Mecânica Quântica II (2013-2014)

1. Um pacote de ondas que representa o movimento de uma partícula livre numa dimensão é, em unidades $\hbar = c = 1$, dado pela seguinte expressão

$$\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \varphi(k) \exp\left\{i\left(kx - \omega(k)t\right)\right\} \quad ,$$

onde ($\bar{k}$ constante e $\left|\bar{k}\right| \gg \Delta k > 0$)

$$\varphi(k) \;=\; \frac{1}{\sqrt{2\Delta k}}\; \theta\left((\Delta k)^2 - \left(k-\bar{k}\right)^2\right) \;=\; \begin{cases} \dfrac{1}{\sqrt{2\Delta k}} & ,\left|k-\bar{k}\right| \leq \Delta k \\ 0 & ,\left|k-\bar{k}\right| > \Delta k \end{cases} \quad , \tag{1}$$

e

$$\omega(k) \;=\; \frac{k^2}{2m} \quad .$$

a Mostre que no instante $t = 0$ a função de onda é dada por

$$\psi(x, t=0) \;=\; \frac{1}{\sqrt{\pi\Delta k}}\, e^{i\bar{k}x}\, \frac{\sin\left(\Delta k\, x\right)}{x} \quad ,$$

e faça um esquema de $\left|\psi(x,t=0)\right|^2$ em função de x.

b Determine graficamente Δx e $\Delta x \Delta k$ e compare o resultado com a relação de incerteza de Heisenberg.

2. Considere de novo o pacote de ondas do problema anterior (1) que representa o movimento de uma partícula livre numa dimensão em unidades $\hbar = c = 1$.

a Determine
$$\int_{-\infty}^{\infty} dk \ |\varphi(k)|^2 \quad .$$

b Determine (O integral número 11 da tabela das integrais na página http://www.sosmath.com/tables/integral/integ37/integ37.html do web pode ser útil.)
$$\int_{-\infty}^{\infty} dx \ |\psi(x, t = 0)|^2$$
e interprete o resultado.

c Demonstre a seguinte relação
$$\int_{-\infty}^{\infty} dx \ |\psi(x, t = 0)|^2 \ = \ \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} dk' \ \varphi^*(k)\varphi(k') \ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \ e^{i(k' - k)x} \quad .$$

d A expressão
$$\delta(k' - k) \ = \ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \ e^{i(k' - k)x}$$
é designada **a função delta de Dirac** e tem a seguinte propriedade
$$\int_{-\infty}^{\infty} dk' \ F(k') \ \delta(k' - k) \ = \ F(k)$$
para funções F "bem comportadas".
Demonstre
$$\int_{-\infty}^{\infty} dx \ |\psi(x, t = 0)|^2 \ = \ \int_{-\infty}^{\infty} dk \ |\varphi(k)|^2$$
e verifique o resultado com as alineas a) e b).

3. Considere mais uma vez o pacote de ondas do problema (1) que representa o movimento de uma partícula livre numa dimensão em unidades $\hbar = c = 1$.

a Faça outros esquemas de $|\psi(x, t = 1)|^2$ e $|\psi(x, t = 2)|^2$ na aproximação
$$\omega(k) \ = \ \frac{\bar{k}^2}{2m} \ + \ \frac{\bar{k}}{m} \ \left(k - \bar{k}\right) \quad ,$$
em função de x e tire uma conclusão relativamente à velocidade do pacote de ondas.

b Mostre que o pacote de ondas é solução da seguinte equação de onda
$$i \ \frac{\partial}{\partial t} \ \psi(x, t) \ = \ -\frac{1}{2m} \ \frac{\partial^2}{\partial x^2} \ \psi(x, t) \quad ,$$
e interprete este resultado.

4. Considera um pacote de ondas que representa o movimento de uma partícula livre numa dimensão em unidades $\hbar = c = 1$, dado pela seguinte expressão

$$\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) \exp\left\{ i \left(kx - \omega(k)t \right) \right\} \quad , \tag{2}$$

com

$$\omega(k) \;=\; \sqrt{k^2 + m^2} \quad \text{(relação de Einstein)} \quad .$$

a Mostra que o pacote de ondas é solução da seguinte equação da onda (equação de Klein e Gordon)

$$\frac{\partial^2}{\partial t^2}\, \psi(x,t) \;=\; \left(\frac{\partial^2}{\partial x^2} \;-\; m^2 \right) \psi(x,t) \quad .$$

b Considera a seguinte transformação de Lorentz para um referêncial (x', t') em movimento relativamente ao referêncial (x, t) com velocidade β

$$x' \;=\; \gamma \left(x - \beta t \right) \quad \text{e} \quad t' \;=\; \gamma \left(t - \beta x \right) \quad \text{com} \quad \gamma^2 \;=\; \frac{1}{1 - \beta^2} \quad .$$

Determina a equação da onda nas coordenadas (x', t'). para o pacote de ondas $\psi'(x', t') = \psi(x(x', t'), t(x', t'))$.

5. Considera um pacote de ondas que representa o movimento de uma partícula livre em três dimensões em unidades $\hbar = c = 1$, dado pela seguinte expressão

$$\psi(\vec{x},t) \;=\; \left(\frac{1}{2\pi}\right)^{3/2} \int d^3k\, \varphi\left(\vec{k}\right) \exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0) - E\left(\vec{k}\right)t\right]\right\} \quad ,$$

onde $\vec{x}_0$ representa a "posição" da partícula no instante $t = 0$, e $E\left(\vec{k}\right)$ é dado por

$$E\left(\vec{k}\right) \;=\; \frac{\vec{k}^{\,2}}{2m} \quad .$$

Caso

$$\varphi\left(\vec{k}\right) \;=\; \prod_{i=1}^{3} \frac{1}{\sqrt{2\Delta k_i}}\; \theta\left(\left(\Delta k_i\right)^2 - \left(k_i - \bar{k}_i\right)^2\right)$$

$$= \begin{cases} \dfrac{1}{2\sqrt{2\Delta k_1 \Delta k_2 \Delta k_3}} & ,\left|k_i - \bar{k}_i\right| \leq \Delta k_i \quad i=1, \;\text{ e }\; i=2, \;\text{ e }\; i=3 \\ 0 & ,\left|k_i - \bar{k}_i\right| > \Delta k_i \quad i=1, \;\text{ ou }\; i=2, \;\text{ ou }\; i=3 \end{cases}$$

mostra que

a

$$\psi(\vec{x}, t=0) \;=\; e^{i\vec{\bar{k}}\cdot(\vec{x}-\vec{x}_0)} \prod_{i=1}^{3} \frac{1}{\sqrt{\pi\Delta k_i}} \frac{\sin\left(\Delta k_i\,\left[x_i - (\vec{x}_0)_i\right]\right)}{x_i - (\vec{x}_0)_i} \quad ,$$

e enterpreta o resultado.

b o pacote de ondas é solução da equação

$$i\frac{\partial}{\partial t}\psi\left(\vec{r},t\right) \;=\; -\frac{\nabla^2}{2m}\psi\left(\vec{r},t\right) \quad \text{onde} \quad \nabla^2 = \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2} \quad .$$

6. Análise Fourier e função Dirac delta

a Para o intervalo $-L < x < L$, mostrar

$$f(x) \; = \; \frac{1}{2} \sum_{n=-\infty}^{\infty} \left[\, a_n \, \sin\left(\frac{n\pi x}{L}\right) \; + \; b_n \, \cos\left(\frac{n\pi x}{L}\right) \right] \quad ,$$

com

$$a_n \; = \; \frac{1}{L} \int_{-L}^{L} dx \; f(x) \; \sin\left(\frac{n\pi x}{L}\right) \quad \text{e} \quad b_n \; = \; \frac{1}{L} \int_{-L}^{L} dx \; f(x) \; \cos\left(\frac{n\pi x}{L}\right) \quad .$$

b Para o intervalo $-L < x < L$, mostrar

$$f(x) \; = \; \sum_{n=-\infty}^{\infty} c_n \, \exp\left(-i \, \frac{n\pi x}{L}\right) \quad \text{com} \quad c_n \; = \; \frac{1}{2L} \int_{-L}^{L} dx \; f(x) \; \exp\left(i \, \frac{n\pi x}{L}\right) \quad .$$

c Com $\Delta\omega = \pi/L$, $\omega_n = n\pi/L$ e $F_n = 2Lc_n/\sqrt{2\pi}$, mostrar que no limite $L \to \infty$ se obtem

$$f(x) \; = \; \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}} F(\omega) \, e^{-i\omega x} \quad \text{com} \quad F(\omega) \; = \; \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} f(x) \, e^{i\omega x} \quad .$$

d Mostrar (por substituição)

$$\delta(x - \bar{x}) \; = \; \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \; e^{i\omega(x-\bar{x})} \quad .$$

7. A distribuição Gaussiana

a Mostra $\int \, d^3k \, \left|\varphi\left(\vec{k}\right)\right|^2 \; = \; 1$ com $\varphi\left(\vec{k}\right) \; = \; \left(\frac{\alpha}{\pi}\right)^{3/4} \, e^{-\frac{1}{2}\alpha\left(\vec{k} - \vec{\bar{k}}\right)^2}$.

b Determina

$$\psi\left(\vec{r}\right) \; = \; \int \frac{d^3k}{(2\pi)^{3/2}} \, \varphi\left(\vec{k}\right) \; e^{i\vec{k}\cdot\vec{r}} \quad .$$

8. A equação de Schrödinger em coordenadas esféricas $(r,\, \vartheta,\, \varphi)$:

a Mostre

$$\vec{p}^{\,2} \;=\; \frac{L^2}{r^2} \;-\; \hbar^2 \left\{ \frac{1}{r^2}\left(r\frac{\partial}{\partial r}\right)^2 \;+\; \frac{1}{r}\frac{\partial}{\partial r} \right\}$$

$$\text{com}\;\; L^2 \;=\; -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial \vartheta}\sin(\vartheta)\frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial \varphi^2} \right\} \quad .$$

b Considere a substituição seguinte

$$\psi\left(\vec{r}\,\right) \;=\; \frac{u_\ell(r)}{r}\, Y_{\ell m}(\vartheta,\varphi) \;\;,$$

onde o harmónico esférico $Y_{\ell m}(\vartheta,\varphi)$ representa uma solução da equação seguinte

$$L^2 Y_{\ell m}(\vartheta,\varphi) \;=\; \hbar^2 \ell(\ell+1)\, Y_{\ell m}(\vartheta,\varphi) \;\; .$$

Para um potencial esférico simétrico, *i.e.* $V(\vec{r}\,) = V(r)$, a partir da equação de Schrödinger dada por

$$\left\{ \frac{p^2}{2m} \;+\; V(\vec{r}\,) \right\} \psi\left(\vec{r}\,\right) \;=\; E\psi\left(\vec{r}\,\right) \quad ,$$

deduze a relação (Equação radial de Schrödinger)

$$\left\{ -\frac{d^2}{dr^2} \;+\; \frac{\ell(\ell+1)}{r^2} \;+\; U(r) \;-\; k^2 \right\} u_\ell(r) \;=\; 0 \quad ,$$

com

$$U(r) \;=\; \frac{2mV(r)}{\hbar^2} \quad \text{e} \quad k^2 \;=\; \frac{2mE}{\hbar^2} \quad .$$

9. O espectro do átomo de hidrogénio é o conjunto de comprimentos de onda presentes na luz que o átomo de hidrogénio é capaz de emitir quando baixa de nível de energia.

O modelo mais simples do átomo de hidrogénio é representado pelo átomo de Bohr. Neste modelo o espectro de luz é composto de comprimentos de onda discretos, cujos valores são expressos pela fórmula de Rydberg

$$\frac{1}{\lambda_{\mathrm{vac}}} = R_{\mathrm{H}} \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right) \quad ,$$

onde λ_{vac} é o comprimento de onda da luz emitida no vácuo, R_{H} é a constante de Rydberg para o hidrogénio, e n_1 e n_2 são inteiros tais que $n_1 < n_2$.

Deixando n_1 igual a 1 e fazendo n_2 percorrer valores de 2 a infinito, as linhas de espectro conhecidas como série de Lyman convergem para 91 nm. Da mesma maneira:

n_1	n_2		limite (nm)
1	$2 \to \infty$	Série de Lyman	91
2	$3 \to \infty$	Série de Balmer	365
3	$4 \to \infty$	Série de Paschen	821
4	$5 \to \infty$	Série de Brackett	1459
5	$6 \to \infty$	Série de Pfund	2280
6	$7 \to \infty$	Série de Humphreys	3283

a Determine os valores de n_2 para as linhas da série de Balmer (1885), H_α, H_β, H_γ, etc., que têm respectivamente os seguintes comprimentos de onda (em **nm**): no espectro visível 656.3 (vermelho), 486.1 (azul-verde), 434.1 (azul-violeta) e 410.2 (violeta) e no espectro ultra-violeta 397.0, 388.9, 383.5 e 364.6.

b A mesma pergunta para as linhas da série de Lyman, cujas frequências são (em 10^{15} Hz) 3.238, 3.223, 3.198, 3.158, 3.084, 2.924 e 2.467.

10. O termo da energia cinética da equação de Schrödinger é dado por

$$-\frac{\hbar^2}{2m}\bigtriangledown^2\ \psi(\vec{r}\,)\ =\ -\frac{\hbar^2}{2mr}\frac{\partial^2}{\partial r^2}\,r\,\psi(\vec{r}\,)\ +\ \frac{L^2}{2mr^2}\,\psi(\vec{r}\,)\quad ,$$

onde o momento angular ao quadrado L^2 é dado por

$$L^2\ =\ -\hbar^2\left\{\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\ +\ \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\quad .$$

Define ainda o seguinte operador

$$L_z\ =\ -i\,\hbar\,\frac{\partial}{\partial\varphi}\quad .$$

Mostre que as seguintes expressões são simultaneamente funções próprias de L^2 e de L_z e determine os respectivos valores próprios:

a $Y_0^0(\vartheta,\varphi)=\sqrt{1/4\pi}$

b $Y_1^0(\vartheta,\varphi)=\sqrt{3/4\pi}\,\cos(\vartheta)$

c $Y_1^1(\vartheta,\varphi)=-\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{i\varphi}$

d $Y_1^{-1}(\vartheta,\varphi)=\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi}$

e $Y_2^0(\vartheta,\varphi)=\sqrt{5/16\pi}\,\left\{3\cos^2(\vartheta)-1\right\}$

f $Y_2^1(\vartheta,\varphi)=-\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{i\varphi}$

g $Y_2^{-1}(\vartheta,\varphi)=\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{-i\varphi}$

h $Y_2^2(\vartheta,\varphi)=\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{2i\varphi}$

i $Y_2^{-2}(\vartheta,\varphi)=\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{-2i\varphi}$

11. Os operadores de subida L_+ e de descida L_- são dados por

$$L_+\ =\ \hbar\,e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta}\ +\ i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\quad\text{e}\quad L_-\ =\ \hbar\,e^{-i\varphi}\left\{-\frac{\partial}{\partial\vartheta}\ +\ i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\quad .$$

Determine $L_+Y_\ell^m$ e $L_-Y_\ell^m$ para cada uma das funções dadas no exercício (10).

12. Considere a equação de onda para o sistema electrão-protão dada por

$$\left\{ -\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2} r \; + \; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \; - \; \frac{e^2}{4\pi\epsilon_0 r} \right\} R_{n\ell}(r) \; = \; E_n\, R_{n\ell}(r) \quad .$$

Mostre que as seguintes expressões $R_{n\ell}(r)$ para diversos valores de n ($n = 1, 2, 3, \ldots$) e de ℓ ($\ell = 0, 1, 2, \ldots \leq n-1$), são soluções dessa equação e determine os respectivos valores próprios E_n.

a $\quad R_{10}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$

b $\quad R_{20}(r) = \left(\frac{1}{2a_0}\right)^{3/2} \left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}$

c $\quad R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{1}{2a_0}\right)^{3/2} \left\{\frac{r}{a_0}\right\} e^{-r/2a_0}$

d $\quad R_{30}(r) = 2\left(\frac{1}{3a_0}\right)^{3/2} \left\{1 - \frac{2}{3}\frac{r}{a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$

e $\quad R_{31}(r) = \frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{1 - \frac{1}{6}\frac{r}{a_0}\right\} \frac{r}{a_0}\, e^{-r/3a_0}$

f $\quad R_{32}(r) = \frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$

onde a_0 represente o raio de Bohr dado por

$$a_0 \; = \; \frac{4\pi\epsilon_0\hbar^2}{m_e e^2} \quad .$$

13. Considere os resultados dos exercícios (10) e (12).

a Caso $R_{n\ell}(r)$, para $n = 1, 2, 3, \ldots$ e $\ell = 0, 1, 2, \ldots \leq n-1$, é uma das soluções da equação

$$\left\{ -\frac{\hbar^2}{2m_e r} \frac{d^2}{dr^2} r + \frac{\hbar^2 \, \ell(\ell+1)}{2m_e r^2} - \frac{e^2}{4\pi\epsilon_0 r} \right\} R_{n\ell}(r) = E_n \, R_{n\ell}(r) \quad ,$$

e $Y_\ell^m(\vartheta, \varphi)$, para $\ell = 0, 1, 2, \ldots$ e $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$, uma das soluções da equação

$$L^2 \, Y_\ell^m(\vartheta, \varphi) = \hbar^2 \, \ell(\ell+1) \, Y_\ell^m(\vartheta, \varphi)$$

com

$$L^2 = -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)} \frac{\partial}{\partial \vartheta} \sin(\vartheta) \frac{\partial}{\partial \vartheta} + \frac{1}{\sin^2(\vartheta)} \frac{\partial^2}{\partial \varphi^2} \right\} \quad ,$$

então mostre que $\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r) \, Y_\ell^m(\vartheta, \varphi)$ é uma das soluções da equação

$$\left\{ -\frac{\hbar^2}{2m_e} \bigtriangledown^2 - \frac{e^2}{4\pi\epsilon_0 r} \right\} \psi_{n\ell m}(\vec{r}) = E_n \, \psi_{n\ell m}(\vec{r}) \quad .$$

b Caso $R_{n\ell}(r)$ satisfaz a relação

$$\int_0^\infty r^2 dr \, \left| R_{n\ell}(r) \right|^2 = 1 \quad ,$$

e $Y_\ell^m(\vartheta, \varphi)$ satisfaz a relação

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin(\vartheta) d\vartheta \, \left| Y_\ell^m(\vartheta, \varphi) \right|^2 = 1 \quad ,$$

então mostre que $\psi_{n\ell m}(\vec{r}) = R_{n\ell}(r) \, Y_\ell^m(\vartheta, \varphi)$ satisfaz a relação

$$\int_{-\infty}^\infty dx \int_{-\infty}^\infty dy \int_{-\infty}^\infty dz \, \left| \psi_{n\ell m}(x, y, z) \right|^2 = 1 \quad .$$

14. Um estado excitado do átomo de hidrogénio pode-se representar por $H(n, \ell, m)$, onde n, ℓ e m representam respectivamente o número quântico principal, o de momento angular orbital e o magnético ($m = -\ell$, $-\ell + 1$, ..., 0, ..., $+\ell$).
No entanto, da solução da equação de onda para o átomo de hidrogénio deduzimos que o espectro de Coulomb é dado por

$$E_n = -\frac{E_\infty}{n^2} \quad , \quad n = 1, 2, 3, \ldots$$

e ainda a condição $\ell \leq n - 1$ para estados quânticos fisicamente aceitáveis. Portanto, existem vários estados excitados diferentes com a mesma energia. Este fenómeno chama-se *degenerescência*.

a Demostra que o número de estados excitados diferentes com energia E_n, é igual ao quadrado do número quântico principal n.

Do passado existe ainda uma outra classificação dos estados excitados de hidrogénio, classificação em que se consideram como manifestações diferentes do mesmo estado $H(n, \ell)$ (indicado por $n\ell$), os vários estados $H(n, \ell, 0)$, $H(n, \ell, \pm 1)$, $H(n, \ell, \pm 2)$, ..., $H(n, \ell, \pm \ell)$. Neste abordagem o número quântico de momento angular orbital ℓ é representado por uma letra de acordo com o seguinte quadro

ℓ	0	1	2	3	4	5	6	7
letra	s	p	d	f	g	h	i	j

b Faça um quadro para estados quânticos fisicamente aceitáveis onde se indica os estados $H(n, \ell)$ para $n = 1$, ..., 6 e $\ell = 0$, ..., 5.

15. Considere a transição $E_2 \to E_1$ 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 $E_2 \to E_1$ 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 = 5.79×10^{-5} eV/T.

16. 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

$$\left[H \, , \, \vec{L}\right] = H\,\vec{L} - \vec{L}\,H = 0 \quad . \tag{3}$$

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 (3) para a componente L_z.

17. A partícula livre:

a Para uma partícula livre, mostre que substituindo $z = kr$ na equação radial de Schrödinger, se obtém a equação diferencial seguinte

$$\left\{-\frac{d^2}{dz^2} + \frac{\ell(\ell+1)}{z^2} - 1\right\} u_\ell(z) = 0 \quad , \tag{4}$$

e comente os casos (i) $\ell = 0$, (ii) $z \gg 1$ e (iii) $z \ll 1$.

b A seguir, mostre que se $u_\ell(z)$ representa uma solução da equação (4) para o número quântico rotacional igual a ℓ, então

$$u_{\ell+1}(z) = \left\{\frac{\ell+1}{z} - \frac{d}{dz}\right\} u_\ell(z)$$

representa uma solução para o número quântico rotacional igual a $\ell + 1$.

c Deduze a relação

$$u_{\ell+1}(z) = z^{\ell+2} \left(-\frac{1}{z}\frac{d}{dz}\right) \frac{u_\ell(z)}{z^{\ell+1}}$$

d A função esférica de Bessel é dada por

$$j_\ell(z) = z^\ell \left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\sin(z)}{z}$$

Mostre que $u_\ell(z) = z j_\ell(z)$ representa uma solução da equação (4) para o número quântico rotacional igual a ℓ e comente os casos $z \gg 1$ e $z \ll 1$.

e A função esférica de Neumann é dada por

$$n_\ell(z) = -z^\ell \left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{\cos(z)}{z}$$

Mostre que $u_\ell(z) = z n_\ell(z)$ representa uma solução da equação (4) para o número quântico rotacional igual a ℓ e comente os casos $z \gg 1$ e $z \ll 1$.

18. Considere o potencial seguinte

$$V(r) = \begin{cases} U & \text{para} \quad r < a \\ 0 & \text{para} \quad r > a \end{cases} \tag{5}$$

U e a constantes.

a No caso em que $\ell = 0$ determina a função de onda.

b Determine a diferença de fase, δ, entre a função de onda ao infínito para $U = 0$ e a função de onda ao infínito para $U > 0$.

c Determine ainda $S = \exp(2i\delta)$ e $|S - 1|^2$

19.

