\ ,\ S_y\right]S_x + L_y\left[S_y\ ,\ S_y\right] + \left[L_y\ ,\ S_y\right]S_y + L_z\left[S_z\ ,\ S_y\right] + \left[L_z\ ,\ S_y\right]S_z$$

$$=\ i\hbar L_xS_z + 0 + 0 + 0 - i\hbar L_zS_x + 0\ =\ -i\hbar\left[\vec{L}\times\vec{S}\right]_y$$

$$\left[\vec{L}\cdot\vec{S}\ ,\ S_z\right] = \left[L_xS_x + L_yS_y + L_zS_z\ ,\ S_z\right]\ =$$

$$=\ \left[L_xS_x\ ,\ S_z\right] + \left[L_yS_y\ ,\ S_z\right] + \left[L_zS_z\ ,\ S_z\right]$$

$$=\ L_x\left[S_x\ ,\ S_z\right] + \left[L_x\ ,\ S_z\right]S_x + L_y\left[S_y\ ,\ S_z\right] + \left[L_y\ ,\ S_z\right]S_y + L_z\left[S_z\ ,\ S_z\right] + \left[L_z\ ,\ S_z\right]S_z$$

$$=\ -i\hbar L_xS_y + 0 + i\hbar L_yS_x + 0 + 0 + 0\ =\ -i\hbar\left[\vec{L}\times\vec{S}\right]_z$$

Consequently

$$\left[\vec{L}\cdot\vec{S}\ ,\ \vec{S}\right]\ =\ -i\hbar\vec{L}\times\vec{S}\quad .$$

c:

$$\left[\vec{L}\cdot\vec{S}\ ,\ \vec{L}^{\,2}\right] = \left[\vec{L}\cdot\vec{S}\ ,\ L_x^2 + L_y^2 + L_z^2\right]$$

$$=\ \left[\vec{L}\cdot\vec{S}\ ,\ L_x^2\right] + \left[\vec{L}\cdot\vec{S}\ ,\ L_y^2\right] + \left[\vec{L}\cdot\vec{S}\ ,\ L_z^2\right]$$

$$=\ L_x\left[\vec{L}\cdot\vec{S}\ ,\ L_x\right] + \left[\vec{L}\cdot\vec{S}\ ,\ L_x\right]L_x + L_y\left[\vec{L}\cdot\vec{S}\ ,\ L_y\right] + \left[\vec{L}\cdot\vec{S}\ ,\ L_y\right]L_y$$
$$+L_z\left[\vec{L}\cdot\vec{S}\ ,\ L_z\right] + \left[\vec{L}\cdot\vec{S}\ ,\ L_z\right]L_z$$

$$=\ L_xi\hbar\left[\vec{L}\times\vec{S}\right]_x + i\hbar\left[\vec{L}\times\vec{S}\right]_xL_x + L_yi\hbar\left[\vec{L}\times\vec{S}\right]_y + i\hbar\left[\vec{L}\times\vec{S}\right]_yL_y$$
$$+L_zi\hbar\left[\vec{L}\times\vec{S}\right]_z + i\hbar\left[\vec{L}\times\vec{S}\right]_zL_z$$

$$=\ L_xi\hbar\left[\vec{L}\times\vec{S}\right]_x + L_yi\hbar\left[\vec{L}\times\vec{S}\right]_y + L_zi\hbar\left[\vec{L}\times\vec{S}\right]_z$$

$$+i\hbar\left[\vec{L}\times\vec{S}\right]_x L_x + i\hbar\left[\vec{L}\times\vec{S}\right]_y L_y + i\hbar\left[\vec{L}\times\vec{S}\right]_z L_z$$

$$= \; i\hbar\vec{L}\cdot\left[\vec{L}\times\vec{S}\right] \; + \; i\hbar\left[\vec{L}\times\vec{S}\right]\cdot\vec{L} \; = \; 0 \quad .$$

The last step follows because $\vec{L}$ and $\vec{L}\times\vec{S}$ are perpendicular.

$$\left[\vec{L}\cdot\vec{S}\ ,\ \vec{S}^{\,2}\right] = \left[\vec{L}\cdot\vec{S}\ ,\ S_x^2 + S_y^2 + S_z^2\right]$$

$$= \; \left[\vec{L}\cdot\vec{S}\ ,\ S_x^2\right] + \left[\vec{L}\cdot\vec{S}\ ,\ S_y^2\right] + \left[\vec{L}\cdot\vec{S}\ ,\ S_z^2\right]$$

$$= \; S_x\left[\vec{L}\cdot\vec{S}\ ,\ S_x\right] + \left[\vec{L}\cdot\vec{S}\ ,\ S_x\right]S_x + S_y\left[\vec{L}\cdot\vec{S}\ ,\ S_y\right] + \left[\vec{L}\cdot\vec{S}\ ,\ S_y\right]S_y$$
$$+S_z\left[\vec{L}\cdot\vec{S}\ ,\ S_z\right] + \left[\vec{L}\cdot\vec{S}\ ,\ S_z\right]S_z$$

$$= \; -S_x i\hbar\left[\vec{L}\times\vec{S}\right]_x - i\hbar\left[\vec{L}\times\vec{S}\right]_x S_x - S_y i\hbar\left[\vec{L}\times\vec{S}\right]_y - i\hbar\left[\vec{L}\times\vec{S}\right]_y S_y$$
$$-S_z i\hbar\left[\vec{L}\times\vec{S}\right]_z - i\hbar\left[\vec{L}\times\vec{S}\right]_z S_z$$

$$= \; -S_x i\hbar\left[\vec{L}\times\vec{S}\right]_x - S_y i\hbar\left[\vec{L}\times\vec{S}\right]_y - S_z i\hbar\left[\vec{L}\times\vec{S}\right]_z$$
$$-i\hbar\left[\vec{L}\times\vec{S}\right]_x S_x - i\hbar\left[\vec{L}\times\vec{S}\right]_y S_y - i\hbar\left[\vec{L}\times\vec{S}\right]_z S_z$$

$$= \; -\,i\hbar\vec{S}\cdot\left[\vec{L}\times\vec{S}\right] \; - \; i\hbar\left[\vec{L}\times\vec{S}\right]\cdot\vec{S} \; = \; 0 \quad .$$

The last step follows because $\vec{S}$ and $\vec{L}\times\vec{S}$ are perpendicular.