Neste problema consideramos a seguinte equação diferencial de segunda ordem:

$$-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2}+\tfrac{1}{2}\mu\omega^2r^2\;u(r)\;=\;E\;u(r)\quad . \tag{6}$$

a Considera a substituição $x=\frac{\mu\omega}{\hbar}r^2$. Mostre que

$$\frac{d^2u}{dr^2}\;=\;2\frac{\mu\omega}{\hbar}\left\{\;u'\;+\;2xu''\;\right\},$$

com $u'=du/dx$ e $u''=d^2u/dx^2$.

b Mostre que

$$-2xu''\;-\;u'\;+\;\tfrac{1}{2}xu\;=\;\frac{E}{\hbar\omega}u\quad .$$

c Considere a substituição $u(x)=\sqrt{x}e^{-\frac{1}{2}x}\phi(x)$ e deduza as relações

$$2xu''\;=\;\frac{1}{2\sqrt{x}}e^{-\frac{1}{2}x}\left\{\left(x^2-2x-1\right)\phi\;-\;4\left(x^2-x\right)\phi'\;+4x^2\phi''\right\}$$

$$e\qquad x\phi''\;-\;\left(x-\tfrac{3}{2}\right)\phi'\;+\;s\phi\;=\;0\quad , \tag{7}$$

com $E=\hbar\omega\left(2s+\frac{3}{2}\right)$.

d Para a função hipergeométrica confluente ${}_1F_1$, definida por

$$\begin{aligned}{}_1F_1(a,b,x)\;&=\;1\;+\;\frac{a}{b}x\;+\;\frac{a(a+1)}{b(b+1)}\frac{x^2}{2}\;+\;\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!}\;+\;\cdots\\&=\;\sum_{n=0}^{\infty}\frac{(a)_n}{(b)_n}\frac{x^n}{n!}\end{aligned}$$

$$\text{com}\;\;(p)_n\;=\;p(p+1)(p+2)\cdots(p+n-1)\;\;\text{e}\;\;(p)_0\;=\;1\;,$$

mostre as seguintes relações:

$$\frac{d}{dx}{}_1F_1(a,b,x)\;=\;\frac{a}{b}{}_1F_1(a+1,b+1,x)\quad ,$$

$$\begin{aligned}&(a+1)x\;{}_1F_1(a+2,b+2,x)+(b+1)(b-x)\;{}_1F_1(a+1,b+1,x)\;=\\&=\;b(b+1)\;{}_1F_1(a,b,x)\quad .\end{aligned}$$

e Mostre que ${}_1F_1\left(-s,\frac{3}{2},x\right)$ e $x^{-1/2}{}_1F_1\left(-s-\frac{1}{2},\frac{1}{2},x\right)$ resolvem a equação (7).

20. Considere o potencial seguinte

$$V(r) \;=\; \lambda\, \delta(r-b) \tag{8}$$

λ e b constantes.

a Mostre que em $r = b$ para a função de onda se tem as seguintes condições.

$$-\left.\frac{du}{dr}\right|_{r\downarrow b} + \left.\frac{du}{dr}\right|_{r\uparrow b} + \lambda\, u(b) \;=\; 0 \quad \text{and} \quad u\,(r\downarrow b) \;=\; u\,(r\uparrow b) \quad .$$

b No caso em que $\ell = 0$ determina a função de onda.

c Determine a diferença de fase, δ, entre a função de onda ao infínito para $\lambda = 0$ e a função de onda ao infínito para $\lambda > 0$.

d Determine ainda $S = \exp(2i\delta)$ e $|S-1|^2$

21. Considere o propagador $\mathcal{G}\,(r_2, r_1)$ que relaciona a função de onda $u\,(r_1)$ e a sua derivada $u'\,(r_1)$ na posição $r = r_1$ com a função de onda $u\,(r_2)$ e a sua derivada $u'\,(r_2)$ na posição $r = r_2 > r_1$ e que é dado por

$$\begin{pmatrix} u\,(r_2) \\ u'\,(r_2) \end{pmatrix} \;=\; \mathcal{G}\,(r_2, r_1) \begin{pmatrix} u\,(r_1) \\ u'\,(r_1) \end{pmatrix} \quad .$$

a Mostre as seguintes relações:

$$\mathcal{G}\,(r_1, r_1) = \mathbf{1} \;\;,\;\; \mathcal{G}\,(r_3, r_1) = \mathcal{G}\,(r_3, r_2)\, \mathcal{G}\,(r_2, r_1) \quad \text{e} \quad \mathcal{G}^{-1}\,(r_2, r_1) = \mathcal{G}\,(r_1, r_2) \;.$$

b No caso em que o potencial é nulo e para $\ell = 0$ mostre que

$$\mathcal{G}\,(r_2, r_1) \;=\; \begin{pmatrix} \sin\,(kr_2) & -\dfrac{\cos\,(kr_2)}{k} \\ k\cos\,(kr_2) & \sin\,(kr_2) \end{pmatrix} \begin{pmatrix} \sin\,(kr_1) & \dfrac{\cos\,(kr_1)}{k} \\ -k\cos\,(kr_1) & \sin\,(kr_1) \end{pmatrix} \quad .$$

c No caso em que o potencial é dado por $V(r) \;=\; \lambda\, \delta(r-b)$ (problema 20), mostre que

$$\begin{pmatrix} u\,(r\downarrow b) \\ u'\,(r\downarrow b) \end{pmatrix} \;=\; \begin{pmatrix} 1 & 0 \\ \lambda & 1 \end{pmatrix} \begin{pmatrix} u\,(r\uparrow b) \\ u'\,(r\uparrow b) \end{pmatrix} \quad .$$

22. 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 $[S_z\ ,\ S_x]$.

23. 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 22) 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 $\vec{L}\cdot\vec{S} = L_xS_x + L_yS_y + L_zS_z$, 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 $\left[\vec{L}\cdot\vec{S}\ ,\ S^2\right]$.

24. O movimento orbital do electrão dentro do interior do átomo de hidrogénio causa um momento magnético proporcional ao momento angular orbital $\vec{L}$. Consequentemente, o momento magnético intrínseco do electrão, proporcional ao spin $\vec{S}$ sofre uma força, proporcional com $\vec{L}\cdot\vec{S}$ (*acoplamento spin-orbital*). Portanto, a forma mais completa do Hamiltoniano do átomo de hidrogénio é igual a

$$H' \;=\; \frac{p^2}{2\mu_{\rm e}} - \frac{e^2}{4\pi\epsilon_0 r} + W(r)\vec{L}\cdot\vec{S} \quad ,$$

onde $W(r)$ é uma função da distância entre o protão e o electrão.
Utilizando os resultados dos problemas (22) e (23), mostra que $\left[H'\ ,\ \vec{S}\right] \neq 0$, $\left[H'\ ,\ \vec{L}\right] \neq 0$, $[H'\ ,\ S^2] = 0$ e $[H'\ ,\ L^2] = 0$ e tira uma conclusão relativamente aos observáveis L_z, S_z, L^2 e S^2.

25. Devido às conclusões do problema (24) é preciso encontrar um novo observável para rotular os estados próprios do Hamiltoniano H'.
Defina-se o *momento angular total* $\vec{J} = \vec{L} + \vec{S}$ do átomo de hidrogénio.
Utilizando os resultados dos problemas (22) e (23), mostra que $\left[H'\ ,\ \vec{J}\right] = 0$ e $[H'\ ,\ J^2] = 0$ e tira uma conclusão relativamente aos observáveis J_z e J^2.

26. Considere, em três dimensões, dois sistemas de coordenadas $\mathcal{S}$ e $\mathcal{S}$'. As origens, O e O', dos dois sistemas coincidem. No sistema $\mathcal{S}$ uma base ortonormal é dada por $\boldsymbol{e}_1$, $\boldsymbol{e}_2$ e $\boldsymbol{e}_3 = \boldsymbol{e}_1 \times \boldsymbol{e}_2$, e no sistema $\mathcal{S}$' por $\boldsymbol{e}'_1$, $\boldsymbol{e}'_2$ e $\boldsymbol{e}'_3 = \boldsymbol{e}'_1 \times \boldsymbol{e}'_2$. Sejam as relações entre as duas bases dadas por:

$$\boldsymbol{e}'_i = \sum_{j=1}^{3} R_{ji} \boldsymbol{e}_j \ ,$$

onde R representa uma rotação (transformação ortogonal).
Sejam ainda as componentes de um vector $\vec{r}$ no sistema $\mathcal{S}$ dadas por $\vec{r} = x_1 \boldsymbol{e}_1 + x_2 \boldsymbol{e}_2 + x_3 \boldsymbol{e}_3$, e no sistema $\mathcal{S}$' por $\vec{r} = x'_1 \boldsymbol{e}'_1 + x'_2 \boldsymbol{e}'_2 + x'_3 \boldsymbol{e}'_3$.

a Mostre que as relações entre $\left\{x'_i \ , \ i = 1,2,3\right\}$ e $\left\{x_j \ , \ j = 1,2,3\right\}$ são dadas por:

$$x'_i = \sum_{j=1}^{3} \left[R^{-1}\right]_{ij} x_j \quad \text{e} \quad x_j = \sum_{i=1}^{3} R_{ji} x'_i \ ,$$

b e ainda que $\displaystyle\sum_{i=1}^{3} \left(x'_i\right)^2 = \sum_{j=1}^{3} \left(x_j\right)^2$.

c Mostre que uma função Hamiltoniana, H, dada no sistema $\mathcal{S}$ pela seguinte expressão:

$$H\left(x_i, p_i, i = 1,2,3\right) = \tfrac{1}{2} \sum_{i=1}^{3} \left(p_i\right)^2 + V(r) \ , \text{com } r = \sqrt{\sum_{j=1}^{3} \left(x_j\right)^2} \ ,$$

é no sistema $\mathcal{S}'$ dada por:

$$\tfrac{1}{2} \sum_{i=1}^{3} \left(p'_i\right)^2 + V(r') = H\left(x'_i, p'_i, i = 1,2,3\right) \ , \text{com } r' = \sqrt{\sum_{j=1}^{3} \left(x'_j\right)^2}.$$

d Seja o valor de uma função (de onda) escalar num ponto P (P indicado pelo vector posição $\vec{r} = x_1\boldsymbol{e}_1 + x_2\boldsymbol{e}_2 + x_3\boldsymbol{e}_3$) dado por $\psi\left(x_i\right) \equiv \psi\left(x_1, x_2, x_3\right)$ no sistema $\mathcal{S}$, e por $\psi'\left(x'_i\right) \equiv \psi'\left(x'_1, x'_2, x'_3\right)$ no sistema $\mathcal{S}$'. Suponha que o valor da função não depende do sistema dos eixos, então $\psi'\left(x'_i\right) = \psi\left(x_i\right)$, ou seja $\psi'\left(x'_i\right) = \psi\left(R_{ij}x'_j\right)$, ou ainda $\psi'\left(x_i\right) = \psi\left(R_{ij}x_j\right)$.
No caso em que R representa uma rotação em torno do eixo dos zz com ângulo α, temos $R_{1j}x_j = x\cos(\alpha) - y\sin(\alpha) \approx x - \frac{1}{2}\alpha^2 x - \alpha y$, $R_{2j}x_j = x\sin(\alpha) + y\cos(\alpha) \approx y - \frac{1}{2}\alpha^2 y + \alpha x$ e $R_{3j}x_j = z$. Mostre que (expansão de Taylor até a segunda ordem em α):

$$\psi\left(R_{ij}x_j\right) =$$

$$= \psi\left(x_i\right) + \alpha\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\psi\left(x_i\right) + \tfrac{1}{2}\alpha^2\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)^2\psi\left(x_i\right) + \cdots$$

$$= \exp\left\{\alpha\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right\}\psi\left(x_i\right)$$

27. Considere, em três dimensões, um conjunto de três matrizes, A_1, A_2 e A_3, cujas elementos da matriz são dados por:

$$\left[A_i\right]_{jk} = -\epsilon_{ijk} \quad .$$

a Mostre, para um vector espacial $\vec{n} = n_1\boldsymbol{e}_1 + n_2\boldsymbol{e}_2 + n_3\boldsymbol{e}_3$, a seguinte igualdade:

$$\vec{n}\cdot\vec{A} \equiv n_1A_1 + n_2A_2 + n_3A_3 = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \quad .$$

b Para $\vec{n} = \alpha\boldsymbol{e}_3$, mostre que

$$\begin{aligned} \exp\left(\vec{n}\cdot\vec{A}\right) &\equiv \mathbf{1} + \vec{n}\cdot\vec{A} + \tfrac{1}{2!}\left(\vec{n}\cdot\vec{A}\right)^2 + \tfrac{1}{3!}\left(\vec{n}\cdot\vec{A}\right)^3 + \tfrac{1}{4!}\left(\vec{n}\cdot\vec{A}\right)^4 + \cdots \\ &= \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv R\left(\hat{z},\alpha\right) \quad . \end{aligned}$$

c Mostre que para o comutador entre as matrizes A_i e A_j se tem:

$$\left[A_i\ ,\ A_j\right] = \sum_{m=1}^{3} \epsilon_{ijm}A_m \quad .$$

d Para $\vec{n} = \alpha\hat{n}$ (direcção arbitrária), mostre que

$$\left(\vec{n}\cdot\vec{A}\right)^3 = -\alpha^2\left(\vec{n}\cdot\vec{A}\right) \quad ,$$

e e ainda que

$$\exp\left(\vec{n}\cdot\vec{A}\right) = \mathbf{1} + \sin(\alpha)\left(\hat{n}\cdot\vec{A}\right) + \left[1-\cos(\alpha)\right]\left(\hat{n}\cdot\vec{A}\right)^2 \quad .$$

28. Neste problema pretende-se mostrar que a expressão do problema anterior (27e) pode ser identificada com a rotação $R(\hat{n}, \alpha)$.

a Mostre que $\left(\vec{n} \cdot \vec{A}\right) \vec{n} = 0$ e então $\exp\left(\vec{n} \cdot \vec{A}\right) \vec{n} = \vec{n}$ (isto é: a transformação $\exp\left(\vec{n} \cdot \vec{A}\right)$ deixa o vector $\vec{n}$ invariante, ou seja, indica o eixo da rotação).

b Para os vectores $\vec{v}$ e $\vec{w}$ definidos por

$$\vec{v} = \begin{pmatrix} n_2 - n_3 \\ n_3 - n_1 \\ n_1 - n_2 \end{pmatrix} \quad \text{e} \quad \vec{w} = \hat{n} \times \vec{v} \ ,$$

mostre que $\left(\hat{n} \cdot \vec{A}\right) \vec{v} = \vec{w}$ e $\left(\hat{n} \cdot \vec{A}\right) \vec{w} = -\vec{v}$,

c e ainda que

$$\begin{aligned} \vec{v}\,' &= \exp\left(\vec{n} \cdot \vec{A}\right) \vec{v} = \vec{v} \cos(\alpha) + \vec{w} \sin(\alpha) \ , \quad \text{e} \\ \vec{w}\,' &= \exp\left(\vec{n} \cdot \vec{A}\right) \vec{w} = -\vec{v} \sin(\alpha) + \vec{w} \cos(\alpha) \ . \end{aligned}$$

d Indique então as razões por que $\exp\left(\vec{n} \cdot \vec{A}\right)$ pode ser identificado com a rotação $R(\hat{n}, \alpha)$.

29. Neste problema pretende-se estudar o comportamento de uma função vectorial sob uma rotação do sistema de coordenadas. Considere as transformações estudadas no problema (28) e em particular uma rotação em torno do eixo dos zz, $R(\hat{z}, \alpha)$, dada por

$$\boldsymbol{e'}_1 = \boldsymbol{e}_1 \cos(\alpha) + \boldsymbol{e}_2 \sin(\alpha) \ , \ \boldsymbol{e'}_2 = -\boldsymbol{e}_1 \sin(\alpha) + \boldsymbol{e}_2 \cos(\alpha) \text{ e } \boldsymbol{e'}_3 = \boldsymbol{e}_3 \ ,$$

e uma função vectorial, $\vec{\psi}(\vec{r}\,)$, dada por

$$\vec{\psi}(\vec{r}\,) = \psi_1(\vec{r}\,)\boldsymbol{e}_1 + \psi_2(\vec{r}\,)\boldsymbol{e}_2 + \psi_3(\vec{r}\,)\boldsymbol{e}_3 \ \ .$$

Para as componentes da função vectorial, que são funções escalares, tem-se:

$$\psi_j(\vec{r}\,) \xRightarrow{R(\hat{z},\alpha)} e^{-i\alpha L_z}\psi_j(\vec{r}\,) \ \ (j=1,2,3) \ \ , \ \ \text{com} \ \ L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \ ,$$

então

$$\vec{\psi}'(\vec{r}\,) = \left\{e^{-i\alpha L_z}\psi_1(\vec{r}\,)\right\}\boldsymbol{e'}_1 + \left\{e^{-i\alpha L_z}\psi_2(\vec{r}\,)\right\}\boldsymbol{e'}_2 + \left\{e^{-i\alpha L_z}\psi_3(\vec{r}\,)\right\}\boldsymbol{e'}_3$$

a Qual o aspecto de $\vec{\psi}'(\vec{r}\,) = \psi'_1(\vec{r}\,)\boldsymbol{e}_1 + \psi'_2(\vec{r}\,)\boldsymbol{e}_2 + \psi'_3(\vec{r}\,)\boldsymbol{e}_3$ na base $\boldsymbol{e'}_1$, $\boldsymbol{e'}_2$ e $\boldsymbol{e'}_3$?

b Mostre que

$$\begin{pmatrix} \psi'_1(\vec{r}\,) \\ \psi'_2(\vec{r}\,) \\ \psi'_3(\vec{r}\,) \end{pmatrix} = e^{-i\alpha L_z} e^{-i\alpha S_z} \begin{pmatrix} \psi_1(\vec{r}\,) \\ \psi_2(\vec{r}\,) \\ \psi_3(\vec{r}\,) \end{pmatrix} \ \ , \ \ \text{com} \ \ S_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \ .$$

c Determine os vectores próprios de S_z.

30. Considere funções de onda de duas componentes, $\psi(\vec{r}\,)$, dadas por

$$\psi(\vec{r}\,) = \begin{pmatrix} \psi_1(\vec{r}\,) \\ \\ \psi_2(\vec{r}\,) \end{pmatrix} \quad ,$$

e uma rotação $R(\hat{n}, \alpha)$ do sistema de coordenadas.
No espaço das funções de onda de duas componentes esperamos sob a transformação de coordenadas do sistema $\mathcal{S}$ para as coordenadas do sistema $\mathcal{S}$', uma transformação da seguinte forma para a função da onda $\psi(\vec{r}\,)$:

$$\psi(\vec{r}\,) \xRightarrow{R(\hat{n},\alpha)} \psi'(\vec{r}\,) = \begin{pmatrix} u_{11}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_1(\vec{r}\,) + u_{12}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_2(\vec{r}\,) \\ \\ u_{21}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_1(\vec{r}\,) + u_{22}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_2(\vec{r}\,) \end{pmatrix},$$

onde u_{ij} $(i,j = 1,2)$ são constantes que só dependem da orientação do sistema $\mathcal{S}$' relativamente ao sistema $\mathcal{S}$.

a Mostre que $e^{-i\alpha\hat{n}\cdot\vec{L}}$ e $U(\hat{n},\alpha)$ comutam e que $\psi'(\vec{r}\,) = e^{-i\alpha\hat{n}\cdot\vec{L}}U(\hat{n},\alpha)\psi(\vec{r}\,)$, com

$$U(\hat{n},\alpha) = \begin{pmatrix} u_{11}(\hat{n},\alpha) & u_{12}(\hat{n},\alpha) \\ \\ u_{21}(\hat{n},\alpha) & u_{22}(\hat{n},\alpha) \end{pmatrix} \quad .$$

b Mostre que $|\psi'(\vec{r}\,)|^2 = |\psi(\vec{r}\,)|^2$ implica $UU^\dagger = \mathbf{1}$ e ainda que $\det(U) = \pm 1$.

c Mostre que a forma mais geral de uma matriz 2×2 para que $UU^\dagger = \mathbf{1}$ e $\det(U) = 1$, é dada por $U(\hat{n},\alpha) = \mathbf{1}\cos\left(\frac{\alpha}{2}\right) - i\hat{n}\cdot\vec{\sigma}\sin\left(\frac{\alpha}{2}\right)$, onde σ_1, σ_2 e σ_3 representam as matrizes σ de Pauli, definidas por

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad .$$

d Mostre que $U(\hat{n},\alpha) = \exp\left(-i\frac{\alpha}{2}\hat{n}\cdot\vec{\sigma}\right)$, e então

$$\psi'(\vec{r}\,) \;=\; e^{-i\alpha\hat{n}\cdot\left(\vec{L}+\frac{\vec{\sigma}}{2}\right)}\psi(\vec{r}\,) \quad .$$

e Determine os vectores próprios de $S_z = \frac{1}{2}\vec{\sigma}_3$.

31. Rotações deixam invariante uma esfera em torno da origem. As coordenadas da esfera são os ângulos polares ϑ e φ.
Qualquer função f, função de ϑ e φ, $f = f(\vartheta, \varphi)$, pode ser expandida na base das funções esféricas harmónicas $Y_{\ell m}(\vartheta, \varphi)$, de acordo com

$$f(\vartheta, \varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} B_{\ell m} Y_{\ell m}(\vartheta, \varphi), \text{ com } B_{\ell m} = \int d\Omega Y^*_{\ell m}(\vartheta, \varphi) f(\vartheta, \varphi).$$

As funções esféricas harmónicas são funções próprias dos operadores L_z e $L^2 = (L_x)^2 + (L_y)^2 + (L_z)^2$, com os respectivos valores próprios dados por ($\hat{r} = (\vartheta, \varphi)$):

$$L_z Y_{\ell m}(\hat{r}) = m Y_{\ell m}(\hat{r}) \text{ e } L^2 Y_{\ell m}(\hat{r}) \ell(\ell+1) Y_{\ell m}(\hat{r}) \ .$$

Os operadores de escada, $L_{\pm} = L_x \pm i L_y$, actuam nas funções esféricas harmónicas da seguinte maneira:

$$L_{\pm} Y_{\ell,\, m}(\hat{r}) = \sqrt{\ell(\ell+1) - m(m \pm 1)}\, Y_{\ell,\, m \pm 1}(\hat{r}) \ .$$

Considere para $\ell = 1$ no espaço de funções de duas componentes a seguinte base de seis estados:

$$\begin{pmatrix} Y_{1,\, m}(\hat{r}) \\ 0 \end{pmatrix} \ , \ \begin{pmatrix} 0 \\ Y_{1,\, m}(\hat{r}) \end{pmatrix} \ , \text{ com } m = 0, \pm 1 \ .$$

a Mostre que

$$(L_x \sigma_1 + L_y \sigma_2) \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} L_- \psi_2 \\ L_+ \psi_1 \end{pmatrix} \text{ e } L_z \sigma_3 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} L_z \psi_1 \\ -L_z \psi_2 \end{pmatrix} \ .$$

b Seja $\vec{J} = \vec{L} + \frac{\vec{\sigma}}{2}$, então mostre que

$$J^2 \begin{pmatrix} Y_{1,\, m} \\ 0 \end{pmatrix} = \begin{pmatrix} \left(\frac{11}{4} + L_z\right) Y_{1,\, m} \\ L_+ Y_{1,\, m} \end{pmatrix} \text{ e } J^2 \begin{pmatrix} 0 \\ Y_{1,\, m} \end{pmatrix} = \begin{pmatrix} L_- Y_{1,\, m} \\ \left(\frac{11}{4} - L_z\right) Y_{1,\, m} \end{pmatrix}.$$

c Mostre que as funções $\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}} \equiv \begin{pmatrix} Y_{1,\,+1} \\ 0 \end{pmatrix}$, $J_- \mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$, $(J_-)^2 \mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$ e $(J_-)^3 \mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$ são funções próprias dos operadores J^2 e J_z.

32. Neste problema pretende-se mostrar que $\{2\} \otimes \{3\} = \{4\} \oplus \{2\}$.

a Determine os valores próprios de L^2, L_z, $\left(\frac{\vec{\sigma}}{2}\right)^2$ e $\frac{\sigma_z}{2}$ de cada um dos seguintes seis estados

$$\begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} \; , \; \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} \; , \; \text{com} \;\; m = 0, \pm 1 \;\; .$$

b Estes estados formam uma base ortonormal do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 1\}$. Temos por exemplo:

$$\left| s = \tfrac{1}{2}, s_z = +\tfrac{1}{2} \right\rangle \otimes |\ell = 1, \ell_z = +1\rangle = \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} \; .$$

Determine relações semelhantes para os outros cinco estados.

c Uma outra base ortonormal do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 1\}$ é dada por:

$$\begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} , \begin{pmatrix} \sqrt{\frac{2}{3}} Y_{1,0} \\ \sqrt{\frac{1}{3}} Y_{1,+1} \end{pmatrix} , \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix} , \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} ,$$

$$\begin{pmatrix} -\sqrt{\frac{1}{3}} Y_{1,0} \\ \sqrt{\frac{2}{3}} Y_{1,+1} \end{pmatrix} \; \text{e} \; \begin{pmatrix} -\sqrt{\frac{2}{3}} Y_{1,-1} \\ \sqrt{\frac{1}{3}} Y_{1,0} \end{pmatrix} \; .$$

Determine, se possível, os valores próprios de L^2, L_z, $\left(\frac{\vec{\sigma}}{2}\right)^2$, $\frac{\sigma_z}{2}$, e ainda de $J^2 = \left(\vec{L} + \frac{\vec{\sigma}}{2}\right)^2$ e $J_z = L_z + \frac{\sigma_z}{2}$ de cada um destes seis estados.

d Verifica-se que podemos dividir o espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 1\}$ em dois subespaços: $\left\{j = \frac{3}{2}\right\}$ de quatro dimensões e $\left\{j = \frac{1}{2}\right\}$ de duas dimensões. Os estados destes últimos espaços são designados por $|j, j_z\rangle$. Temos por exemplo:

$$\left| j = \tfrac{3}{2}, j_z = +\tfrac{3}{2} \right\rangle = \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} = \left| s = \tfrac{1}{2}, s_z = +\tfrac{1}{2} \right\rangle \otimes |\ell = 1, \ell_z = +1\rangle \; .$$

Determine relações semelhantes para os outros cinco estados da alínea (c).

e Os coeficientes destas relações chamam-se coeficientes de Clebsch-Gordan (CCG), designados por:

$$\begin{pmatrix} \ell & s & j \\ \ell_z & s_z & j_z \end{pmatrix} \ .$$

Da relação dada na alínea (d) determina-se por exemplo:

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ +1 & +\frac{1}{2} & +\frac{3}{2} \end{pmatrix} = 1 \ .$$

Determine os outros CCG das relações entre as bases dos subespaços $\left\{j = \frac{3}{2}\right\}$ e $\left\{j = \frac{1}{2}\right\}$ e a base do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 1\}$.

33. Em virtude de se estar a estudar o espectro rotacional de uma molécula polar diatómica, considere que os dois núcleos atómicos, de massas m_1 e m_2, giram em volta do seu centro de massa comum.

a Determine uma relação entre a energia total deste sistema, o momento angular total $\vec{K}$, a massa reduzida e a distância entre os núcleos.

b Sabendo que K^2 apenas pode ter valores $\hbar^2 K(K+1)$, com $K = 0, 1, 2, ...$, que o espectro rotacional de $HC\ell$ contém os comprimentos de onda (em μm) 120.3, 96.0, 80.4, 68.9 e 60.4, e ainda que apenas ocorem transições dipolares com $\Delta K = \pm 1$, determine a distância entre os núcleos de hidrogénio $({}_1H^1)$ e cloro $({}_{17}C\ell^{35})$ da molécula de $HC\ell$.

34. Oscilações pequenas de um sistema de duas partículas, ligadas por uma mola (constante de mola C), cujos movimentos estão restritos a uma dimensão (coordenada r), são classicamente descritas pela equação dinâmica $\mu\ddot{r} = -C\,(r - r_0)$, onde r_0 representa a distância de equilíbrio do sistema das duas partículas e μ a sua massa reduzida.

a Mostre que o Hamiltoniano deste sistema é dado por

$$H \;=\; \tfrac{1}{2}\left\{\frac{p^2}{\mu} + \mu\omega^2 x^2\right\} \quad ,$$

com $x = r - r_0$ e $\omega = \sqrt{C/\mu}$.

b A correspondente equação de onda na Mecânica Quântica obtém-se pela substituição $p \rightarrow -i\,\hbar\,\partial/\partial x$ e é dada por

$$H \;=\; \frac{1}{2\mu}\left\{-\hbar^2\frac{\partial^2}{\partial x^2} + (\mu\omega x)^2\right\} \quad . \tag{9}$$

Mostre que a função de onda, dada por

$$\psi_0(x) \;=\; \left[\frac{\mu\omega}{\pi\hbar}\right]^{1/4}\; e^{-\frac{1}{2}\mu\omega x^2/\hbar} \quad , \tag{10}$$

representa uma solução normalizada da equação de Schrödinger $H\psi = E\psi$ para $E = E_0 = \hbar\omega/2$.

c Os operadores de criação e aniquilação são respectivamente definidos por

$$a^\dagger \;=\; \sqrt{\frac{\mu\omega}{2\hbar}}\left(x \;-\; \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) \quad \text{e} \quad a \;=\; \sqrt{\frac{\mu\omega}{2\hbar}}\left(x \;+\; \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) \quad . \tag{11}$$

Mostre (i) $a\psi_0 = 0$, (ii) $H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$, (iii) $\left[a\ ,\ a^\dagger\right] = 1$, (iv) $\left[H\ ,\ a^\dagger\right] = \hbar\omega\, a^\dagger$ e (v) $[H\ ,\ a] = -\hbar\omega\, a$.

d Mostre que, se ψ é uma solução própria com valor próprio E da equação $H\psi = E\psi$, então $a^\dagger\psi$ é uma solução própria com valor próprio $E + \hbar\omega$ da mesma equação.

35. Numa notação devida ao físico P.A.M. Dirac, os estados próprios normalizados do oscilador harmónico numa dimensão são designados por $|\nu\rangle$. O estado fundamental é dado por $|0\rangle = \psi_0(x)$, onde $\psi_0(x)$ é dada por

$$\psi_0(x) \;=\; \mathcal{N}_0 \, e^{-\frac{1}{2}\mu\omega x^2/\hbar} \quad , \tag{12}$$

onde $\mathcal{N}_0$ representa a constante de normalização, $\mathcal{N}_0 = \left[\frac{\mu\omega}{\pi\hbar}\right]^{1/4}$

a Mostre que é igual a $\hbar\omega/2$ o valor próprio de $|0\rangle$ sob o efeito do Hamiltoniano dado no exercício (34) e igual a $\hbar\omega\left(\nu + \frac{1}{2}\right)$ o valor próprio de $\left(a^\dagger\right)^\nu |0\rangle$ (aplicar ν vezes o operador $a^\dagger$ definido no exercício 34).

b Na notação acima definida, o valor expectável de um operador A, caso o sistema se encontre no estado excitado $|\nu\rangle = \psi_\nu(x)$, é denotado por

$$\langle A\rangle \;=\; \langle \nu\,|A|\,\nu\rangle \;=\; \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, A\, \psi_\nu(x) \quad .$$

Determine o valor expectável do Hamiltoniano dado no exercício (34) para o estado $\left(a^\dagger\right)^\nu |0\rangle$.

c O estado $a^\dagger|\nu\rangle$ é proporcional ao estado $|\nu + 1\rangle$ (porquê?). Utilizando o resultado da alínea **b**, mostre que a constante de proporcionalidade é igual a $\sqrt{\nu + 1}$.

d Mostre que o valor expectável do operador x (exprimir em a e $a^\dagger$) para a transição de um estado $|\nu\rangle$ para um estado $|\nu + m\rangle$ se anula, salvo nos casos $m = \pm 1$.

36. Em virtude de se estar a estudar o espectro vibracional de uma molécula polar diatómica, considere que os dois núcleos atómicos estão ligados por uma mola (frequência de mola $\omega = 2\pi\nu$) e cujos movimentos estão restritos a uma dimensão (x).

a Utilizando os resultados do exercício (35), mostre que o espectro deste oscilador é dado por

$$E_v \;=\; \hbar\omega \left(v + \frac{1}{2} \right) \;, \qquad v = 0,\ 1,\ 2,\ 3,\ \ldots \quad .$$

b A probabilidade de ocorrer uma transição dipolar entre os estados $|n\rangle$ e $|n+m\rangle$ é dada pelo integral $\int_{-\infty}^{+\infty} dx\, \psi_n^*(x)\, x\, \psi_{n+m}(x)$. Utilizando os resultados do exercício (35), determine as regras de selecção para transições dipolares.

c No entanto, o potencial entre os núcleos atómicos de uma molécula polar diatómica na realidade não é dado por um oscilador harmónico. O espectro real é dado por

$$E_v \;=\; \hbar\omega \left(v + \frac{1}{2} \right) \left\{ 1 \,-\, a_1 \left(v + \frac{1}{2} \right) \,-\, a_2 \left(v + \frac{1}{2} \right)^2 \,-\, \ldots \right\} \,,$$

$$v = 0,\ 1,\ 2,\ 3,\ \ldots \quad ,$$

onde os parâmetros a_1, a_2, ... variam de molécula para molécula. Também as regras de selecção são mais flexíveis na realidade, embora as transições $\Delta v = \pm 1$ sejam mais intensas do que as transições $\Delta v = \pm 2$, etc..
Numa aproximação linear ($a_2 = a_3 = \ldots = 0$), determine $\hbar\omega$ e a_1 para a molécula $HC\ell$, caso o espectro de vibração de $HC\ell$ mostre uma linha intensa com frequência 2886 cm^{-1}, uma linha mais fraca com frequência 5668 cm^{-1} e ainda uma linha muito fraca com frequência 8347 cm^{-1}.

37. Considere a seguinte função de ondas de duas componentes

$$\begin{pmatrix} \psi_c\left(\vec{r}\,\right) \\ \\ \psi_s\left(\vec{r}\,\right) \end{pmatrix} = \begin{pmatrix} \dfrac{u_c(r)}{r} \\ \\ \dfrac{u_s(r)}{r} \end{pmatrix} \quad ,$$

e a seguinte equação radial de Schrödinger

$$\begin{pmatrix} h_c & \lambda V(r) \\ \\ \lambda V(r) & h_s \end{pmatrix} \begin{pmatrix} u_c \\ \\ u_s \end{pmatrix} = E \begin{pmatrix} u_c \\ \\ u_s \end{pmatrix} \quad ,$$

onde

$$\begin{aligned} h_c &= -\frac{1}{2\mu_c}\frac{d^2}{dr^2} + m_q + m_{\bar{q}} + \tfrac{1}{2}\mu_c\omega^2 r^2 \quad , \\ \\ h_s &= -\frac{1}{2\mu_s}\frac{d^2}{dr^2} + M_1 + M_2 \\ &\text{e} \\ V &= \frac{1}{2\mu_c a}\,\delta\left(r-a\right) \quad . \end{aligned}$$

Deduza as condições fronteiras

$$\left\{ \begin{array}{l} \dfrac{1}{2\mu_c}\left(-\left.\dfrac{d\,u_c(r)}{dr}\right|_{r\downarrow a} + \left.\dfrac{d\,u_c(r)}{dr}\right|_{r\uparrow a}\right) + \dfrac{\lambda}{2\mu_c a}u_s(a) \; = \; 0 \\ \\ \dfrac{\lambda}{2\mu_c a}u_c(a) + \dfrac{1}{2\mu_s}\left(-\left.\dfrac{d\,u_s(r)}{dr}\right|_{r\downarrow a} + \left.\dfrac{d\,u_s(r)}{dr}\right|_{r\uparrow a}\right) \; = \; 0 \end{array} \right. \quad ,$$

e

$$\left\{ \begin{array}{l} u_c(r\uparrow a) \; = \; u_c(r\downarrow a) \\ \\ u_s(r\uparrow a) \; = \; u_s(r\downarrow a) \end{array} \right. \quad .$$

38. Os níveis energéticos do oscilador harmónico numa dimensão, $H_c = -\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2$, são dados por

$$E_n \;=\; \omega\left(n + \frac{1}{2}\right) \qquad (n = 0,\, 1,\, 2,\, \ldots) \quad .$$

Determine as correcções de primeira ordem em λ aos níveis energéticos do oscilador harmónico numa dimensão, quando se aplica uma perturbação da forma

a $\Delta V(x) = \lambda x^4$,

b $\Delta V(x) = \lambda x^3$,

utilizando os operadores a e $a^\dagger$ definidos no exercío 34c.

39. Determine a correcção de segunda ordem em λ ao nível energético do estado principal do oscilador harmónico numa dimensão, quando se aplica uma perturbação da forma

$$\begin{pmatrix} -\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 & \lambda\,\delta\,(x) \\ \lambda\,\delta\,(x) & -\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}\mu\omega^2 x^2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = E \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad .$$

40. Mostra que a equação radial de Schrödinger

$$\left[-\frac{1}{2\mu}\frac{d^2}{dr^2} + m_q + m_{\bar{q}} + \tfrac{1}{2}\mu\omega^2 r^2 \right] u(r) = E\, u(r) \quad ,$$

tem soluções

$$F(\nu, r) = \sqrt{\mu\omega r^2}\, e^{-\frac{1}{2}\mu\omega r^2} \phi\left(-\nu; \tfrac{3}{2}; \mu\omega r^2\right)$$

e

$$G(\nu, r) = \sqrt{\mu\omega r^2}\, e^{-\frac{1}{2}\mu\omega r^2} \psi\left(-\nu; \tfrac{3}{2}; \mu\omega r^2\right) \quad ,$$

onde o número quântico radial ν se defina por

$$E = \omega\left(2\nu + \tfrac{3}{2}\right) + m_q + m_{\bar{q}} \quad ,$$

e as funções ϕ e ψ por (utiliza o resultado do problema 19)

$$\phi(a; b; z) = \sum_{n=0}^{\infty} \frac{(a)_n z^n}{(b)_n n!} \quad \text{with} \quad (a)_0 = 1 \quad \text{and} \quad (a)_{n+1} = (a+n)(a)_n$$

e

$$\psi\left(a; \tfrac{3}{2}; z\right) = \frac{1}{\Gamma\left(a - \frac{1}{2}\right)} \phi\left(a; \tfrac{3}{2}; z\right) - \frac{1}{\Gamma(a)} z^{-1/2} \phi\left(a - \tfrac{1}{2}; \tfrac{1}{2}; z\right) \quad .$$

41. Uma solução geral da seguinte equação radial de Schrödinger

$$\begin{pmatrix} -\frac{1}{2\mu}\frac{d^2}{dr^2} + \frac{1}{2}\mu\omega^2 r^2 & \lambda\,\delta(r-a) \\ \lambda\,\delta(r-a) & -\frac{1}{2\mu}\frac{d^2}{dr^2} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = E \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad .$$

é dada por

$$\begin{pmatrix} u_c(r) \\ u_s(r) \end{pmatrix} = \begin{cases} \begin{pmatrix} F(\nu, r)\ A_c \\ \sin(kr)\ \ A_s \end{pmatrix} & r < a \\ \\ \begin{pmatrix} G(\nu, r)\ B_c \\ \sin(kr + \delta)\ \ B_s \end{pmatrix} & r > a \end{cases}$$

determina, por eliminação de A_c, A_s e B_s, uma expressão para cotg(δ).

42. Seja a amplitude da probabiblidade de transição entre o estado s e o estado k dada por

$$c_k(+\infty) \; = \; -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt' \; V_{ks} \; e^{i\omega_{ks} t'} \quad ,$$

onde $V_{ks} = \langle k \, |V| \, s \rangle$ e V hermítico. Mostrar que a amplitude da probabiblidade de transição entre o estado s e o estado k, dada por

$$c'_s(+\infty) \; = \; -\frac{i}{\hbar} \int_{-\infty}^{+\infty} dt' \; V_{sk} \; e^{i\omega_{sk} t'} \quad ,$$

tem a seguinte propriedade (*detailed balancing*)

$$c'_s(+\infty) \; = \; -\left\{ c_k(+\infty) \right\}^* \quad .$$

43. Mostrar que para radiação polarizada (na direcção $\hat{e}$), dada por

$$\vec{A}(\vec{r}, t) \; = \; \int_{-\infty}^{+\infty} d\omega A(\omega) \hat{e} \; e^{-i\omega \left(t - \dfrac{\hat{n} \cdot \vec{r}}{c} \right)} \quad ,$$

o vector Poynting é dado por

$$\vec{N} \; = \; -\frac{\hat{n}}{4\pi c} \int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\omega' \; A(\omega) A(\omega') \; e^{-i(\omega + \omega') \left(t - \dfrac{\hat{n} \cdot \vec{r}}{c} \right)} \quad .$$

44. Para a amplitude de transição, dada por

$$f\left(\vec{k}, \hat{r} \right) \; = \; -\sqrt{2\pi} \; \mu \int d^3 r' \; e^{-ik\hat{r} \cdot \vec{r}\,'} V\left(\vec{r}\,' \right) \psi^{(+)}\left(\vec{k}, \vec{r}\,' \right) \quad ,$$

deduza a seguinte relação

$$f\left(\vec{k}, \hat{r} \right) \; = \; -4\pi^2 \mu \sum_{\ell=0}^{\infty} (2\ell + 1) \; P_\ell\left(\hat{k} \cdot \hat{r} \right) \; T_\ell(k) \quad ,$$

onde $T_\ell(k, k')$ se defina por

$$\left\langle \vec{k} \; | T\left(k^2 + i\epsilon \right) | \; \vec{k}\,' \right\rangle \; = \; \sum_{\ell=0}^{\infty} (2\ell + 1) \; P_\ell\left(\hat{k} \cdot \hat{k}\,' \right) \; T_\ell(k, k') \quad .$$

45. A equação de Schrödinger para um potencial não-local tem a seguinte forma

$$-\frac{1}{2\mu} \nabla_r^2 \ \psi(\vec{r}\,) \ + \ \int d^3r' \ V\left(\vec{r}\,,\vec{r}\,'\right) \ \psi\left(\vec{r}\,'\right) \ = \ E\,\psi(\vec{r}\,) \quad ,$$

onde E representa a energia total do sistema.
Mostra que no espaço dos momentos lineares a equação correspondente é dada por

$$\frac{k^2}{2\mu}\,\phi\left(\vec{k}\,\right) \ + \ \int d^3k' \ V\left(\vec{k}\,,\vec{k}\,'\right) \ \phi\left(\vec{k}\,'\right) \ = \ E\,\phi\left(\vec{k}\,\right) \quad .$$

Qual a relação entre $\psi(\vec{r}\,)$ e $\phi\left(\vec{k}\,\right)$?

46. Considere o seguinte sistema de equações acopladas

$$(E - H_c) \ \psi_c(\vec{r}\,) \ = \ V_t\,\psi_f(\vec{r}\,) \quad \text{and} \quad (E - H_f) \ \psi_f(\vec{r}\,) \ = \ V_t\,\psi_c(\vec{r}\,) \quad ,$$

Onde o espectro discreto de H_c é dado por

$$H_c\,Y_m^{(\ell_c)}(\hat{r}) \ \mathcal{F}_{n\ell_c}(r) \ = \ E_{n\ell_c}\,Y_m^{(\ell_c)}(\hat{r}) \ \mathcal{F}_{n\ell_c}(r) \ \text{ com } \left\{ \begin{array}{l} n = 0,\,1,\,2,\,\ldots\,, \\ \\ \ell_c = 0,\,1,\,2,\,\ldots\,, \\ \\ m = -\ell_c,\,\ldots,\,+\ell_c\,. \end{array} \right. \quad ,$$

e onde H_f e V_t são dados por

$$H_f \ = \ -\frac{1}{2}\,\mu^{-1} \ \nabla_r^2 \ + M_1 \ + \ M_2 \quad , \quad \text{e} \quad V_t \ = \ \frac{\lambda}{a^{3/2}}\,\bar{V}_t\,\delta(r-a) \quad .$$

a. Mostra que o operador de dispersão na onda parcial ℓ é dado por

$$S_\ell(E) \ = \ \left[1 \ - \ 2i\frac{\lambda^2}{pa}\,\mu\,J(a)\,H^{(2)}(a) \ \left[\bar{V}_t\right]^2 \ \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell_c}(a)\right|^2}{E - E_{n\ell_c}} \ \right]$$

$$\times\left[1 \ + \ 2i\frac{\lambda^2}{pa}\,\mu\,J(a)\,H^{(1)}(a) \ \left[\bar{V}_t\right]^2 \ \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell_c}(a)\right|^2}{E - E_{n\ell_c}} \ \right]^{-1} \quad ,$$

com

$$J(a) \ = \ pa\,j_\ell(pa) \quad \text{e} \quad H^{(1,2)}(a) \ = \ pa\,h_\ell^{(1,2)}(pa) \quad .$$

47. Considere a dispersão de uma partícula num potencial esférico cuja dinâmica é dada pela seguinte equação

$$\Big(-\bigtriangledown^2 + g\delta(r-a)\Big)\,\psi\,(\vec{r}\,) \;=\; k^2\psi\,(\vec{r}\,) \tag{13}$$

a Mostre, para onda S ($\ell = 0$), a solução da equação (13) é dada por (A e B constantes)

$$\psi\,(\vec{r}\,) = \frac{u(r)}{r} Y_0^0\,(\hat{r}\,)\,, \quad \text{onde} \quad u(r) = \begin{cases} A\sin(kr) & \text{para} \quad r < a \\ B\sin(kr+\delta) & \text{para} \quad r > a \end{cases},$$

demostre que

$$\text{cotg}(\delta) \;=\; = -\text{cotg}(ka) - \frac{k}{g\sin^2(ka)}$$

e determine a relação entre A e B.

b Demostre que a amplitude de dispersão na aproximação de Born é dada por

$$f(k,\hat{r}) = -\frac{m}{2\pi}\int d^3r'\; e^{i\left(\vec{k}-k\hat{r}\right)\cdot\vec{r}\,'}\,V\,(\vec{r}\,') =$$

$$= -\frac{gm}{2\pi}\int d^3r'\; e^{i\left(\vec{k}-k\hat{r}\right)\cdot\vec{r}\,'}\,\delta(a-r'\,) = -\frac{2gm}{\left|\vec{k}-k\hat{r}\right|}\,a\sin\left(\left|\vec{k}-k\hat{r}\right|a\right)$$

c Utilizando o resultado da alínea (**a**) determine o termo em ordem g para $g\downarrow 0$ da expressão

$$f(k) \;=\; \frac{2m}{k}\,e^{i\delta}\,\sin(\delta)$$

d Utilizando o resultado da alínea (**b**) determine a componente da onda S dada pela expressão

$$f(k) \;=\; \int\frac{d\Omega}{4\pi}\,f(k,\hat{r})$$

48. Considere o sistema electrão-protão cuja dinâmica é dada por

$$H_0 = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{r} \tag{14}$$

a Mostre que o estado próprio principal $\psi_0^{(0)}$ é dado por

$$\psi_0^{(0)}(\vec{r}) = \mathcal{N} e^{-r/a}$$

pela energia própria igual a $E_0 = -e^2/2a$, onde $\mathcal{N}$ é uma constante de normalização e onde o raio de Bohr, a, é dado por $a = \hbar^2/\mu e^2$.

b Para um operador $F = F(\vec{r}) = -\frac{\mu a}{\hbar^2}\left(\frac{1}{2}r + a\right) z$ demonstre que

$$[F\ ,\ H_0] = \frac{\hbar^2}{2\mu}\left\{\left(\nabla^2 F\right) + 2\left(\nabla F\right)\nabla\right\} \quad \Longleftrightarrow \quad [F\ ,\ H_0]\,\psi_0^{(0)} = z\psi_0^{(0)} \quad .$$

c Para um campo eléctrico fraco, dado por $\vec{E} = E\hat{z}$, o termo quadrático do efeito de Stark no estado principal é dado por

$$e^2E^2\sum_{k\neq 0}\frac{z_{0k}z_{k0}}{E_0^{(0)} - E_k^{(0)}}$$

Utilizando o resultado da alínea (**b**) mostre que

$$z_{k0} \quad = \quad \langle k\,|z|\,0\rangle = \left(E_0^{(0)} - E_k^{(0)}\right)\langle k\,|F|\,0\rangle$$

e, ainda, que

$$e^2E^2\sum_{k\neq 0}\frac{z_{0k}z_{k0}}{E_0^{(0)}-E_k^{(0)}} = e^2E^2\sum_{k\neq 0}\langle 0\,|z|\,k\rangle\langle k\,|F|\,0\rangle =$$

$$= e^2E^2\left\{\sum_k \langle 0\,|z|\,k\rangle\langle k\,|F|\,0\rangle - \langle 0\,|z|\,0\rangle\langle 0\,|F|\,0\rangle\right\}$$

$$= e^2E^2\left\{\langle 0\,|Fz|\,0\rangle - \langle 0\,|z|\,0\rangle\langle 0\,|F|\,0\rangle\right\}$$

d Demonstre que $\langle 0\,|z|\,0\rangle = 0$ e portanto

$$e^2E^2\sum_{k\neq 0}\frac{z_{0k}z_{k0}}{E_0^{(0)}-E_k^{(0)}} = -\tfrac{1}{3}E^2\left\langle 0\left|\left(\tfrac{1}{2}r + a\right)z^2\right|0\right\rangle$$

e Utilizando a simetria esférica do estado principal $\psi_0^{(0)}$ e o resultado da alínea (**d**) demonstre que

$$\langle 0\,|f(r)x^2|\,0\rangle = \langle 0\,|f(r)y^2|\,0\rangle = \langle 0\,|f(r)z^2|\,0\rangle \quad = \quad \tfrac{1}{3}\langle 0\,|f(r)r^2|\,0\rangle$$

e portanto, com $E_0^{(1)} = 0$, temos

$$E_0 = E_0^{(0)} + E_0^{(2)} + \ldots \quad = \quad -\frac{e^2}{2a} - \tfrac{1}{3}E^2\left\{\tfrac{1}{2}\langle 0\,|r^3|\,0\rangle + a\langle 0\,|r^2|\,0\rangle\right\} + \ldots$$

$$= \quad -\frac{e^2}{2a} - \tfrac{9}{4}a^3E^2 + \ldots$$

49. Neste problema pretende-se mostrar que $\{2\} \otimes \{5\} = \{6\} \oplus \{4\}$.

a Determine os valores próprios de L^2, L_z, $\left(\frac{\vec{\sigma}}{2}\right)^2$ e $\frac{\sigma_z}{2}$ de cada um dos seguintes dez estados

$$\begin{pmatrix} Y_{2,m}(\hat{r}) \\ 0 \end{pmatrix} \quad , \quad \begin{pmatrix} 0 \\ Y_{2,m}(\hat{r}) \end{pmatrix} \quad , \quad \text{com} \;\; m = 0, \pm 1, \pm 2 \;\; .$$

b Estes estados formam uma base ortonormal do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 2\}$. Temos por exemplo:

$$\left| s = \tfrac{1}{2}, s_z = +\tfrac{1}{2} \right\rangle \otimes |\ell = 2, \ell_z = +2\rangle = \begin{pmatrix} Y_{2,+2} \\ 0 \end{pmatrix} \; .$$

Determine relações semelhantes para os outros nove estados.

c Uma outra base ortonormal do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 2\}$ é dada por:

$$\begin{pmatrix} Y_{2,+2} \\ 0 \end{pmatrix}, \begin{pmatrix} \sqrt{\frac{4}{5}} Y_{2,+1} \\ \sqrt{\frac{1}{5}} Y_{2,+2} \end{pmatrix}, \begin{pmatrix} \sqrt{\frac{3}{5}} Y_{2,0} \\ \sqrt{\frac{2}{5}} Y_{2,+1} \end{pmatrix}, \begin{pmatrix} \sqrt{\frac{2}{5}} Y_{2,-1} \\ \sqrt{\frac{3}{5}} Y_{2,0} \end{pmatrix}, \begin{pmatrix} \sqrt{\frac{1}{5}} Y_{2,-2} \\ \sqrt{\frac{4}{5}} Y_{2,-1} \end{pmatrix}, \begin{pmatrix} 0 \\ Y_{2,-2} \end{pmatrix},$$

$$\begin{pmatrix} -\sqrt{\frac{1}{5}} Y_{2,+1} \\ \sqrt{\frac{4}{5}} Y_{2,+2} \end{pmatrix}, \begin{pmatrix} -\sqrt{\frac{2}{5}} Y_{2,0} \\ \sqrt{\frac{3}{5}} Y_{2,+1} \end{pmatrix}, \begin{pmatrix} -\sqrt{\frac{3}{5}} Y_{2,-1} \\ \sqrt{\frac{2}{5}} Y_{2,0} \end{pmatrix} \text{ e } \begin{pmatrix} -\sqrt{\frac{4}{5}} Y_{2,-2} \\ \sqrt{\frac{1}{5}} Y_{1,-1} \end{pmatrix}.$$

Determine, se possível, os valores próprios de L^2, L_z, $\left(\frac{\vec{\sigma}}{2}\right)^2$, $\frac{\sigma_z}{2}$, e ainda de $J^2 = \left(\vec{L} + \frac{\vec{\sigma}}{2}\right)^2$ e $J_z = L_z + \frac{\sigma_z}{2}$ de cada um destes dez estados.

d Verifica-se que podemos dividir o espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 2\}$ em dois subespaços: $\left\{j = \frac{5}{2}\right\}$ de seis dimensões e $\left\{j = \frac{3}{2}\right\}$ de quatro dimensões. Os estados destes últimos espaços são designados por $|j, j_z\rangle$. Temos por exemplo:

$$\left| j = \tfrac{5}{2}, j_z = +\tfrac{5}{2} \right\rangle = \begin{pmatrix} Y_{2,+2} \\ 0 \end{pmatrix} = \left| s = \tfrac{1}{2}, s_z = +\tfrac{1}{2} \right\rangle \otimes |\ell = 2, \ell_z = +2\rangle \; .$$

Determine relações semelhantes para os outros nove estados da alínea (c).

e Os coeficientes destas relações chamam-se coeficientes de Clebsch-Gordan (CCG), designados por:

$$\begin{pmatrix} \ell & s & j \\ \ell_z & s_z & j_z \end{pmatrix} \ .$$

Da relação dada na alínea (d) determina-se por exemplo:

$$\begin{pmatrix} 2 & \frac{1}{2} & \frac{5}{2} \\ +2 & +\frac{1}{2} & +\frac{5}{2} \end{pmatrix} = 1 \ .$$

Determine os outros CCG das relações entre as bases dos subespaços $\left\{j = \frac{5}{2}\right\}$ e $\left\{j = \frac{3}{2}\right\}$ e a base do espaço $\{s = \frac{1}{2}\} \otimes \{\ell = 2\}$.

50. Considere um sistema de dois estados descrito pelo seguinte Hamiltoniano:

$$H = \begin{pmatrix} A & \frac{B}{r} \\ Br & A \end{pmatrix} \quad \text{com} \quad \left\{ \begin{array}{l} A = M + \frac{1}{2}\left(\Delta M - \frac{1}{2}i\left(\gamma_1 + \gamma_2\right)\right) \\ B = -\frac{1}{2}\left(\Delta M + \frac{1}{2}i\left(\gamma_1 - \gamma_2\right)\right) \end{array} \right. \quad . \tag{15}$$

O parâmetro complexo r é dado pela expressão $r = 1 - 2\varepsilon$ onde $|\varepsilon| \ll 1$. Notar que H não é hermítico e portanto $H^\dagger \neq H$.

a Mostre que os dois estados próprios normalizados do Hamiltoniano (15) são dados por

$$\phi_\pm = \frac{1}{\sqrt{1 + |r|^2}} \begin{pmatrix} 1 \\ \pm r \end{pmatrix}$$

e determine os valores próprios $E_\pm$.

b Seja um estado abitrário $\psi(t)$ deste sistema no instant $t = 0$ dado pelo "*pacote de ondas*" ($c_\pm$ constantes)

$$\psi(0) = c_+\phi_+ + c_-\phi_- \quad .$$

Mostre que o desenvolvimento temporal $\psi(t) = e^{-iHt}\psi(0)$ pode ser dado por

$$\psi(t) = \frac{1}{E_+ - E_-}\left\{(E_+ - H)\, e^{-iE_- t} - (E_- - H)\, e^{-iE_+ t}\right\}\psi(0) \quad .$$

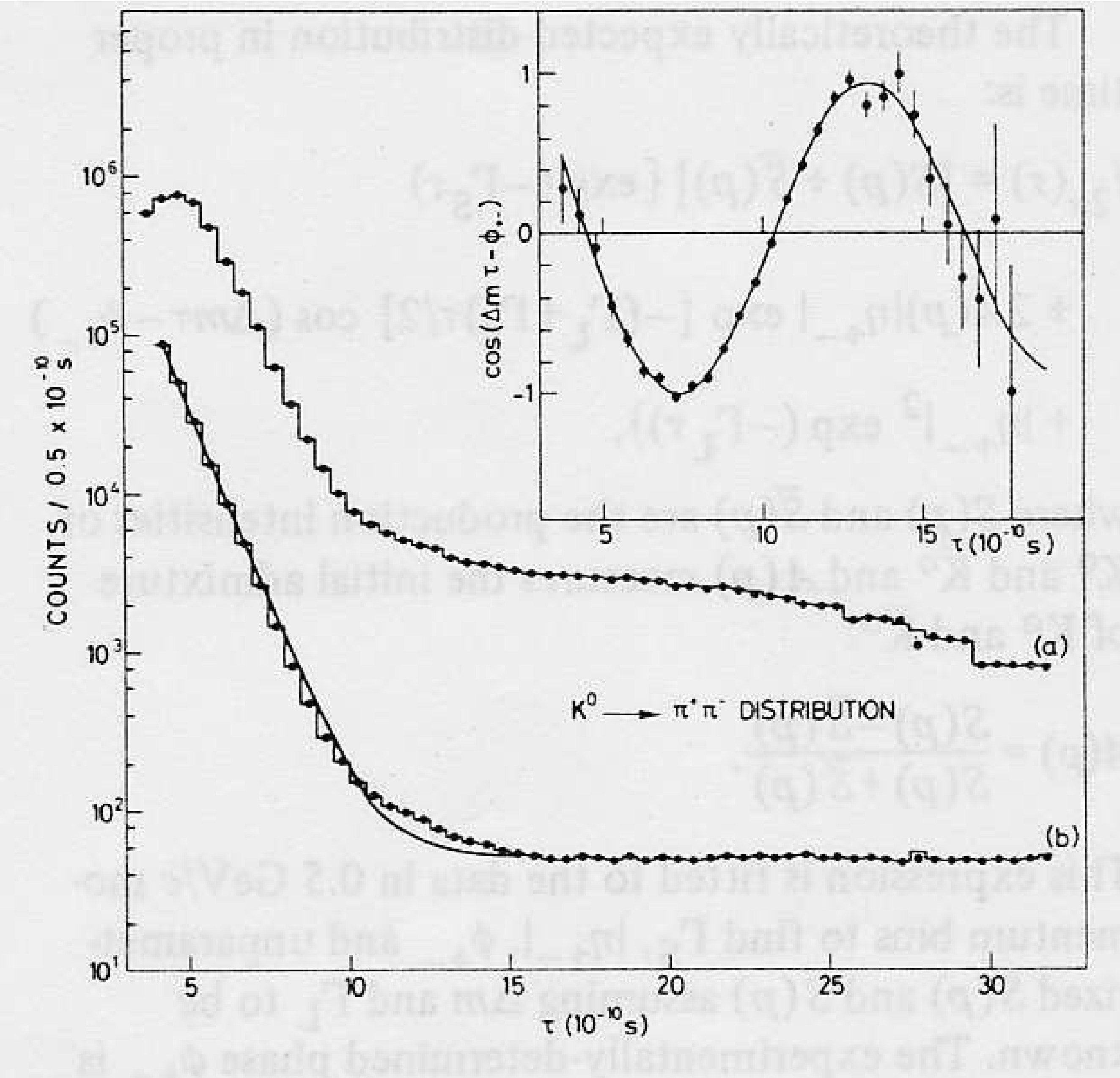
c Determine a amplitude da probabiblidade de transição, $\left\langle \downarrow \left| e^{-iHt} \right| \uparrow \right\rangle$, entre os estados

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{e} \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

e mostre que

$$\left|\left\langle \downarrow \left| e^{-iHt} \right| \uparrow \right\rangle\right|^2 = \tfrac{1}{4}|r|^2 \left\{ e^{-\gamma_1 t} + e^{-\gamma_2 t} - 2e^{-\frac{1}{2}\left(\gamma_1 + \gamma_2\right)t} \cos(\Delta M t) \right\} \quad .$$

d A figura na página seguinte mostra as observações experimentais da desintegração do mesão Kaon neutro. O Kaon neutro é um estado misto do sistema de dois níveis que consiste dos estados próprios K_S de vida curta e K_L de vida longa. As massas do K_S e K_L são aproximadamente idênticas, nomeadamente $M_S \approx M_L \approx 500$ MeV. Os tempos de vida média de K_S e K_L são respectivamente $\gamma_1^{-1} = 0.90 \times 10^{-10}$ s e $\gamma_2^{-1} = 5.2 \times 10^{-8}$ s.
Determine, a partir das observações experimentais, a diferença de massa em eV entre os dois estados próprios, $\Delta M = M_L - M_S$.
Notar que $1 = 0.66 \times 10^{-15}$ eVs em unidades $\hbar = c = 1$.



De C. Geweniger *et al.*, Physics Letters 48B, 483 (1974).

Solutions

Exercício 1

a. The example we study here for φ is a function of k which peaks around a certain value $k = \bar{k}$ and which vanishes rapidly for large values of $|k|$. For the sake of calculational simplicity we choose a Fourier transform which vanishes everywhere at the k-axis except for a small interval where it has a constant value different from zero, as is shown in figure (1a). The wave packet ψ

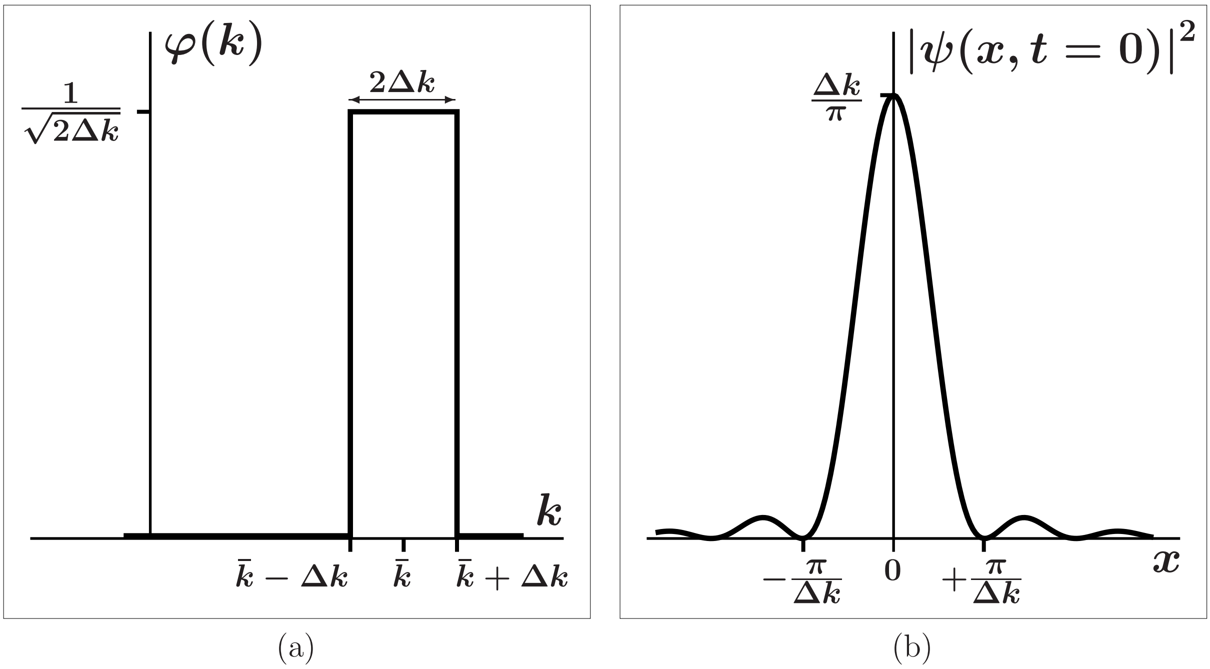


Figure 1: (a) The Fourier transform in one dimension of a wave packet which differs from zero only in a small region of width $2\Delta k$ around a central value $k = \bar{k}$. (b) The corresponding wave packet at the instant $t = 0$.

which follows for the above choice of Fourier transform φ can readily be determined to be given by

$$
\begin{aligned}
\psi(x, t = 0) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \varphi(k)\, e^{ikx} = \frac{1}{\sqrt{2\pi}} \int_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} dk\, \frac{1}{\sqrt{2\Delta k}}\, e^{ikx} \\
&= \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2\Delta k}} \left[\frac{e^{ikx}}{ix} \right]_{\bar{k} - \Delta k}^{\bar{k} + \Delta k} = \frac{1}{2\sqrt{\pi \Delta k}} \frac{e^{i\left(\bar{k} + \Delta k\right)x} - e^{i\left(\bar{k} - \Delta k\right)x}}{ix} \\
&= \frac{e^{i\bar{k}x}}{x\sqrt{\pi\Delta k}} \frac{e^{i\Delta kx} - e^{-i\Delta kx}}{2i} = \frac{1}{\sqrt{\pi\Delta k}}\, e^{i\bar{k}x}\, \frac{\sin\left(\Delta k\, x\right)}{x} \quad , \qquad (16)
\end{aligned}
$$

the probability distribution of which expression is given by

$$
|\psi(x, t = 0)|^2 = \frac{\Delta k}{\pi} \left(\frac{\sin\left(\Delta k\, x\right)}{\Delta k x} \right)^2
$$

and is depicted in figure (1b).

b. From Fig. 1a we read for the uncertainty in k the value Δk, since

$$k = \bar{k} \pm \Delta k$$

whereas, for the uncertainty in x, we find $\Delta x = \pi/\Delta k$, since

$$x = 0 \pm \frac{\pi}{\Delta k}$$

Hence

$$\Delta x \Delta k = \frac{\pi}{\Delta k}\Delta k = \pi \geq 1 \quad \text{(Heisenberg)}$$

Exercício 2

a.

$$\int_{-\infty}^{\infty} dk \ |\varphi(k)|^2 = \int_{\bar{k}-\Delta k}^{\bar{k}+\Delta k} dk \ \frac{1}{2\Delta k} = 1 \quad .$$

b.

$$\int_{-\infty}^{\infty} dx \ |\psi(x, t = 0)|^2 \ = \ \int_{-\infty}^{\infty} dx \ \frac{\Delta k}{\pi} \ \left(\frac{\sin(\Delta k \ x)}{\Delta k x}\right)^2$$

From integral number 11 of the integral tabel at the web page http://www.sosmath.com/tables/-integral/integ37/integ37.html we learn

$$\int_0^{\infty} dx \ \left(\frac{\sin(px)}{x}\right)^2 \ = \ \frac{\pi p}{2}$$

Hence

$$\int_{-\infty}^{\infty} dx \ \frac{\Delta k}{\pi} \ \left(\frac{\sin(\Delta k \ x)}{\Delta k x}\right)^2 \ = \ \frac{1}{\pi \Delta k} \ 2 \int_0^{\infty} dx \ \left(\frac{\sin(\Delta k \ x)}{x}\right)^2 \ = \ \frac{1}{\pi \Delta k} \ 2 \ \frac{\pi \Delta k}{2} \ = \ 1 \quad .$$

c e **d**.

$$\int_{-\infty}^{\infty} dx \ |\psi(x, t = 0)|^2 \ = \ \int_{-\infty}^{\infty} dx \ \psi^*(x, t = 0)\psi(x, t = 0) \ =$$

$$= \int_{-\infty}^{\infty} dx \ \left\{\frac{1}{\sqrt{2\pi}} \ \int_{-\infty}^{\infty} dk \ \varphi(k) \ e^{ikx}\right\}^* \left\{\frac{1}{\sqrt{2\pi}} \ \int_{-\infty}^{\infty} dk' \ \varphi(k') \ e^{ik'x}\right\} \ =$$

$$= \int_{-\infty}^{\infty} dk \ \int_{-\infty}^{\infty} dk' \ \varphi^*(k) \ \varphi(k') \ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \ e^{-ikx} e^{ik'x} \ =$$

$$= \int_{-\infty}^{\infty} dk \ \int_{-\infty}^{\infty} dk' \ \varphi^*(k) \ \varphi(k') \ \frac{1}{2\pi} \int_{-\infty}^{\infty} dx \ e^{i(k'-k)x} \ =$$

$$= \int_{-\infty}^{\infty} dk \ \varphi^*(k) \ \int_{-\infty}^{\infty} dk' \ \varphi(k') \ \delta(k' - k) = \int_{-\infty}^{\infty} dk \ \varphi^*(k) \ \varphi(k) \ = \ \int_{-\infty}^{\infty} dk \ |\varphi(k)|^2$$

Exercício 3

The general expression for the time development of a wave packet is as follows:

$$\psi(x,t) \;=\; \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\,\varphi(k)\exp\left\{i\left(kx-\omega(k)t\right)\right\} \quad , \tag{17}$$

where $\omega(k)$ is some function of momentum k.

In order to study the above expression (17), we assume that ω is linear in k, at least for values where the Fourier transform φ is maximal, *i.e.*

$$\omega(k) \;=\; \bar{\omega} \;+\; \bar{\omega}'(k-\bar{k}) \quad . \tag{18}$$

Such choice for ω leads for the wave packet (17) to the expression

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\,\varphi(k)\exp\left\{i\left(kx-\left[\bar{\omega}\;+\;\bar{\omega}'(k-\bar{k})\right]t\right)\right\}\\ &= \frac{1}{\sqrt{2\pi}}\exp\left\{i\left(-\bar{\omega}t+\bar{\omega}'\bar{k}t\right)\right\}\int_{-\infty}^{\infty} dk\,\varphi(k)\exp\left\{ik\left(x-\bar{\omega}'t\right)\right\}\\ &= \exp\left\{it\left(-\bar{\omega}+\bar{\omega}'\bar{k}\right)\right\}\;\psi(x-\bar{\omega}'t,0) \quad ,\end{aligned} \tag{19}$$

which implies that apart from a phase factor and a translation along the x-axis, the wave packet at the instant t has the same form as the wave packet at the instant $t=0$. For the probability distribution one finds consequently

$$\left|\psi(x,t)\right|^2 \;=\; \left|\psi(x-\bar{\omega}'t,0)\right|^2 \quad . \tag{20}$$

From the latter formula we read that the central peak in the probability distribution, which according to figure (1b) at $t=0$ is found at the origin of the x-axis, is located at the position $x=\bar{\omega}'t$ at the instant of time t. Consequently, for ω linear in k as in formula (18), the wave packet moves with a constant velocity $\bar{\omega}'$ and hence represents a freely moving particle. The general idea is depicted in figure (2).

Notice, that for ω linear in k as in formula (18), the wave packet does not spread as time develops. A feature which at first sight also seems quite reasonable for a point particle in the absence of external forces. However, in general ω is not linear in k as in formula (18). Hence, also quadratic and higher order terms must be considered which in general leads to spreading.

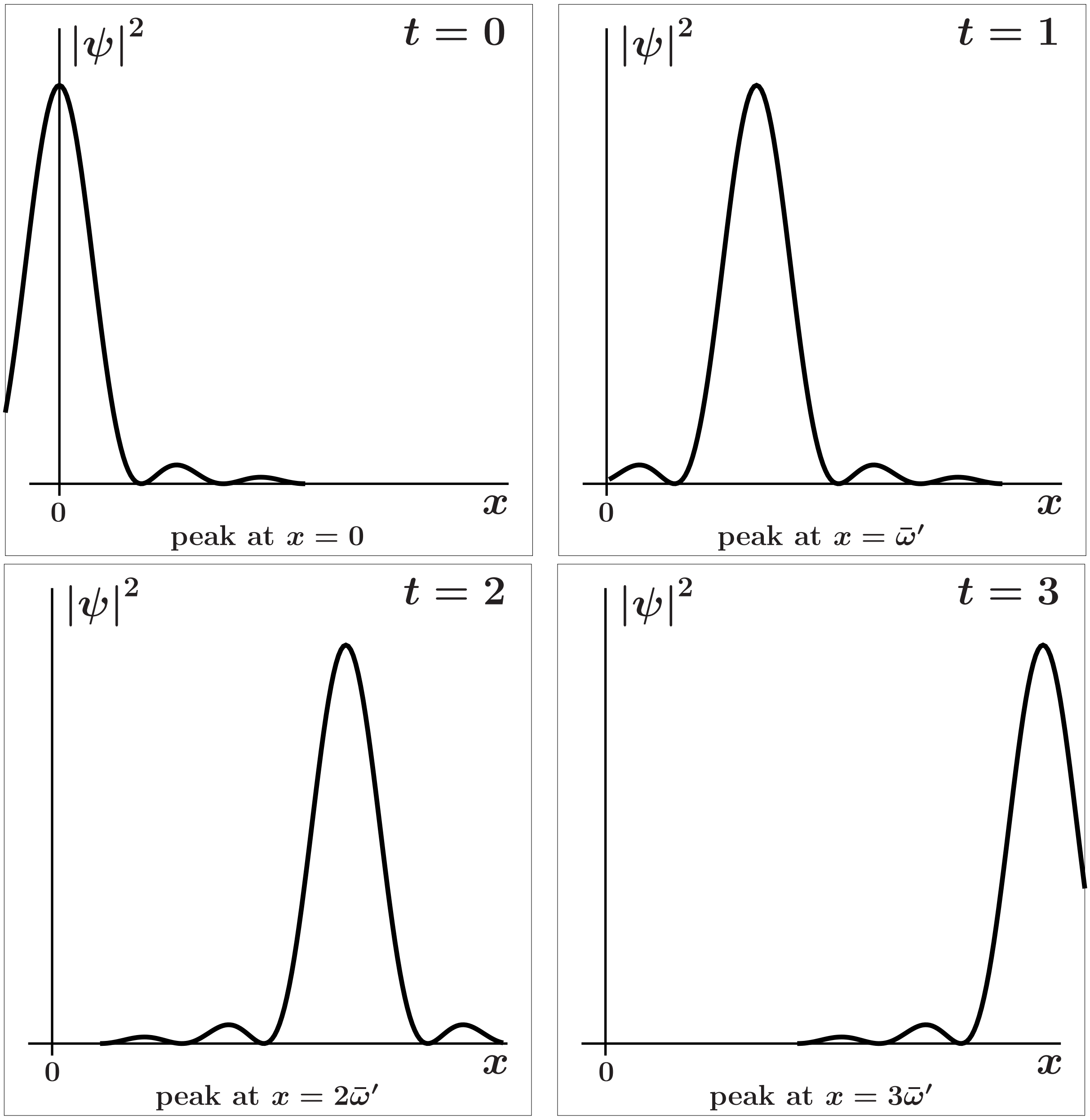


Figure 2: The probability distribution (20) in space (x) of wave packet (19) for the momentum distribution (1) at four different instances, $t = 0$, 1, 2 and 3. The position of the maximum probability, which represents the most probable place where the particle can be found, moves at constant velocity $\bar{\omega}'$.

b. From expression (17) we obtain

$$\begin{aligned}
i\frac{\partial}{\partial t}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k) i\frac{\partial}{\partial t}\exp\left\{i\left(kx-\omega(k)t\right)\right\} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\omega(k)\exp\left\{i\left(kx-\omega(k)t\right)\right\} \quad ,
\end{aligned} \tag{21}$$

and

$$\begin{aligned}
-\frac{1}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\left(-\frac{1}{2m}\frac{\partial^2}{\partial x^2}\right)\exp\left\{i\left(kx-\omega(k)t\right)\right\} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\frac{k^2}{2m}\exp\left\{i\left(kx-\omega(k)t\right)\right\} \quad ,
\end{aligned} \tag{22}$$

With $\omega(k) = \frac{k^2}{2m}$ and the results (21) and (22), we find that the wave function satisfies the Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = -\frac{1}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t)$$

Exercício 4

For expression (2) we find

$$\begin{aligned}
\frac{\partial^2}{\partial t^2}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\frac{\partial^2}{\partial t^2}\exp\left\{i\left(kx-\omega(k)t\right)\right\} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\left(-\omega^2(k)\right)\exp\left\{i\left(kx-\omega(k)t\right)\right\} \quad ,
\end{aligned} \tag{23}$$

and

$$\begin{aligned}
\frac{\partial^2}{\partial x^2}\psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\frac{\partial^2}{\partial x^2}\exp\left\{i\left(kx-\omega(k)t\right)\right\} \\
&= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\ \varphi(k)\left(-k^2\right)\exp\left\{i\left(kx-\omega(k)t\right)\right\} \quad ,
\end{aligned} \tag{24}$$

With $-\omega^2(k) = -k^2 - m^2$ and the results (23) and (24), we find that the wave function satisfies the Klein-Gordon equation

$$\frac{\partial^2}{\partial t^2}\psi(x,t) = \left(-k^2-m^2\right)\psi(x,t) = \left(\frac{\partial^2}{\partial x^2}-m^2\right)\psi(x,t) \tag{25}$$

b. First we need the inverse transformations

$$\gamma x' + \gamma\beta t' = \gamma^2\left(x-\beta t\right) + \gamma^2\beta\left(t-\beta x\right) = \gamma^2\left(1-\beta^2\right)x = x$$

and

$$\gamma t' + \gamma\beta x' = \gamma^2\left(t-\beta x\right) + \gamma^2\beta\left(x-\beta t\right) = \gamma^2\left(1-\beta^2\right)t = t$$

Hence

$$x \;=\; \gamma\left(x' + \beta t'\right) \quad \text{and} \quad t \;=\; \gamma\left(t' + \beta x'\right) \tag{26}$$

Then, we substitute those relations into expression (2), which leads to

$$\begin{aligned}
\psi'(x',t') &= \psi(x(x',t'),t(x',t')) \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) \exp\left\{i\left[k\gamma\left(x' + \beta t'\right) - \omega\gamma\left(t' + \beta x'\right)\right]\right\} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) \exp\left\{i\left[\gamma\left(k - \beta\omega\right)x' - \gamma\left(\omega - \beta k\right)t'\right]\right\}
\end{aligned}$$

Now, when we define

$$k'(k) \;=\; \gamma\left(k - \beta\omega\right) \quad \text{and} \quad \omega'(k) \;=\; \gamma\left(\omega - \beta k\right) \quad ,$$

then we find

$$\begin{aligned}
\left(\omega'\right)^2 - \left(k'\right)^2 &= \gamma^2\left(\omega - \beta k\right)^2 - \gamma^2\left(k - \beta\omega\right)^2 \\
&= \gamma^2\left(\omega^2 - 2\beta\omega k + \beta^2 k^2 - k^2 + 2\beta\omega k - \beta^2\omega^2\right) \\
&= \gamma^2\left(1 - \beta^2\right)\left(\omega^2 - k^2\right) = \omega^2 - k^2 = m^2
\end{aligned} \tag{27}$$

We find for the new wave function

$$\begin{aligned}
\psi'(x',t') &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) \exp\left\{i\left[\gamma\left(k - \beta\omega\right)x' - \gamma\left(\omega - \beta k\right)t'\right]\right\} \\
&= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\; \varphi(k) \exp\left\{i\left[k'(k)x' - \omega'(k)t'\right]\right\}
\end{aligned}$$

which, because of relation (27), obviously satisfies a wave equation of the same form as the Klein-Gordon equation (25), namely

$$\frac{\partial^2}{\partial\left(t'\right)^2}\psi'(x',t') \;=\; \left(\frac{\partial^2}{\partial\left(x'\right)^2} - m^2\right)\psi'(x',t')$$

Exercício 5

a. First, we notice

$$\begin{aligned}
\varphi\left(\vec{k}\right) &= \prod_{i=1}^{3} \frac{1}{\sqrt{2\Delta k_i}}\; \theta\left(\left(\Delta k_i\right)^2 - \left(k_i - \bar{k}_i\right)^2\right) \\
&= \begin{cases} \dfrac{1}{\sqrt{2\Delta k_1}}\dfrac{1}{\sqrt{2\Delta k_2}}\dfrac{1}{\sqrt{2\Delta k_3}} & ,\left|k_i - \bar{k}_i\right| \leq \Delta k_i \quad i = 1, \;\text{ e }\; i = 2, \;\text{ e }\; i = 3 \\[2ex] 0 & ,\left|k_i - \bar{k}_i\right| > \Delta k_i \quad i = 1, \;\text{ ou }\; i = 2, \;\text{ ou }\; i = 3 \end{cases}
\end{aligned}$$

Hence

$$\varphi\left(\vec{k}\right) = \begin{cases} \prod_{i=1}^{3}\frac{1}{\sqrt{2\Delta k_i}} & ,\left|k_1-\bar{k}_1\right| \leq \Delta k_1 \text{ and } \left|k_2-\bar{k}_2\right| \leq \Delta k_2 \text{ and } \left|k_3-\bar{k}_3\right| \leq \Delta k_3 \\ 0 & ,\left|k_1-\bar{k}_1\right| > \Delta k_1 \text{ or } \left|k_2-\bar{k}_2\right| > \Delta k_2 \text{ or } \left|k_3-\bar{k}_3\right| > \Delta k_3 \end{cases}$$

Furthermore

$$\vec{k}\cdot(\vec{x}-\vec{x}_0) - E\left(\vec{k}\right)t =$$
$$= k_1\left(x_1-(\vec{x}_0)_1\right) + k_2\left(x_2-(\vec{x}_0)_2\right) + k_3\left(x_3-(\vec{x}_0)_3\right) - \frac{1}{2m}\left(k_1^2+k_2^2+k_3^2\right)t$$

Hence

$$\exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0) - E\left(\vec{k}\right)t\right]\right\} = \prod_{i=1}^{3}\exp\left\{i\left[k_i\left(x_i-(\vec{x}_0)_i\right) - \frac{1}{2m}k_i^2 t\right]\right\}$$

Moreover

$$\left(\frac{1}{2\pi}\right)^{3/2}\int d^3k = \prod_{i=1}^{3}\frac{1}{\sqrt{2\pi}}\int dk_i$$

So, we arrive at

$$\psi(\vec{x},t=0) = \prod_{i=1}^{3}\frac{1}{\sqrt{2\pi}}\int_{\bar{k}_i-\Delta k_i}^{\bar{k}_i+\Delta k_i} dk_i \frac{1}{\sqrt{2\Delta k_i}}\exp\left\{i\left[k_i\left(x_i-(\vec{x}_0)_i\right)\right]\right\}$$

The integral has been calculated for exercise 1a. We obtain

$$\begin{aligned}\psi(\vec{x},t=0) &= \prod_{i=1}^{3}\frac{1}{\sqrt{\pi\Delta k_i}}\, e^{i\bar{k}_i\left(x_i-(\vec{x}_0)_i\right)}\, \frac{\sin\left(\Delta k_i\left[x_i-(\vec{x}_0)_i\right]\right)}{x_i-(\vec{x}_0)_i} \\ &= e^{i\vec{\bar{k}}\cdot(\vec{x}-\vec{x}_0)}\prod_{i=1}^{3}\frac{1}{\sqrt{\pi\Delta k_i}}\,\frac{\sin\left(\Delta k_i\left[x_i-(\vec{x}_0)_i\right]\right)}{x_i-(\vec{x}_0)_i}\end{aligned}$$

The probability distribution is given by

$$|\psi(\vec{x},t=0)|^2 = \prod_{i=1}^{3}\frac{1}{\pi\Delta k_i}\,\frac{\sin^2\left(\Delta k_i\left[x_i-(\vec{x}_0)_i\right]\right)}{\left(x_i-(\vec{x}_0)_i\right)^2}$$

It has its maximum at $x_1=(\vec{x}_0)_1$, $x_2=(\vec{x}_0)_2$ and $x_3=(\vec{x}_0)_3$, or, equivalently, at $\vec{x}=\vec{x}_0$.

b. We determine

$$\begin{aligned} i\frac{\partial}{\partial t}\psi(\vec{x},t) &= \left(\frac{1}{2\pi}\right)^{3/2}\int d^3k\,\varphi\left(\vec{k}\right)E\left(\vec{k}\right)\exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0)-E\left(\vec{k}\right)t\right]\right\} \\ &= \left(\frac{1}{2\pi}\right)^{3/2}\int d^3k\,\varphi\left(\vec{k}\right)\frac{\vec{k}^{\,2}}{2m}\exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0)-E\left(\vec{k}\right)t\right]\right\}\end{aligned}$$

Furthermore

$$-\frac{\partial^2}{\partial {x_1}^2}\psi(\vec{x},t) \;=\; \left(\frac{1}{2\pi}\right)^{3/2}\int d^3k\,\varphi\left(\vec{k}\right)k_1^2\exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0)-E\left(\vec{k}\right)t\right]\right\}$$

Hence

$$-\frac{\nabla^2}{2m}\psi\left(\vec{r},t\right) \;=\; \left(\frac{1}{2\pi}\right)^{3/2}\int d^3k\,\varphi\left(\vec{k}\right)\frac{\vec{k}^{\,2}}{2m}\exp\left\{i\left[\vec{k}\cdot(\vec{x}-\vec{x}_0)-E\left(\vec{k}\right)t\right]\right\}$$

Consequently

$$i\frac{\partial}{\partial t}\psi\left(\vec{r},t\right) \;=\; -\frac{\nabla^2}{2m}\psi\left(\vec{r},t\right)$$

Exercício 6

a. Jean Baptiste Joseph Fourier (1768–1830) discovered that one can represent any periodically repeating function as the sum of a sine, a cosine, and all of their overtones; that is, he discovered that

$$f(x)=\tfrac{1}{2}b_0+\sum_{n=1}^{\infty}a_n\sin\left(\frac{n\pi x}{L}\right)+\sum_{n=1}^{\infty}b_n\cos\left(\frac{n\pi x}{L}\right)\quad .$$

When we define $a_{-n}=-a_n$ and $b_{-n}=b_n$, we obtain

$$\begin{aligned}
a_n\sin\left(\frac{n\pi x}{L}\right) &= \tfrac{1}{2}\left[a_n\sin\left(\frac{n\pi x}{L}\right)+a_{-n}\sin\left(\frac{-n\pi x}{L}\right)\right]\\
b_n\cos\left(\frac{n\pi x}{L}\right) &= \tfrac{1}{2}\left[b_n\cos\left(\frac{n\pi x}{L}\right)+b_{-n}\cos\left(\frac{-n\pi x}{L}\right)\right]\\
\tfrac{1}{2}b_0 &= \tfrac{1}{2}b_0\cos\left(\frac{0\pi x}{L}\right)\\
0 &= a_0\sin\left(\frac{0\pi x}{L}\right)
\end{aligned}$$

So, we arrive at

$$f(x) \;=\; \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n\sin\left(\frac{n\pi x}{L}\right)+b_n\cos\left(\frac{n\pi x}{L}\right)\right]$$

The coefficients a_n and b_n are determined as follows

$$\begin{aligned}
&\frac{1}{L}\int_{-L}^{L}dx f(x)\sin\left(\frac{m\pi x}{L}\right)=\\
&\quad=\frac{1}{L}\int_{-L}^{L}dx\frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n\sin\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)+b_n\cos\left(\frac{n\pi x}{L}\right)\sin\left(\frac{m\pi x}{L}\right)\right]\\
&\quad=\frac{1}{L}\int_{-L}^{L}dx\frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n\frac{1}{2}\left\{\cos\left(\frac{(n-m)\pi x}{L}\right)-\cos\left(\frac{(n+m)\pi x}{L}\right)\right\}+\right.\\
&\quad\left.+b_n\frac{1}{2}\left\{\sin\left(\frac{(n-m)\pi x}{L}\right)+\sin\left(\frac{(n+m)\pi x}{L}\right)\right\}\right]
\end{aligned}$$

The integrals over the sine and cosine functions in the interval $x \in [-L, L]$ vanish, unless the argument equals zero for the cosine. Hence,

$$\begin{aligned}
&\frac{1}{L}\int_{-L}^{L} dx f(x) \sin\left(\frac{m\pi x}{L}\right) = \\
&\quad = \frac{1}{L}\int_{-L}^{L} dx \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \frac{1}{2}\left\{\delta_{n,m} - \delta_{n,-m}\right\} + b_n \frac{1}{2}\left\{0+0\right\}\right] \\
&\quad = \frac{1}{L}\int_{-L}^{L} dx \frac{1}{4}\left\{a_m - a_{-m}\right\} = \frac{a_m}{2L}\int_{-L}^{L} dx = \frac{a_m}{2L}2L = a_m
\end{aligned}$$

Similarly,

$$\begin{aligned}
&\frac{1}{L}\int_{-L}^{L} dx f(x) \cos\left(\frac{m\pi x}{L}\right) = \\
&= \frac{1}{L}\int_{-L}^{L} dx \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \sin\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right) + b_n \cos\left(\frac{n\pi x}{L}\right)\cos\left(\frac{m\pi x}{L}\right)\right] \\
&= \frac{1}{L}\int_{-L}^{L} dx \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \frac{1}{2}\left\{\sin\left(\frac{(n-m)\pi x}{L}\right) + \sin\left(\frac{(n+m)\pi x}{L}\right)\right\} + \right. \\
&\left. + b_n \frac{1}{2}\left\{\cos\left(\frac{(n-m)\pi x}{L}\right) + \cos\left(\frac{(n+m)\pi x}{L}\right)\right\}\right] \\
&= \frac{1}{L}\int_{-L}^{L} dx \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \frac{1}{2}\left\{0+0\right\} + b_n \frac{1}{2}\left\{\delta_{n,m} + \delta_{n,-m}\right\}\right] \\
&= \frac{1}{L}\int_{-L}^{L} dx \frac{1}{4}\left\{b_m + b_{-m}\right\} = \frac{b_m}{2L}\int_{-L}^{L} dx = \frac{b_m}{2L}2L = b_m
\end{aligned}$$

b.

$$\begin{aligned}
f(x) &= \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \sin\left(\frac{n\pi x}{L}\right) + b_n \cos\left(\frac{n\pi x}{L}\right)\right] = \\
&= \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \tfrac{-i}{2}\left\{\exp\left(\frac{in\pi x}{L}\right) - \exp\left(\frac{-in\pi x}{L}\right)\right\} + b_n \tfrac{1}{2}\left\{\exp\left(\frac{in\pi x}{L}\right) + \exp\left(\frac{-in\pi x}{L}\right)\right\}\right] \\
&= \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[\tfrac{1}{2}\left\{b_n - ia_n\right\}\exp\left(\frac{in\pi x}{L}\right) + \tfrac{1}{2}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right)\right] \\
&= \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_n - ia_n\right\}\exp\left(\frac{in\pi x}{L}\right) + \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right) \\
&= \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_{-n} - ia_{-n}\right\}\exp\left(\frac{-in\pi x}{L}\right) + \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right) \\
&= \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right) + \sum_{n=-\infty}^{\infty}\tfrac{1}{4}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right) \\
&= \sum_{n=-\infty}^{\infty}\tfrac{1}{2}\left\{b_n + ia_n\right\}\exp\left(\frac{-in\pi x}{L}\right)
\end{aligned}$$

Hence, with $c_n = \frac{1}{2}\left\{b_n + ia_n\right\}$, we have

$$f(x) \quad = \quad \frac{1}{2}\sum_{n=-\infty}^{\infty}\left[a_n \sin\left(\frac{n\pi x}{L}\right) + b_n \cos\left(\frac{n\pi x}{L}\right)\right] = \sum_{n=-\infty}^{\infty} c_n \exp\left(\frac{-in\pi x}{L}\right)$$

Furthermore

$$
\begin{aligned}
c_m &= \tfrac{1}{2}\left\{b_m + i a_m\right\} = \\
&= \tfrac{1}{2}\left\{\frac{1}{L}\int_{-L}^{L} dx f(x)\cos\left(\frac{m\pi x}{L}\right) + i\frac{1}{L}\int_{-L}^{L} dx f(x)\sin\left(\frac{m\pi x}{L}\right)\right\} \\
&= \frac{1}{2L}\int_{-L}^{L} dx f(x)\left\{\cos\left(\frac{m\pi x}{L}\right) + i\sin\left(\frac{m\pi x}{L}\right)\right\} = \frac{1}{2L}\int_{-L}^{L} dx f(x)\exp\left(\frac{im\pi x}{L}\right)
\end{aligned}
$$

c. First, notice that $\Delta\omega$ vanishes in the limit $L \uparrow \infty$, *i.e.*

$$
\Delta\omega = \frac{\pi}{L} \underset{L\uparrow\infty}{\longrightarrow} 0
$$

Furthermore,

$$
\omega_{n+1} - \omega_n = \frac{(n+1)\pi}{L} - \frac{n\pi}{L} = \frac{\pi}{L} = \Delta\omega
$$

Hence, in the limit $L \uparrow \infty$ the discrete variable ω_n turns into a continuous variable, say ω. Let us write

$$
F(\omega_n) = F_n = \frac{2L}{\sqrt{2\pi}} c_n
$$

We obtain then

$$
\begin{aligned}
f(x) &= \sum_{n=-\infty}^{\infty} c_n \exp\left(\frac{-in\pi x}{L}\right) = \\
&= \sum_{n=-\infty}^{\infty} \frac{\sqrt{2\pi}}{2L} F(\omega_n)\exp(-i\omega_n x) = \sum_{n=-\infty}^{\infty} \frac{\Delta\omega}{\sqrt{2\pi}} F(\omega_n)\exp(-i\omega_n x) \\
&\underset{L\uparrow\infty}{\longrightarrow} \int_{-\infty}^{\infty} \frac{d\omega}{\sqrt{2\pi}} F(\omega)\exp(-i\omega x)
\end{aligned}
$$

and

$$
F(\omega_n) = \frac{2L}{\sqrt{2\pi}} c_n = \frac{2L}{\sqrt{2\pi}}\frac{1}{2L}\int_{-L}^{L} dx f(x)\exp\left(i\frac{n\pi x}{L}\right) = \int_{-L}^{L}\frac{dx}{\sqrt{2\pi}} f(x)\exp(i\omega_n x)
$$

Hence,

$$
F(\omega_n) \underset{L\uparrow\infty}{\longrightarrow} F(\omega) = \int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}} f(x)\exp(i\omega x)
$$

d.

$$
\begin{aligned}
&\int_{-\infty}^{\infty} dx f(x)\delta(x-\bar{x}) = f(\bar{x}) = \int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{2\pi}} F(\omega)\exp(-i\omega\bar{x}) = \\
&= \int_{-\infty}^{\infty}\frac{d\omega}{\sqrt{2\pi}}\left\{\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}} f(x)\exp(i\omega x)\right\}\exp(-i\omega\bar{x}) = \int_{-\infty}^{\infty} dx f(x)\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\exp(i\omega(x-\bar{x}))
\end{aligned}
$$

Hence,

$$\delta(x-\bar{x}) \quad = \quad \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \exp\left(i\omega(x-\bar{x})\right)$$

Exercício 8

a. First, we consider the transformation from Cartesian coordinates (x, y, z) to cylindrical coordinates (ρ, φ, z), related by

$$x = \rho\cos(\varphi) \quad , \quad y = \rho\sin(\varphi) \quad , \quad z = z \quad , \tag{28}$$

and

$$\rho = \sqrt{x^2+y^2} \quad , \quad \varphi = \operatorname{arctg}\left(\frac{y}{x}\right) \quad , \quad z = z \quad . \tag{29}$$

To begin with, we must determine the derivatives of ρ and φ with respect to x and y. For that, we need the derivatives of $\operatorname{arctg}\left(\frac{y}{x}\right)$. Let $a = \operatorname{tg}(b)$, hence $b = \operatorname{arctg}(a)$. Then

$$\frac{db}{da} = \frac{1}{\frac{da}{db}} = \cos^2(b) = \frac{\cos^2(b)}{\cos^2(b)+\sin^2(b)} = \frac{1}{1+\operatorname{tg}^2(b)} = \frac{1}{1+a^2} \quad . \tag{30}$$

Using the result (30) and the relations (29), we obtain then

$$\begin{array}{ccc} \dfrac{\partial\rho}{\partial x} = \dfrac{x}{\sqrt{x^2+y^2}} = \cos(\varphi) & , & \dfrac{\partial\rho}{\partial y} = \dfrac{y}{\sqrt{x^2+y^2}} = \sin(\varphi) \\ \dfrac{\partial\varphi}{\partial x} = \dfrac{-\frac{y}{x^2}}{1+\left(\frac{y}{x}\right)^2} = \dfrac{-y}{x^2+y^2} = -\dfrac{\sin(\varphi)}{\rho} & , & \dfrac{\partial\varphi}{\partial y} = \dfrac{\frac{1}{x}}{1+\left(\frac{y}{x}\right)^2} = \dfrac{x}{x^2+y^2} = \dfrac{\cos(\varphi)}{\rho} \quad . \end{array} \tag{31}$$

Next, consider the function

$$\psi = \psi\left(\rho(x,y), \varphi(x,y), z\right) \quad . \tag{32}$$

Its first order derivatives are given by

$$\begin{aligned} \frac{\partial}{\partial x}\psi &= \frac{\partial\rho}{\partial x}\frac{\partial\psi}{\partial\rho} + \frac{\partial\varphi}{\partial x}\frac{\partial\psi}{\partial\varphi} = \left\{\cos(\varphi)\frac{\partial}{\partial\rho} - \frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\right\}\psi \\ \text{and} \quad \frac{\partial}{\partial y}\psi &= \frac{\partial\rho}{\partial y}\frac{\partial\psi}{\partial\rho} + \frac{\partial\varphi}{\partial y}\frac{\partial\psi}{\partial\varphi} = \left\{\sin(\varphi)\frac{\partial}{\partial\rho} + \frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\right\}\psi \quad , \end{aligned} \tag{33}$$

whereas, by the use of the results (33), for the second order derivatives we find

$$\begin{aligned} \frac{\partial^2}{\partial x^2}\psi &= \left\{\cos(\varphi)\frac{\partial}{\partial\rho} - \frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\right\}^2\psi \\ &= \left\{\cos(\varphi)\frac{\partial}{\partial\rho}\cos(\varphi)\frac{\partial}{\partial\rho} - \cos(\varphi)\frac{\partial}{\partial\rho}\frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi} + \right. \end{aligned}$$

$$-\frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\cos(\varphi)\frac{\partial}{\partial\rho}+\frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\frac{\sin(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\bigg\}\psi$$

$$= \bigg\{\cos^2(\varphi)\frac{\partial^2}{\partial\rho^2}+\frac{\cos(\varphi)\sin(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}-\frac{\cos(\varphi)\sin(\varphi)}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}+$$

$$+\frac{\sin^2(\varphi)}{\rho}\frac{\partial}{\partial\rho}-\frac{\sin(\varphi)\cos(\varphi)}{\rho}\frac{\partial^2}{\partial\varphi\partial\rho}+\frac{\sin(\varphi)\cos(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}+\frac{\sin^2(\varphi)}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\bigg\}\psi$$

$$= \bigg\{\cos^2(\varphi)\frac{\partial^2}{\partial\rho^2}+\frac{2\cos(\varphi)\sin(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}-\frac{2\cos(\varphi)\sin(\varphi)}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}+$$

$$+\frac{\sin^2(\varphi)}{\rho}\frac{\partial}{\partial\rho}+\frac{\sin^2(\varphi)}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\bigg\}\psi \quad , \tag{34}$$

and

$$\frac{\partial^2}{\partial y^2}\psi = \bigg\{\sin(\varphi)\frac{\partial}{\partial\rho}+\frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\bigg\}^2\psi$$

$$= \bigg\{\sin(\varphi)\frac{\partial}{\partial\rho}\sin(\varphi)\frac{\partial}{\partial\rho}+\sin(\varphi)\frac{\partial}{\partial\rho}\frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}+$$

$$+\frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\sin(\varphi)\frac{\partial}{\partial\rho}+\frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\frac{\cos(\varphi)}{\rho}\frac{\partial}{\partial\varphi}\bigg\}\psi$$

$$= \bigg\{\sin^2(\varphi)\frac{\partial^2}{\partial\rho^2}-\frac{\sin(\varphi)\cos(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}+\frac{\sin(\varphi)\cos(\varphi)}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}+$$

$$+\frac{\cos^2(\varphi)}{\rho}\frac{\partial}{\partial\rho}+\frac{\cos(\varphi)\sin(\varphi)}{\rho}\frac{\partial^2}{\partial\varphi\partial\rho}-\frac{\cos(\varphi)\sin(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}+\frac{\cos^2(\varphi)}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\bigg\}\psi$$

$$= \bigg\{\sin^2(\varphi)\frac{\partial^2}{\partial\rho^2}-\frac{2\sin(\varphi)\cos(\varphi)}{\rho^2}\frac{\partial}{\partial\varphi}+\frac{2\sin(\varphi)\cos(\varphi)}{\rho}\frac{\partial^2}{\partial\rho\partial\varphi}+$$

$$+\frac{\cos^2(\varphi)}{\rho}\frac{\partial}{\partial\rho}+\frac{\cos^2(\varphi)}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\bigg\}\psi \quad . \tag{35}$$

By taking the sum of relations (34) and (35), we obtain

$$\left\{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right\}\psi=\left\{\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}\right\}\psi \quad . \tag{36}$$

Hence, for the Laplacian operator we obtain

$$\bigtriangledown^2\psi=\left\{\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right\}\psi=\left\{\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2}+\frac{\partial^2}{\partial z^2}\right\}\psi \quad . \tag{37}$$

Next, we introduce spherical coordinates (r,ϑ,φ), given by

$$\rho=r\sin(\vartheta) \quad , \quad \varphi=\varphi \quad , \quad z=r\cos(\vartheta) \quad , \tag{38}$$

and

$$r = \sqrt{\rho^2 + z^2} \quad , \quad \vartheta = \text{arctg}\left(\frac{\rho}{z}\right) \quad , \quad \varphi = \varphi \quad . \tag{39}$$

Using the result (30) and the relations (39), we obtain for the derivatives of r and ϑ with respect to ρ and z

$$\begin{array}{ccc} \dfrac{\partial r}{\partial \rho} = \dfrac{\rho}{\sqrt{\rho^2+z^2}} = \sin(\vartheta) & , & \dfrac{\partial r}{\partial z} = \dfrac{z}{\sqrt{\rho^2+z^2}} = \cos(\vartheta) \\ & & \\ \dfrac{\partial \vartheta}{\partial \rho} = \dfrac{\frac{1}{z}}{1+\left(\frac{\rho}{z}\right)^2} = \dfrac{z}{z^2+\rho^2} = \dfrac{\cos(\vartheta)}{r} & , & \dfrac{\partial \vartheta}{\partial z} = \dfrac{-\frac{\rho}{z^2}}{1+\left(\frac{\rho}{z}\right)^2} = \dfrac{-\rho}{z^2+\rho^2} = -\dfrac{\sin(\vartheta)}{r} \quad . \end{array} \tag{40}$$

Next, consider the function

$$\psi = \psi\left(r(\rho,z), \vartheta(\rho,z), \varphi\right) \quad . \tag{41}$$

Its first order derivatives are given by

$$\begin{array}{rcl} \dfrac{\partial}{\partial \rho}\psi & = & \dfrac{\partial r}{\partial \rho}\dfrac{\partial \psi}{\partial r} + \dfrac{\partial \vartheta}{\partial \rho}\dfrac{\partial \psi}{\partial \vartheta} = \left\{\sin(\vartheta)\dfrac{\partial}{\partial r} + \dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\right\}\psi \\ & & \\ \text{and} \quad \dfrac{\partial}{\partial z}\psi & = & \dfrac{\partial r}{\partial z}\dfrac{\partial \psi}{\partial r} + \dfrac{\partial \vartheta}{\partial z}\dfrac{\partial \psi}{\partial \vartheta} = \left\{\cos(\vartheta)\dfrac{\partial}{\partial r} - \dfrac{\sin(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\right\}\psi \quad , \end{array} \tag{42}$$

whereas, by the use of the results (42), for the second order derivatives we find

$$\begin{array}{rcl} \dfrac{\partial^2}{\partial \rho^2}\psi & = & \left\{\sin(\vartheta)\dfrac{\partial}{\partial r} + \dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\right\}^2 \psi \\ & & \\ & = & \left\{\sin(\vartheta)\dfrac{\partial}{\partial r}\sin(\vartheta)\dfrac{\partial}{\partial r} + \sin(\vartheta)\dfrac{\partial}{\partial r}\dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta} + \right. \\ & & \\ & & \left. + \dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\sin(\vartheta)\dfrac{\partial}{\partial r} + \dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\dfrac{\cos(\vartheta)}{r}\dfrac{\partial}{\partial \vartheta}\right\}\psi \\ & & \\ & = & \left\{\sin^2(\vartheta)\dfrac{\partial^2}{\partial r^2} - \dfrac{\sin(\vartheta)\cos(\vartheta)}{r^2}\dfrac{\partial}{\partial \vartheta} + \dfrac{\sin(\vartheta)\cos(\vartheta)}{r}\dfrac{\partial^2}{\partial r \partial \vartheta} + \right. \\ & & \\ & & \left. + \dfrac{\cos^2(\vartheta)}{r}\dfrac{\partial}{\partial r} + \dfrac{\cos(\vartheta)\sin(\vartheta)}{r}\dfrac{\partial^2}{\partial \vartheta \partial r} - \dfrac{\cos(\vartheta)\sin(\vartheta)}{r^2}\dfrac{\partial}{\partial \vartheta} + \dfrac{\cos^2(\vartheta)}{r^2}\dfrac{\partial^2}{\partial \vartheta^2}\right\}\psi \\ & & \\ & = & \left\{\sin^2(\vartheta)\dfrac{\partial^2}{\partial r^2} - \dfrac{2\sin(\vartheta)\cos(\vartheta)}{r^2}\dfrac{\partial}{\partial \vartheta} + \dfrac{2\sin(\vartheta)\cos(\vartheta)}{r}\dfrac{\partial^2}{\partial r \partial \vartheta} + \right. \\ & & \\ & & \left. + \dfrac{\cos^2(\vartheta)}{r}\dfrac{\partial}{\partial r} + \dfrac{\cos^2(\vartheta)}{r^2}\dfrac{\partial^2}{\partial \vartheta^2}\right\}\psi \quad , \end{array} \tag{43}$$

and

$$
\begin{aligned}
\frac{\partial^2}{\partial z^2}\psi &= \left\{\cos(\vartheta)\frac{\partial}{\partial r} - \frac{\sin(\vartheta)}{r}\frac{\partial}{\partial\vartheta}\right\}^2 \psi \\
&= \left\{\cos(\vartheta)\frac{\partial}{\partial r}\cos(\vartheta)\frac{\partial}{\partial r} - \cos(\vartheta)\frac{\partial}{\partial r}\frac{\sin(\vartheta)}{r}\frac{\partial}{\partial\vartheta} + \right. \\
&\qquad \left. -\frac{\sin(\vartheta)}{r}\frac{\partial}{\partial\vartheta}\cos(\vartheta)\frac{\partial}{\partial r} + \frac{\sin(\vartheta)}{r}\frac{\partial}{\partial\vartheta}\frac{\sin(\vartheta)}{r}\frac{\partial}{\partial\vartheta}\right\}\psi \\
&= \left\{\cos^2(\vartheta)\frac{\partial^2}{\partial r^2} + \frac{\cos(\vartheta)\sin(\vartheta)}{r^2}\frac{\partial}{\partial\vartheta} - \frac{\cos(\vartheta)\sin(\vartheta)}{r}\frac{\partial^2}{\partial r\partial\vartheta} + \right. \\
&\qquad \left. +\frac{\sin^2(\vartheta)}{r}\frac{\partial}{\partial r} - \frac{\sin(\vartheta)\cos(\vartheta)}{r}\frac{\partial^2}{\partial\vartheta\partial r} + \frac{\sin(\vartheta)\cos(\vartheta)}{r^2}\frac{\partial}{\partial\vartheta} + \frac{\sin^2(\vartheta)}{r^2}\frac{\partial^2}{\partial\vartheta^2}\right\}\psi \\
&= \left\{\cos^2(\vartheta)\frac{\partial^2}{\partial r^2} + \frac{2\cos(\vartheta)\sin(\vartheta)}{r^2}\frac{\partial}{\partial\vartheta} - \frac{2\cos(\vartheta)\sin(\vartheta)}{r}\frac{\partial^2}{\partial r\partial\vartheta} + \right. \\
&\qquad \left. +\frac{\sin^2(\vartheta)}{r}\frac{\partial}{\partial r} + \frac{\sin^2(\vartheta)}{r^2}\frac{\partial^2}{\partial\vartheta^2}\right\}\psi \quad . \qquad (44)
\end{aligned}
$$

By taking the sum of relations (43) and (44), we obtain

$$
\left\{\frac{\partial^2}{\partial\rho^2} + \frac{\partial^2}{\partial z^2}\right\}\psi = \left\{\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\vartheta^2}\right\}\psi \quad . \qquad (45)
$$

Hence, also using formulas (37) and (42), for the Laplacian operator we obtain

$$
\begin{aligned}
\bigtriangledown^2\psi &= \left\{\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}\right\}\psi \\
&= \left\{\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\vartheta^2} + \frac{1}{r\sin(\vartheta)}\left[\sin(\vartheta)\frac{\partial}{\partial r} + \frac{\cos(\vartheta)}{r}\frac{\partial}{\partial\vartheta}\right] + \frac{1}{r^2\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\psi \\
&= \left\{\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\vartheta^2} + \frac{\cos(\vartheta)}{r^2\sin(\vartheta)}\frac{\partial}{\partial\vartheta} + \frac{1}{r^2\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\psi \\
&= \left\{\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{1}{r^2}\left[\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right]\right\}\psi \quad . \qquad (46)
\end{aligned}
$$

Exercício 10

In order to obtain the wanted results, we must study the following derivatives.

$$
\begin{aligned}
\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\cos(\vartheta) &= \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\,[-\sin(\vartheta)] = \\
&= -\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin^2(\vartheta) = -\frac{1}{\sin(\vartheta)}\,[2\cos(\vartheta)\sin(\vartheta)] = -2\cos(\vartheta) \quad , \qquad (47)
\end{aligned}
$$

$$\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\ \sin(\vartheta)\ =\ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\ [\cos(\vartheta)]\ =$$

$$=\ \frac{1}{\sin(\vartheta)}\left[\cos^2(\vartheta)-\sin^2(\vartheta)\right]=\frac{1}{\sin(\vartheta)}\left[1-2\sin^2(\vartheta)\right]=\left[\frac{1}{\sin^2(\vartheta)}-2\right]\sin(\vartheta)\ , \tag{48}$$

$$\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\ \left\{3\cos^2(\vartheta)-1\right\}\ =\ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\ [-6\sin(\vartheta)\cos(\vartheta)]\ =$$

$$=\ -6\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin^2(\vartheta)\cos(\vartheta)\ =\ -6\frac{1}{\sin(\vartheta)}\left[2\sin(\vartheta)\cos^2(\vartheta)-\sin^3(\vartheta)\right]$$

$$=\ -12\cos^2(\vartheta)+6\sin^2(\vartheta)\ =\ -18\cos^2(\vartheta)+6\quad , \tag{49}$$

$$\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\ \sin(2\vartheta)\ =\ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\,2\sin(\vartheta)\cos(\vartheta)\ =$$

$$=\ 2\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\ \left[\cos^2(\vartheta)-\sin^2(\vartheta)\right]\ =\ 2\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\ \left[1-2\sin^2(\vartheta)\right]$$

$$=\ 2\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\left[\sin(\vartheta)-2\sin^3(\vartheta)\right]\ =\ 2\frac{1}{\sin(\vartheta)}\left[\cos(\vartheta)-6\sin^2(\vartheta)\cos(\vartheta)\right]$$

$$=\ \frac{\sin(2\vartheta)}{\sin^2(\vartheta)}-6\sin(2\vartheta)\quad , \tag{50}$$

$$\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\ \sin^2(\vartheta)\ =\ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\ [2\sin(\vartheta)\cos(\vartheta)]\ =$$

$$=\ 2\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin^2(\vartheta)\cos(\vartheta)\ =\ 2\frac{1}{\sin(\vartheta)}\left[2\sin(\vartheta)\cos^2(\vartheta)-\sin^3(\vartheta)\right]$$

$$=\ 4\cos^2(\vartheta)-2\sin^2(\vartheta)\ =\ 4-6\sin^2(\vartheta)\quad , \tag{51}$$

and

$$\frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}e^{im\varphi}\ =\ -\ \frac{1}{\sin^2(\vartheta)}m^2\,e^{im\varphi}\ . \tag{52}$$

a: $\boldsymbol{Y_0^0(\vartheta,\varphi)=\sqrt{1/4\pi}}$.

Since the derivatives of a constant function are all equal to zero, we find here

$$L^2Y_0^0(\vartheta,\varphi)\ =\ -\hbar^2\ \left\{\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\ +\ \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\sqrt{1/4\pi}\ =\ 0$$

and

$$L_zY_0^0(\vartheta,\varphi)\ =\ -i\,\hbar\,\frac{\partial}{\partial\varphi}\sqrt{1/4\pi}\ =\ 0\quad .$$

We find that the eigenvalues of Y_0^0 are zero with respect to the differential operators L^2 and L_z.

b: $\boldsymbol{Y_1^0(\vartheta,\varphi) = \sqrt{3/4\pi}\ \cos(\vartheta)}$.

Using formula (47), we obtain

$$\begin{aligned} L^2 Y_1^0(\vartheta,\varphi) &= -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} \ + \ \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2} \right\} \sqrt{3/4\pi}\ \cos(\vartheta) \\ &= -\hbar^2\ \sqrt{3/4\pi}\ \{-2\cos(\vartheta)\ +\ 0\} \ = \ 2\hbar^2 Y_1^0(\vartheta,\varphi) \end{aligned}$$

Furthermore, since Y_1^0 does not depend on φ, we have

$$L_z Y_1^0(\vartheta,\varphi) \ = \ -i\,\hbar\,\frac{\partial}{\partial\varphi}\sqrt{3/4\pi}\ \cos(\vartheta) \ = \ 0 \quad .$$

We find that the eigenvalues of Y_1^0 equal $\hbar^2\ell(\ell+1)$ for $\ell = 1$ with respect to the differential operator L^2, and $m\hbar$ for $m = 0$ with respect to the differential operator L_z.

c: $\boldsymbol{Y_1^1(\vartheta,\varphi) = -\sqrt{3/8\pi}\ \sin(\vartheta)\, e^{i\varphi}}$.

Using formulas (48) and (52), we obtain

$$\begin{aligned} L^2 Y_1^1(\vartheta,\varphi) &= -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} \ + \ \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2} \right\} \left[-\sqrt{3/8\pi}\ \sin(\vartheta)\, e^{i\varphi}\right] = \\ &= \hbar^2\sqrt{3/8\pi}\ \left\{ \left[\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\sin(\vartheta)\right] e^{i\varphi} \ + \ \frac{1}{\sin^2(\vartheta)}\sin(\vartheta)\left[\frac{\partial^2}{\partial\varphi^2}e^{i\varphi}\right]\right\} \\ &= \hbar^2\sqrt{3/8\pi}\ \left\{ \left[\frac{1}{\sin^2(\vartheta)} - 2\right]\sin(\vartheta)\, e^{i\varphi} \ + \ \frac{1}{\sin^2(\vartheta)}\sin(\vartheta)\left[-e^{i\varphi}\right]\right\} \\ &= -2\hbar^2\sqrt{3/8\pi}\ \sin(\vartheta)\, e^{i\varphi} \ = \ 2\hbar^2 Y_1^1(\vartheta,\varphi) \end{aligned}$$

and

$$\begin{aligned} L_z Y_1^1(\vartheta,\varphi) &= -i\,\hbar\,\frac{\partial}{\partial\varphi}\left[-\sqrt{3/8\pi}\ \sin(\vartheta)\, e^{i\varphi}\right] \ = \ i\,\hbar\,\sqrt{3/8\pi}\sin(\vartheta)\ \left[\frac{\partial}{\partial\varphi}e^{i\varphi}\right] \\ &= i\,\hbar\,\sqrt{3/8\pi}\sin(\vartheta)\ \left[ie^{i\varphi}\right] \ = \ -\hbar\,\sqrt{3/8\pi}\sin(\vartheta)\ \left[e^{i\varphi}\right] \ = \ \hbar\, Y_1^1(\vartheta,\varphi) \quad . \end{aligned}$$

We find that the eigenvalues of Y_1^1 equal $\hbar^2\ell(\ell+1)$ for $\ell = 1$ with respect to the differential operator L^2, and $m\hbar$ for $m = 1$ with respect to the differential operator L_z.

d: $\boldsymbol{Y_1^{-1}(\vartheta,\varphi) = \sqrt{3/8\pi}\ \sin(\vartheta)\, e^{-i\varphi}}$.

Using formulas (48) and (52), we obtain

$$L^2 Y_1^{-1}(\vartheta,\varphi) \ = \ -\hbar^2 \left\{ \frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} \ + \ \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2} \right\} \sqrt{3/8\pi}\ \sin(\vartheta)\, e^{-i\varphi} \ =$$

$$= -\hbar^2\sqrt{3/8\pi}\left\{\left[\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\sin(\vartheta)\right]e^{-i\varphi} + \frac{1}{\sin^2(\vartheta)}\sin(\vartheta)\left[\frac{\partial^2}{\partial\varphi^2}e^{-i\varphi}\right]\right\}$$

$$= -\hbar^2\sqrt{3/8\pi}\left\{\left[\frac{1}{\sin^2(\vartheta)} - 2\right]\sin(\vartheta)\,e^{-i\varphi} + \frac{1}{\sin^2(\vartheta)}\sin(\vartheta)\left[-e^{-i\varphi}\right]\right\}$$

$$= 2\hbar^2\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi} = 2\hbar^2 Y_1^{-1}(\vartheta,\varphi)$$

and

$$L_z Y_1^{-1}(\vartheta,\varphi) = -i\hbar\frac{\partial}{\partial\varphi}\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi} = -i\hbar\sqrt{3/8\pi}\sin(\vartheta)\left[\frac{\partial}{\partial\varphi}e^{-i\varphi}\right]$$

$$= -i\hbar\sqrt{3/8\pi}\sin(\vartheta)\left[-ie^{-i\varphi}\right] = -\hbar\sqrt{3/8\pi}\sin(\vartheta)\left[e^{-i\varphi}\right] = -\hbar\, Y_1^{-1}(\vartheta,\varphi) \quad .$$

We find that the eigenvalues of Y_1^{-1} equal $\hbar^2\ell(\ell+1)$ for $\ell = 1$ with respect to the differential operator L^2, and $m\hbar$ for $m = -1$ with respect to the differential operator L_z.

e: $\mathbf{Y_2^0(\boldsymbol{\vartheta},\boldsymbol{\varphi}) = \sqrt{5/16\boldsymbol{\pi}}\ \{3\cos^2(\boldsymbol{\vartheta}) - 1\}}$.

Using formulas (49) and (52), we obtain

$$L^2 Y_2^0(\vartheta,\varphi) = -\hbar^2\left\{\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\sqrt{5/16\pi}\left\{3\cos^2(\vartheta) - 1\right\} =$$

$$= -\hbar^2\sqrt{5/16\pi}\left\{\left[\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\left\{3\cos^2(\vartheta) - 1\right\}\right] + 0\right\}$$

$$= -\hbar^2\sqrt{5/16\pi}\left\{-18\cos^2(\vartheta) + 6\right\} = 6\hbar^2\sqrt{5/16\pi}\left\{3\cos^2(\vartheta) - 1\right\} = 6\hbar^2 Y_2^0(\vartheta,\varphi)$$

Furthermore, since Y_2^0 does not depend on φ, we have

$$L_z Y_2^0(\vartheta,\varphi) = -i\hbar\frac{\partial}{\partial\varphi}\sqrt{5/16\pi}\left\{3\cos^2(\vartheta) - 1\right\} = 0 \quad .$$

We find that the eigenvalues of Y_2^0 equal $\hbar^2\ell(\ell+1)$ for $\ell = 2$ with respect to the differential operator L^2, and $m\hbar$ for $m = 0$ with respect to the differential operator L_z.

f: $\mathbf{Y_2^1(\boldsymbol{\vartheta},\boldsymbol{\varphi}) = -\sqrt{15/32\boldsymbol{\pi}}\ \sin(2\boldsymbol{\vartheta})\,e^{i\boldsymbol{\varphi}}}$.

Using formulas (50) and (52), we obtain

$$L^2 Y_2^1(\vartheta,\varphi) = -\hbar^2\left\{\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} + \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}\left[-\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{i\varphi}\right] =$$

$$= \hbar^2\sqrt{15/32\pi}\left\{\left[\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\sin(2\vartheta)\right]e^{i\varphi} + \frac{1}{\sin^2(\vartheta)}\sin(2\vartheta)\left[\frac{\partial^2}{\partial\varphi^2}e^{i\varphi}\right]\right\}$$

$$= \hbar^2\sqrt{15/32\pi}\,\left\{\left[\frac{\sin(2\vartheta)}{\sin^2(\vartheta)} - 6\sin(2\vartheta)\right]\,e^{i\varphi}\;+\;\frac{1}{\sin^2(\vartheta)}\,\sin(2\vartheta)\,\left[-e^{i\varphi}\right]\right\}$$

$$= -6\hbar^2\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{i\varphi}\;=\;6\hbar^2 Y_2^1(\vartheta,\varphi)$$

and

$$L_z Y_2^1(\vartheta,\varphi) \;=\; -i\,\hbar\,\frac{\partial}{\partial\varphi}\left[-\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{i\varphi}\right] = i\,\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[\frac{\partial}{\partial\varphi}e^{i\varphi}\right] =$$

$$= \; i\,\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[ie^{i\varphi}\right] \;=\; -\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[e^{i\varphi}\right] \;=\; \hbar\,Y_2^1(\vartheta,\varphi) \quad .$$

We find that the eigenvalues of Y_2^1 equal $\hbar^2\ell(\ell+1)$ for $\ell = 2$ with respect to the differential operator L^2, and $m\hbar$ for $m = 1$ with respect to the differential operator L_z.

g: $\boldsymbol{Y_2^{-1}(\vartheta,\varphi) = \sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{-i\varphi}}$.

Using formulas (50) and (52), we obtain

$$L^2 Y_2^{-1}(\vartheta,\varphi) \;=\; -\hbar^2\,\left\{\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\;+\;\frac{1}{\sin^2(\vartheta)}\,\frac{\partial^2}{\partial\varphi^2}\right\}\left[\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{-i\varphi}\right] \;=$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\,\sin(2\vartheta)\right]\,e^{-i\varphi}\;+\;\frac{1}{\sin^2(\vartheta)}\,\sin(2\vartheta)\,\left[\frac{\partial^2}{\partial\varphi^2}\,e^{-i\varphi}\right]\right\}$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[\frac{\sin(2\vartheta)}{\sin^2(\vartheta)} - 6\sin(2\vartheta)\right]\,e^{-i\varphi}\;+\;\frac{1}{\sin^2(\vartheta)}\,\sin(2\vartheta)\,\left[-e^{-i\varphi}\right]\right\}$$

$$= 6\hbar^2\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{-i\varphi}\;=\;6\hbar^2 Y_2^{-1}(\vartheta,\varphi)$$

and

$$L_z Y_2^{-1}(\vartheta,\varphi) \;=\; -i\,\hbar\,\frac{\partial}{\partial\varphi}\left[\sqrt{15/32\pi}\,\sin(2\vartheta)\,e^{-i\varphi}\right] = -i\,\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[\frac{\partial}{\partial\varphi}e^{-i\varphi}\right] =$$

$$= \; -i\,\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[-ie^{-i\varphi}\right] \;=\; -\hbar\,\sqrt{15/32\pi}\sin(2\vartheta)\,\left[e^{-i\varphi}\right] \;=\; -\hbar\,Y_2^{-1}(\vartheta,\varphi) \quad .$$

We find that the eigenvalues of Y_2^{-1} equal $\hbar^2\ell(\ell+1)$ for $\ell = 2$ with respect to the differential operator L^2, and $m\hbar$ for $m = -1$ with respect to the differential operator L_z.

h: $\boldsymbol{Y_2^{2}(\vartheta,\varphi) = \sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{2i\varphi}}$.

Using formulas (51) and (52), we obtain

$$L^2 Y_2^{2}(\vartheta,\varphi) \;=\; -\hbar^2\,\left\{\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\;+\;\frac{1}{\sin^2(\vartheta)}\,\frac{\partial^2}{\partial\varphi^2}\right\}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{2i\varphi}\right] \;=$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\,\sin^2(\vartheta)\right]\,e^{2i\varphi}\;+\;\frac{1}{\sin^2(\vartheta)}\,\sin^2(\vartheta)\,\left[\frac{\partial^2}{\partial\varphi^2}\,e^{2i\varphi}\right]\right\}$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[4-6\sin^2(\vartheta)\right]\,e^{2i\varphi} \;+\; \left[-4e^{2i\varphi}\right]\right\}$$

$$= 6\hbar^2\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{2i\varphi} \;=\; 6\hbar^2 Y_2^2(\vartheta,\varphi)$$

and

$$L_z Y_2^2(\vartheta,\varphi) \;=\; -i\,\hbar\,\frac{\partial}{\partial\varphi}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{2i\varphi}\right] = -i\,\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[\frac{\partial}{\partial\varphi}e^{2i\varphi}\right] =$$

$$= \;-i\,\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[2ie^{2i\varphi}\right] \;=\; 2\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[e^{2i\varphi}\right] \;=\; 2\hbar\,Y_2^2(\vartheta,\varphi) \quad .$$

We find that the eigenvalues of Y_2^2 equal $\hbar^2\ell(\ell+1)$ for $\ell = 2$ with respect to the differential operator L^2, and $m\hbar$ for $m = 2$ with respect to the differential operator L_z.

i: $\boldsymbol{Y_2^{-2}(\vartheta,\varphi) = \sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{-2i\varphi}}$.

Using formulas (51) and (52), we obtain

$$L^2 Y_2^2(\vartheta,\varphi) \;=\; -\hbar^2\,\left\{\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta} \;+\; \frac{1}{\sin^2(\vartheta)}\,\frac{\partial^2}{\partial\varphi^2}\right\}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{-2i\varphi}\right] \;=$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[\frac{1}{\sin(\vartheta)}\,\frac{\partial}{\partial\vartheta}\,\sin(\vartheta)\,\frac{\partial}{\partial\vartheta}\,\sin^2(\vartheta)\right]\,e^{-2i\varphi} \;+\; \frac{1}{\sin^2(\vartheta)}\,\sin^2(\vartheta)\,\left[\frac{\partial^2}{\partial\varphi^2}\,e^{-2i\varphi}\right]\right\}$$

$$= -\hbar^2\sqrt{15/32\pi}\,\left\{\left[4-6\sin^2(\vartheta)\right]\,e^{-2i\varphi} \;+\; \left[-4e^{-2i\varphi}\right]\right\}$$

$$= 6\hbar^2\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{-2i\varphi} \;=\; 6\hbar^2 Y_2^2(\vartheta,\varphi)$$

and

$$L_z Y_2^{-2}(\vartheta,\varphi) \;=\; -i\,\hbar\,\frac{\partial}{\partial\varphi}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\,e^{-2i\varphi}\right] = -i\,\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[\frac{\partial}{\partial\varphi}e^{-2i\varphi}\right] =$$

$$= \;-i\,\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[-2ie^{-2i\varphi}\right] \;=\; -2\hbar\,\sqrt{15/32\pi}\,\sin^2(\vartheta)\,\left[e^{-2i\varphi}\right] \;=\; \hbar\,Y_2^{-2}(\vartheta,\varphi) \quad .$$

We find that the eigenvalues of Y_2^{-2} equal $\hbar^2\ell(\ell+1)$ for $\ell = 2$ with respect to the differential operator L^2, and $m\hbar$ for $m = -2$ with respect to the differential operator L_z.

In the following table we collect the results of the preceding calculus.

		angular momentum eigenvalue L^2		magnetic quantum number eigenvalue L_z
Y_ℓ^m	ℓ	$\ell(\ell+1)\hbar^2$	m	$m\hbar$
Y_0^0	0	0	0	0
Y_1^1	1	$2\hbar^2$	1	$\hbar$
Y_1^0	1	$2\hbar^2$	0	0
Y_1^{-1}	1	$2\hbar^2$	-1	$-\hbar$
Y_2^2	2	$6\hbar^2$	2	$2\hbar$
Y_2^1	2	$6\hbar^2$	1	$\hbar$
Y_2^0	2	$6\hbar^2$	0	0
Y_2^{-1}	2	$6\hbar^2$	-1	$-\hbar$
Y_2^{-2}	2	$6\hbar^2$	-2	$-2\hbar$

Exercício 11

a: $\boldsymbol{Y_0^0(\vartheta,\varphi)=\sqrt{1/4\pi}}$.

Since the derivatives of a constant function are all equal to zero, we find here

$$L_+Y_0^0(\vartheta,\varphi) \;=\; \hbar\, e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\sqrt{1/4\pi} \;=\; 0$$

and

$$L_-Y_0^0(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi}\left\{-\,\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\sqrt{1/4\pi} \;=\; 0$$

We find $L_+Y_0^0=0$ and $L_-Y_0^0=0$

b: $\boldsymbol{Y_1^0(\vartheta,\varphi)=\sqrt{3/4\pi}\,\cos(\vartheta)}$.

$$L_+Y_1^0(\vartheta,\varphi) \;=\; \hbar\, e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\sqrt{3/4\pi}\,\cos(\vartheta) \;=$$

$$=\;\hbar\sqrt{3/4\pi}\,e^{i\varphi}\,\{-\sin(\vartheta)\;+\;0\}\;=\;-\hbar\sqrt{2}\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{i\varphi}\;=\;\hbar\sqrt{2}\,Y_1^1(\vartheta,\varphi)$$

and

$$L_-Y_1^0(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi}\left\{-\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\sqrt{3/4\pi}\,\cos(\vartheta) \;=$$

$$=\;\hbar\sqrt{3/4\pi}\,e^{-i\varphi}\,\{\sin(\vartheta)\;+\;0\}\;=\;\hbar\sqrt{2}\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi}\;=\;\hbar\sqrt{2}\,Y_1^{-1}(\vartheta,\varphi).$$

We find $L_+Y_1^0 = \hbar\sqrt{2}\,Y_1^1$ and $L_-Y_1^0 = \hbar\sqrt{2}\,Y_1^{-1}$.

c: $\boldsymbol{Y_1^1(\vartheta,\varphi) = -\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{i\varphi}}$.

$$L_+Y_1^1(\vartheta,\varphi) \;=\; \hbar\,e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[-\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{i\varphi}\right] \;=$$

$$=\; -\hbar\,\sqrt{3/8\pi}\,e^{i\varphi}\left\{\cos(\vartheta)\,e^{i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\left[\sin(\vartheta)\,i\,e^{i\varphi}\right]\right\} \;=\; 0$$

and

$$L_-Y_1^1(\vartheta,\varphi) \;=\; \hbar\,e^{-i\varphi}\left\{-\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[-\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{i\varphi}\right] \;=$$

$$=\; -\hbar\,\sqrt{3/8\pi}\,e^{-i\varphi}\left\{-\;\cos(\vartheta)\,e^{i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\left[\sin(\vartheta)\,i\,e^{i\varphi}\right]\right\}$$

$$=\; \hbar\,2\sqrt{3/8\pi}\,\cos(\vartheta) =\; \hbar\,\sqrt{2}\,Y_1^0(\vartheta,\varphi).$$

We find $L_+Y_1^1 = 0$ and $L_-Y_1^1 = \hbar\sqrt{2}\,Y_1^0$.

d: $\boldsymbol{Y_1^{-1}(\vartheta,\varphi) = \sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi}}$.

$$L_+Y_1^{-1}(\vartheta,\varphi) \;=\; \hbar\,e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi}\right] \;=$$

$$=\; \hbar\,\sqrt{3/8\pi}\,e^{i\varphi}\left\{\;\cos(\vartheta)\,e^{-i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\left[\sin(\vartheta)\,(-i)\,e^{-i\varphi}\right]\right\}$$

$$=\; \hbar\,2\sqrt{3/8\pi}\,\cos(\vartheta) =\; \hbar\,\sqrt{2}\,Y_1^0(\vartheta,\varphi)$$

and

$$L_-Y_1^{-1}(\vartheta,\varphi) \;=\; \hbar\,e^{-i\varphi}\left\{-\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[\sqrt{3/8\pi}\,\sin(\vartheta)\,e^{-i\varphi}\right] \;=$$

$$=\; \hbar\,\sqrt{3/8\pi}\,e^{-i\varphi}\left\{-\;\cos(\vartheta)\,e^{-i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\left[\sin(\vartheta)\,(-i)\,e^{-i\varphi}\right]\right\} \;=\; 0.$$

We find $L_+Y_1^{-1} = \hbar\sqrt{2}\,Y_1^0$ and $L_-Y_1^{-1} = 0$.

e: $\boldsymbol{Y_2^0(\vartheta,\varphi) = \sqrt{5/16\pi}\,\{3\cos^2(\vartheta) - 1\}}$.

$$L_+Y_2^0(\vartheta,\varphi) \;=\; \hbar\, e^{i\varphi} \left\{ \frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{5/16\pi}\; \left\{ 3\cos^2(\vartheta) - 1 \right\} \right] \;=$$

$$=\; \hbar\,\sqrt{5/16\pi}\, e^{i\varphi}\; \{-6\sin(\vartheta)\cos(\vartheta) \;+\; 0\} \;=\; -\hbar\,\sqrt{6}\,\sqrt{15/32\pi}\;\sin(2\vartheta)\, e^{i\varphi} \;=\; \hbar\,\sqrt{6}\, Y_2^1(\vartheta,\varphi)$$

and

$$L_-Y_2^0(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi} \left\{ -\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{5/16\pi}\; \left\{ 3\cos^2(\vartheta) - 1 \right\} \right] \;=$$

$$=\; \hbar\,\sqrt{5/16\pi}\, e^{-i\varphi}\; \{6\sin(\vartheta)\cos(\vartheta) \;+\; 0\} \;=\; \hbar\,\sqrt{6}\,\sqrt{15/32\pi}\;\sin(2\vartheta)\, e^{-i\varphi} \;=\; \hbar\,\sqrt{6}\, Y_2^{-1}(\vartheta,\varphi)$$

We find $L_+Y_2^0 = \hbar\,\sqrt{6}\,Y_2^1$ and $L_-Y_2^0 = \hbar\,\sqrt{6}\,Y_2^{-1}$.

f: $\boldsymbol{Y_2^1(\vartheta,\varphi) = -\sqrt{15/32\pi}\;\sin(2\vartheta)\, e^{i\varphi}}$.

Let us first determine the derivative of $\sin(2\vartheta)$.

$$\frac{\partial}{\partial\vartheta}\,\sin(2\vartheta) \;=\; 2\cos(2\vartheta) \;=$$

$$=\; 2\left[\cos^2(\vartheta) - \sin^2(\vartheta)\right] \;=\; 2\left[2\cos^2(\vartheta) - 1\right] \;=\; 2\left[1 - 2\sin^2(\vartheta)\right] \quad .$$

Using either of the final results, we obtain

$$L_+Y_2^1(\vartheta,\varphi) \;=\; \hbar\, e^{i\varphi} \left\{ \frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[-\sqrt{15/32\pi}\;\sin(2\vartheta)\, e^{i\varphi} \right] \;=$$

$$=\; -\hbar\,\sqrt{15/32\pi}\, e^{i\varphi} \left\{ 2\left[\cos^2(\vartheta) - \sin^2(\vartheta)\right] e^{i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\sin(2\vartheta)\,\left[\, i\, e^{i\varphi}\right] \right\}$$

$$=\; -\hbar\,\sqrt{15/32\pi}\, e^{i\varphi} \left\{ 2\left[\cos^2(\vartheta) - \sin^2(\vartheta)\right] e^{i\varphi} \;-\; \frac{\cos(\vartheta)}{\sin(\vartheta)}\, 2\sin(\vartheta)\cos(\vartheta)\, e^{i\varphi} \right\}$$

$$=\; 2\hbar\,\sqrt{15/32\pi}\;\sin^2(\vartheta)\, e^{2i\varphi} \;=\; 2\hbar\, Y_2^2(\vartheta,\varphi)$$

and

$$L_-Y_2^1(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi} \left\{ -\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[-\sqrt{15/32\pi}\;\sin(2\vartheta)\, e^{i\varphi} \right] \;=$$

$$=\; -\hbar\,\sqrt{15/32\pi}\, e^{-i\varphi} \left\{ -2\left[2\cos^2(\vartheta) - 1\right] e^{i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\sin(2\vartheta)\,\left[\, i\, e^{i\varphi}\right] \right\}$$

$$=\; -\hbar\,\sqrt{15/32\pi}\, e^{-i\varphi} \left\{ -2\left[2\cos^2(\vartheta) - 1\right] e^{i\varphi} \;-\; \frac{\cos(\vartheta)}{\sin(\vartheta)}\, 2\sin(\vartheta)\cos(\vartheta)\, e^{i\varphi} \right\}$$

$$=\; 2\hbar\,\sqrt{15/32\pi}\; \left\{ 3\cos^2(\vartheta) - 1 \right\} \;=\; \hbar\sqrt{6}\, Y_2^0(\vartheta,\varphi)$$

We find $L_+ Y_2^1 = \hbar\,\sqrt{4}\, Y_2^2$ and $L_- Y_2^1 = \hbar\,\sqrt{6}\, Y_2^0$.

g: $\boldsymbol{Y_2^{-1}(\vartheta,\varphi) = \sqrt{15/32\pi}\ \sin(2\vartheta)\, e^{-i\varphi}}$.

$$
\begin{aligned}
L_+ Y_2^{-1}(\vartheta,\varphi) \;&=\; \hbar\, e^{i\varphi} \left\{ \frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{15/32\pi}\ \sin(2\vartheta)\, e^{-i\varphi} \right] \;= \\
&=\; \hbar\,\sqrt{15/32\pi}\, e^{i\varphi} \left\{ 2\left[2\cos^2(\vartheta) - 1 \right]\, e^{-i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\ \sin(2\vartheta)\ \left[-i\, e^{-i\varphi} \right] \right\} \\
&=\; \hbar\,\sqrt{15/32\pi}\, e^{i\varphi} \left\{ 2\left[2\cos^2(\vartheta) - 1 \right]\, e^{-i\varphi} \;+\; \frac{\cos(\vartheta)}{\sin(\vartheta)}\, 2\sin(\vartheta)\cos(\vartheta)\, e^{-i\varphi} \right\} \\
&=\; 2\hbar\,\sqrt{15/32\pi}\ \left\{ 3\cos^2(\vartheta) - 1 \right\} \;=\; \hbar\sqrt{6}\, Y_2^0(\vartheta,\varphi)
\end{aligned}
$$

and

$$
\begin{aligned}
L_- Y_2^{-1}(\vartheta,\varphi) \;&=\; \hbar\, e^{-i\varphi} \left\{ -\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{15/32\pi}\ \sin(2\vartheta)\, e^{-i\varphi} \right] \;= \\
&=\; \hbar\,\sqrt{15/32\pi}\, e^{-i\varphi} \left\{ -2\left[\cos^2(\vartheta) - \sin^2(\vartheta) \right]\, e^{-i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\ \sin(2\vartheta)\ \left[-i\, e^{-i\varphi} \right] \right\} \\
&=\; \hbar\,\sqrt{15/32\pi}\, e^{-i\varphi} \left\{ -2\left[\cos^2(\vartheta) - \sin^2(\vartheta) \right]\, e^{-i\varphi} \;+\; \frac{\cos(\vartheta)}{\sin(\vartheta)}\, 2\sin(\vartheta)\cos(\vartheta)\, e^{-i\varphi} \right\} \\
&=\; 2\hbar\,\sqrt{15/32\pi}\ \sin^2(\vartheta)\, e^{-2i\varphi} \;=\; 2\hbar\, Y_2^{-2}(\vartheta,\varphi)
\end{aligned}
$$

We find $L_+ Y_2^{-1} = \hbar\,\sqrt{6}\, Y_2^0$ and $L_- Y_2^{-1} = \hbar\,\sqrt{4}\, Y_2^{-2}$.

h: $\boldsymbol{Y_2^2(\vartheta,\varphi) = \sqrt{15/32\pi}\ \sin^2(\vartheta)\, e^{2i\varphi}}$.

Let us first determine the derivative of $\sin^2(\vartheta)$.

$$
\frac{\partial}{\partial\vartheta}\ \sin^2(\vartheta) \;=\; 2\sin(\vartheta)\cos(\vartheta) \;=\; \sin(2\vartheta) \quad .
$$

Using either of the final results, we obtain

$$
\begin{aligned}
L_+ Y_2^2(\vartheta,\varphi) \;&=\; \hbar\, e^{i\varphi} \left\{ \frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{15/32\pi}\ \sin^2(\vartheta)\, e^{2i\varphi} \right] \;= \\
&=\; \hbar\,\sqrt{15/32\pi}\, e^{i\varphi} \left\{ 2\sin(\vartheta)\cos(\vartheta)\, e^{2i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\ \sin^2(\vartheta)\ \left[2i\, e^{2i\varphi} \right] \right\} \;=\; 0
\end{aligned}
$$

and

$$
L_- Y_2^2(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi} \left\{ -\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi} \right\} \left[\sqrt{15/32\pi}\ \sin^2(\vartheta)\, e^{2i\varphi} \right] \;=
$$

$$= \hbar\sqrt{15/32\pi}\, e^{-i\varphi}\left\{- \sin(2\vartheta)\, e^{2i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\sin^2(\vartheta)\,\left[2i\, e^{2i\varphi}\right]\right\}$$

$$= \hbar\sqrt{15/32\pi}\, e^{-i\varphi}\left\{- \sin(2\vartheta)\, e^{2i\varphi} \;-\; \sin(2\vartheta)\, e^{2i\varphi}\right\}$$

$$= -2\hbar\sqrt{15/32\pi}\,\sin(2\vartheta)\, e^{i\varphi} \;=\; 2\hbar\, Y_2^1(\vartheta,\varphi).$$

We find $L_+Y_2^2 = 0$ and $L_-Y_2^2 = \hbar\sqrt{4}\, Y_2^1$.

i: $\boldsymbol{Y_2^{-2}(\vartheta,\varphi) = \sqrt{15/32\pi}\,\sin^2(\vartheta)\, e^{-2i\varphi}}$.

$$L_+Y_2^{-2}(\vartheta,\varphi) \;=\; \hbar\, e^{i\varphi}\left\{\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\, e^{-2i\varphi}\right] \;=$$

$$= \hbar\sqrt{15/32\pi}\, e^{i\varphi}\left\{\sin(2\vartheta)\, e^{-2i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\sin^2(\vartheta)\,\left[-2i\, e^{-2i\varphi}\right]\right\}$$

$$= \hbar\sqrt{15/32\pi}\, e^{i\varphi}\left\{\sin(2\vartheta)\, e^{-2i\varphi} \;+\; \sin(2\vartheta)\, e^{-2i\varphi}\right\}$$

$$= 2\hbar\sqrt{15/32\pi}\,\sin(2\vartheta)\, e^{-i\varphi} \;=\; 2\hbar\, Y_2^{-1}(\vartheta,\varphi)$$

and

$$L_-Y_2^{-2}(\vartheta,\varphi) \;=\; \hbar\, e^{-i\varphi}\left\{-\frac{\partial}{\partial\vartheta} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\frac{\partial}{\partial\varphi}\right\}\left[\sqrt{15/32\pi}\,\sin^2(\vartheta)\, e^{-2i\varphi}\right] \;=$$

$$= \hbar\sqrt{15/32\pi}\, e^{-i\varphi}\left\{-2\sin(\vartheta)\cos(\vartheta)\, e^{-2i\varphi} \;+\; i\,\frac{\cos(\vartheta)}{\sin(\vartheta)}\,\sin^2(\vartheta)\,\left[-2i\, e^{-2i\varphi}\right]\right\} \;=\; 0 \quad .$$

We find $L_+Y_2^{-2} = \hbar\sqrt{4}\, Y_2^{-1}$ and $L_-Y_2^{-2} = 0$.

In the following table we collect the results of the preceding calculus.

Y_ℓ^m	ℓ	m	raising L_+	lowering L_-
Y_0^0	0	0	0	0
Y_1^1	1	1	0	$\hbar\sqrt{2}\,Y_1^0$
Y_1^0	1	0	$\hbar\sqrt{2}\,Y_1^1$	$\hbar\sqrt{2}\,Y_1^{-1}$
Y_1^{-1}	1	-1	$\hbar\sqrt{2}\,Y_1^0$	0
Y_2^2	2	2	0	$\hbar\sqrt{4}\,Y_2^1$
Y_2^1	2	1	$\hbar\sqrt{4}\,Y_2^2$	$\hbar\sqrt{6}\,Y_2^0$
Y_2^0	2	0	$\hbar\sqrt{6}\,Y_2^1$	$\hbar\sqrt{6}\,Y_2^{-1}$
Y_2^{-1}	2	-1	$\hbar\sqrt{6}\,Y_2^0$	$\hbar\sqrt{4}\,Y_2^{-2}$
Y_2^{-2}	2	-2	$\hbar\sqrt{4}\,Y_2^{-1}$	0

In general one has

$$L_+\,Y_\ell^m \;=\; \sqrt{\ell(\ell+1)-m(m+1)}\;Y_\ell^{m+1}$$

and

$$L_-\,Y_\ell^m \;=\; \sqrt{\ell(\ell+1)-m(m-1)}\;Y_\ell^{m-1} \quad .$$

The signs $+$ or $-$, or in general the phases, of the spherical harmonics are chosen according to the Condon-Shortley phase convention.

One may use the raising, L_+, and lowering, L_-, operators to construct all spherical harmonics, once one finds the solutions Y_ℓ^0, which are independent of φ, of the equation

$$\begin{aligned} \hbar^2\,\ell(\ell+1)\,Y_\ell^0(\vartheta) \;&=\; L^2\,Y_\ell^0(\vartheta) \;= \\ &=\; -\hbar^2\left\{\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta} \;+\; \frac{1}{\sin^2(\vartheta)}\frac{\partial^2}{\partial\varphi^2}\right\}Y_\ell^0(\vartheta) \\ &=\; -\hbar^2\,\frac{1}{\sin(\vartheta)}\frac{\partial}{\partial\vartheta}\sin(\vartheta)\frac{\partial}{\partial\vartheta}\,Y_\ell^0(\vartheta) \quad . \end{aligned}$$

The latter equation, which is called the Legendre differential equation (1785), is not very difficult to be solved (see e.g. http://mathworld.wolfram.com/LegendreDifferentialEquation.html or http://en.wikipedia.org/wiki/Legendre_polynomials).

Exercício 12

Using the definition for the Bohr radius, we may simplify the differential operator to

$$-\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \;-\; \frac{e^2}{4\pi\epsilon_0 r} \;=\; -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r \;-\; \frac{\ell(\ell+1)}{r} \;+\; \frac{2}{a_0}\right\} \quad .$$

a: $\boldsymbol{R_{n=1,\ell=0}(r) = 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}}$.

Since $\ell = 0$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\}$. Hence, we must determine

$$\frac{d^2}{dr^2} r\, e^{-r/a_0} = \frac{d}{dr}\left\{e^{-r/a_0} + r\left[-\frac{1}{a_0}e^{-r/a_0}\right]\right\} = \frac{d}{dr}\left\{1 - \frac{r}{a_0}\right\} e^{-r/a_0}$$

$$= -\frac{1}{a_0}e^{-r/a_0} + \left\{1 - \frac{r}{a_0}\right\}\left[-\frac{1}{a_0}e^{-r/a_0}\right] = \left\{-\frac{2}{a_0} + \frac{r}{a_0^2}\right\} e^{-r/a_0}$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\} R_{10}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\} 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{\frac{d^2}{dr^2} r e^{-r/a_0} + \frac{2}{a_0}e^{-r/a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{\left[-\frac{2}{a_0} + \frac{r}{a_0^2}\right] e^{-r/a_0} + \frac{2}{a_0}e^{-r/a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2}\left\{-\frac{2}{a_0} + \frac{r}{a_0^2} + \frac{2}{a_0}\right\} e^{-r/a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{a_0}\right)^{3/2} \frac{r}{a_0^2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e a_0^2} 2\left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} = -\frac{\hbar^2}{2m_e a_0^2} R_{10}(r) \quad .$$

Consequently, we find for R_{10} the eigenvalue $E_1 = -\hbar^2/\left(2m_e a_0^2\right)$ under the action of the differential operator. Also using the definition $\alpha = e^2/(4\pi\epsilon_0\hbar c) = \hbar/(m_e a_0 c)$, we obtain $E_1 = -\alpha^2 m_e c^2/2$, which is indeed the expression for the Hydrogen ground state energy we have obtained before.

b: $\boldsymbol{R_{n=2,\ell=0}(r) = \left(\frac{1}{2a_0}\right)^{3/2} \left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}}$.

Since $\ell = 0$, we again obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r + \frac{2}{a_0}\right\}$. Here, we determine, using the substitution $a_0 \to 2a_0$ in the result of **a**,

$$\frac{d^2}{dr^2} r\, e^{-r/2a_0} = \left\{-\frac{2}{2a_0} + \frac{r}{4a_0^2}\right\} e^{-r/2a_0} = \left\{-\frac{1}{a_0} + \frac{r}{4a_0^2}\right\} e^{-r/2a_0}$$

Furthermore, we must determine

$$\frac{d^2}{dr^2} r^2\, e^{-r/2a_0} = \frac{d}{dr}\left\{2re^{-r/2a_0} + r^2\left[-\frac{1}{2a_0}e^{-r/2a_0}\right]\right\} = \frac{d}{dr}\left\{2r - \frac{r^2}{2a_0}\right\} e^{-r/2a_0}$$

$$= \left\{2 - \frac{2r}{2a_0}\right\} e^{-r/2a_0} + \left\{2r - \frac{r^2}{2a_0}\right\}\left[-\frac{1}{2a_0}e^{-r/2a_0}\right] = \left\{2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right\} e^{-r/2a_0} \quad .$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r \;+\; \frac{2}{a_0}\right\}R_{20}(r) \;=$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2 - \frac{r}{a_0}\right\} e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2\frac{d^2}{dr^2}re^{-r/2a_0} - \frac{1}{a_0}\frac{d^2}{dr^2}r^2e^{-r/2a_0} + \frac{4}{a_0}e^{-r/2a_0} - \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{2\left[-\frac{1}{a_0} + \frac{r}{4a_0^2}\right]e^{-r/2a_0} - \frac{1}{a_0}\left[2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right]e^{-r/2a_0} + \right.$$

$$\left. + \frac{4}{a_0}e^{-r/2a_0} - \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{-\frac{2}{a_0} + \frac{r}{2a_0^2} - \frac{2}{a_0} + \frac{2r}{a_0^2} - \frac{r^2}{4a_0^3} + \frac{4}{a_0} - \frac{2r}{a_0^2}\right\}e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{2a_0^2} - \frac{r^2}{4a_0^3}\right\}e^{-r/2a_0} \;=\; -\frac{\hbar^2}{8m_e a_0^2}R_{20}(r) \quad .$$

Consequently, we find for R_{20} the eigenvalue $E_2 = -\hbar^2/\left(8m_e a_0^2\right) = -\alpha^2 m_e c^2/8 = E_1/4$ under the action of the differential operator.

c: $\boldsymbol{R_{n=2,\ell=1}(r) = \frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{a_0}\right\}e^{-r/2a_0}}$.

Since $\ell = 1$, we obtain now for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r \;-\; \frac{2}{r} \;+\; \frac{2}{a_0}\right\}$. Also using the results of **b**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r \;-\; \frac{2}{r} \;+\; \frac{2}{a_0}\right\}R_{21}(r) \;=$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r - \frac{2}{r} + \frac{2}{a_0}\right\}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r}{a_0}\right\} e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{1}{a_0}\frac{d^2}{dr^2}r^2e^{-r/2a_0} - \frac{2}{r}\frac{r}{a_0}e^{-r/2a_0} + \frac{2}{a_0}\frac{r}{a_0}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{1}{a_0}\left[2 - \frac{2r}{a_0} + \frac{r^2}{4a_0^2}\right]e^{-r/2a_0} - \frac{2}{a_0}e^{-r/2a_0} + \frac{2r}{a_0^2}e^{-r/2a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{2}{a_0} - \frac{2r}{a_0^2} + \frac{r^2}{4a_0^3} - \frac{2}{a_0} + \frac{2r}{a_0^2}\right\}e^{-r/2a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left\{\frac{r^2}{4a_0^3}\right\} e^{-r/2a_0} = -\frac{\hbar^2}{8m_e a_0^2} R_{21}(r) \quad .$$

Consequently, we find for R_{21} the eigenvalue $E_2 = -\hbar^2/\left(8m_e a_0^2\right) = -\alpha^2 m_e c^2/8 = E_1/4$ under the action of the differential operator. This is the same eigenvalue as for R_{20}. Why?

d: $\boldsymbol{R_{n=3,\ell=0}(r) = 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{2}{3}\frac{r}{a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}}$.

Since $\ell = 0$, we again obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\}$. Here, we determine, using the substitution $a_0 \to 3a_0$ in the result of **a**,

$$\frac{d^2}{dr^2} r\, e^{-r/3a_0} = \left\{-\frac{2}{3a_0} + \frac{r}{9a_0^2}\right\} e^{-r/3a_0}$$

Furthermore, using the substitution $2a_0 \to 3a_0$ in the result of **b**,

$$\frac{d^2}{dr^2} r^2\, e^{-r/3a_0} = \left\{2 - \frac{4r}{3a_0} + \frac{r^2}{9a_0^2}\right\} e^{-r/3a_0} \quad .$$

Finally, we must determine

$$\frac{d^2}{dr^2} r^3\, e^{-r/3a_0} = \frac{d}{dr}\left\{3r^2 e^{-r/3a_0} + r^3\left[-\frac{1}{3a_0}e^{-r/3a_0}\right]\right\} = \frac{d}{dr}\left\{3r^2 - \frac{r^3}{3a_0}\right\} e^{-r/3a_0}$$

$$= \left\{6r - \frac{3r^2}{3a_0}\right\} e^{-r/3a_0} + \left\{3r^2 - \frac{r^3}{3a_0}\right\}\left[-\frac{1}{3a_0}e^{-r/3a_0}\right] = \left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\} e^{-r/3a_0} \quad .$$

We find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\} R_{30}(r) = -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2}r + \frac{2}{a_0}\right\} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{1 - \frac{2}{3}\frac{r}{a_0} + \frac{2}{27}\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{d^2}{dr^2} r e^{-r/3a_0} - \frac{2}{3a_0}\frac{d^2}{dr^2} r^2 e^{-r/3a_0} + \right.$$

$$\left. + \frac{2}{27a_0^2}\frac{d^2}{dr^2} r^3 e^{-r/3a_0} + \frac{2}{a_0}e^{-r/3a_0} - \frac{4r}{3a_0^2}e^{-r/3a_0} + \frac{4r^2}{27a_0^3}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{\left[-\frac{2}{3a_0} + \frac{r}{9a_0^2}\right] e^{-r/3a_0} - \frac{2}{3a_0}\left[2 - \frac{4r}{3a_0} + \frac{r^2}{9a_0^2}\right] e^{-r/3a_0} + \right.$$

$$\left. + \frac{2}{27a_0^2}\left[6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right] e^{-r/3a_0} + \frac{2}{a_0}e^{-r/3a_0} - \frac{4r}{3a_0^2}e^{-r/3a_0} + \frac{4r^2}{27a_0^3}e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2}\left\{-\frac{2}{3a_0} + \frac{r}{9a_0^2} - \frac{4}{3a_0} + \frac{8r}{9a_0^2} - \frac{2r^2}{27a_0^3} + \frac{4r}{9a_0^2} - \frac{4r^2}{27a_0^3} + \frac{2r^3}{27 \times 9a_0^4} + \right.$$

$$\left. + \frac{2}{a_0} - \frac{4r}{3a_0^2} + \frac{4r^2}{27a_0^3}\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r} 2\left(\frac{1}{3a_0}\right)^{3/2} \left\{\frac{r}{9a_0^2} - \frac{2r^2}{27a_0^3} + \frac{2r^3}{27\times 9a_0^4}\right\} e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2} R_{30}(r) \quad .$$

Consequently, we find for R_{30} the eigenvalue $E_3 = -\hbar^2/\left(18m_e a_0^2\right) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator.

e: $\boldsymbol{R_{n=3,\ell=1}(r) = \frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{1 - \frac{1}{6}\frac{r}{a_0}\right\} \frac{r}{a_0} e^{-r/3a_0}}$.

Since $\ell = 1$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{2}{r} + \frac{2}{a_0}\right\}$. Also using the results of **d**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{2}{r} + \frac{2}{a_0}\right\} R_{31}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{2}{r} + \frac{2}{a_0}\right\} \frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{1 - \frac{1}{6}\frac{r}{a_0}\right\} \frac{r}{a_0} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\frac{1}{a_0}\frac{d^2}{dr^2} r^2 e^{-r/3a_0} - \frac{1}{6a_0^2}\frac{d^2}{dr^2} r^3 e^{-r/3a_0} + \right.$$
$$\left. + \left[-\frac{2}{r} + \frac{2}{a_0}\right]\left[1 - \frac{1}{6}\frac{r}{a_0}\right] \frac{r}{a_0} e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\frac{1}{a_0}\left\{2 - \frac{4r}{3a_0} + \frac{r^2}{9a_0^2}\right\} e^{-r/3a_0} - \frac{1}{6a_0^2}\left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\} e^{-r/3a_0} + \right.$$
$$\left. + \left[-\frac{2}{r} + \frac{2}{a_0}\right]\left[1 - \frac{1}{6}\frac{r}{a_0}\right] \frac{r}{a_0} e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\frac{2}{a_0} - \frac{4r}{3a_0^2} + \frac{r^2}{9a_0^3} - \frac{r}{a_0^2} + \frac{r^2}{3a_0^3} - \frac{r^3}{54a_0^4} - \frac{2}{a_0} + \frac{r}{3a_0^2} + \frac{2r}{a_0^2} - \frac{r^2}{3a_0^3}\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{3}{4}\sqrt{2}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\frac{r^2}{9a_0^3} - \frac{r^3}{54a_0^4}\right\} e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2} R_{31}(r) \quad .$$

Consequently, we find for R_{31} the eigenvalue $E_3 = -\hbar^2/\left(18m_e a_0^2\right) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator. This is the same eigenvalue as for R_{30}. Why?

f: $\boldsymbol{R_{n=3,\ell=2}(r) = \frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}}$.

Since $\ell = 2$, we obtain for the differential operator $-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{6}{r} + \frac{2}{a_0}\right\}$. Also using the results of **d**, we find then

$$-\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{6}{r} + \frac{2}{a_0}\right\} R_{32}(r) =$$

$$= -\frac{\hbar^2}{2m_e r}\left\{\frac{d^2}{dr^2} r - \frac{6}{r} + \frac{2}{a_0}\right\} \frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2} \left\{\left(\frac{r}{a_0}\right)^2\right\} e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0^2}\frac{d^2}{dr^2}r^3e^{-r/3a_0} + \left[-\frac{6}{r}+\frac{2}{a_0}\right]\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{1}{a_0^2}\left\{6r - \frac{2r^2}{a_0} + \frac{r^3}{9a_0^2}\right\}e^{-r/3a_0} + \left[-\frac{6}{r}+\frac{2}{a_0}\right]\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\right\}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{\frac{6r}{a_0^2} - \frac{2r^2}{a_0^3} + \frac{r^3}{9a_0^4} - \frac{6r}{a_0^2} + \frac{2r^2}{a_0^3}\right\}e^{-r/3a_0}$$

$$= -\frac{\hbar^2}{2m_e r}\frac{2}{27}\sqrt{\frac{2}{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left\{-\frac{r^3}{9a_0^4}\right\}e^{-r/3a_0} = -\frac{\hbar^2}{18m_e a_0^2}R_{32}(r) \quad .$$

Consequently, we find for R_{32} the eigenvalue $E_3 = -\hbar^2/\left(18m_e a_0^2\right) = -\alpha^2 m_e c^2/18 = E_1/9$ under the action of the differential operator. This is the same eigenvalue as for R_{30}. Why?

In the following table we collect the results of the preceding calculus.

	principal quantum number n and angular momentum ℓ		binding energy
$R_{n\ell}$	n	$\ell < n$	$E_n = -\alpha^2 m_e c^2/2n^2$
R_{10}	1	0	$E_1 = -\alpha^2 m_e c^2/2$
R_{20}	2	0	$E_2 = -\alpha^2 m_e c^2/8$
R_{21}	2	1	$E_2 = -\alpha^2 m_e c^2/8$
R_{30}	3	0	$E_3 = -\alpha^2 m_e c^2/18$
R_{31}	3	1	$E_3 = -\alpha^2 m_e c^2/18$
R_{32}	3	2	$E_3 = -\alpha^2 m_e c^2/18$

Exercício 13

a. In the lectures it has been shown

$$\hbar^2\bigtriangledown^2 = \frac{\hbar^2}{r}\frac{d^2}{dr^2}r - \frac{L^2}{2m_e r^2} \quad .$$

Consequently,

$$\left\{-\frac{\hbar^2}{2m_e}\bigtriangledown^2 - \frac{e^2}{4\pi\epsilon_0 r}\right\}\psi_{n\ell m}(\vec{r}) = \left\{-\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}r + \frac{L^2}{2m_e r^2} - \frac{e^2}{4\pi\epsilon_0 r}\right\}R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) =$$

$$= -\frac{\hbar^2}{2m_e r}\frac{d^2}{dr^2}rR_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) + \frac{L^2}{2m_e r^2}R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi) - \frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; R_{n\ell}(r)\,\frac{L^2}{2m_e r^2}\,Y_\ell^m(\vartheta,\varphi) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; R_{n\ell}(r)\,\frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,Y_\ell^m(\vartheta,\varphi) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= -Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; Y_\ell^m(\vartheta,\varphi)\,\frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,R_{n\ell}(r) \;-\; Y_\ell^m(\vartheta,\varphi)\frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)$$

$$= Y_\ell^m(\vartheta,\varphi)\left\{-\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,rR_{n\ell}(r) \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2}\,R_{n\ell}(r) \;-\; \frac{e^2}{4\pi\epsilon_0 r}R_{n\ell}(r)\right\}$$

$$= Y_\ell^m(\vartheta,\varphi)\left\{-\frac{\hbar^2}{2m_e r}\,\frac{d^2}{dr^2}\,r \;+\; \frac{\hbar^2\,\ell(\ell+1)}{2m_e r^2} \;-\; \frac{e^2}{4\pi\epsilon_0 r}\right\}R_{n\ell}(r)$$

$$= Y_\ell^m(\vartheta,\varphi)\,E_n\,R_{n\ell}(r) \;=\; E_n\,R_{n\ell}(r)Y_\ell^m(\vartheta,\varphi) \;=\; E_n\,\psi_{n\ell m}(\vec{r}) \quad .$$

b. In the lectures it has been shown

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \;=\; \int_0^{\infty} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\vartheta)d\vartheta \quad .$$

Consequently,

$$\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \;|\psi_{n\ell m}(x,y,z)|^2 \;=$$

$$= \int_0^{\infty} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\vartheta)d\vartheta \;\left|R_{n\ell}(r)\,Y_\ell^m(\vartheta,\varphi)\right|^2$$

$$= \int_0^{\infty} r^2 dr \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\vartheta)d\vartheta \;|R_{n\ell}(r)|^2\;|Y_\ell^m(\vartheta,\varphi)|^2$$

$$= \int_0^{\infty} r^2 dr\;|R_{n\ell}(r)|^2 \int_0^{2\pi} d\varphi \int_0^{\pi} \sin(\vartheta)d\vartheta \;|Y_\ell^m(\vartheta,\varphi)|^2$$

$$= 1\times 1 \;= 1 \quad .$$

Exercício 14

a. For $n = 1$ we only have $\ell = 0$ and $m = 0$. Consequently, for $n = 1$ we find one possible state, the *ground state* $|n=1,\ell=0,m=0\rangle$, with energy $E_1 = -E_\infty/1$.

For $n = 2$ we have $\ell = 0$ with $m = 0$ and $\ell = 1$ with $m = -1, 0, +1$. Consequently, for $n = 2$ we find four $(1 + 3 = 2^2)$ possible states, $|n=2,\ell=0,m=0\rangle$, $|n=2,\ell=1,m=-1\rangle$, $|n=2,\ell=1,m=0\rangle$, and $|n=2,\ell=1,m=+1\rangle$, with energy $E_2 = -E_\infty/4$.

For $n = 3$ we have $\ell = 0$ with $m = 0$, $\ell = 1$ with $m = -1, 0, +1$ and $\ell = 2$ with $m = -2, -1, 0, +1, +2$. Consequently, for $n = 3$ we find nine $(1 + 3 + 5 = 3^2)$ possible states,

$|n=3,\ell=0,m=0\rangle$, $|n=3,\ell=1,m=-1\rangle$, $|n=3,\ell=1,m=0\rangle$, $|n=3,\ell=1,m=+1\rangle$, $|n=3,\ell=2,m=-2\rangle$, $|n=3,\ell=2,m=-1\rangle$, $|n=3,\ell=2,m=0\rangle$, $|n=3,\ell=2,m=+1\rangle$, and $|n=3,\ell=2,m=+2\rangle$, with energy $E_3=-E_\infty/9$.

The number of states with the same value for ℓ equals $2\ell+1$.
The maximum value for ℓ equals $n-1$.
Hence, the number of states N_n with the same energy E_n, is given by

$$N_n \ = \ 1 \ + \ 3 \ + \ 5 \ + \ \dots \ + \ (2(n-3)+1) \ + \ (2(n-2)+1) \ + \ (2(n-1)+1) \quad .$$

The trick for adding this series has been found the other day by Carl Friedrich Gauss. Just add it term by term to the same thing but in reversed order. You obtain then

$$N_n+N_n=[1+2(n-1)+1]+[3+2(n-2)+1]+[5+2(n-3)+1]+\dots$$
$$+\dots+[2(n-3)+1+5]+[2(n-2)+1+3]+[2(n-1)+1+1] \quad .$$

The expressions in between the brackets all add up to $2n$.
Furthermore, there are n terms.
Hence,

$$2N_n=n\times 2n \qquad \rightarrow \qquad N_n=n^2 \quad .$$

Consequently, the degeneracy of the energy level E_n equals n^2.

b.

n	s	p	d	f	g	h
1	1s					
2	2s	2p				
3	3s	3p	3d			
4	4s	4p	4d	4f		
5	5s	5p	5d	5f	5g	
6	6s	6p	6d	6f	6g	6h

Exercício 15

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.

Exercício 16

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,

$$L_z \;=\; \left[\vec{r}\times\vec{p}\right]_z \;=\; xp_y - yp_x$$

a.

$$\begin{aligned}
\left[p_x\ ,\ L_z\right] \;&=\; \left[p_x\ ,\ xp_y - yp_x\right] \;= \\
&=\; \left[p_x\ ,\ xp_y\right] - \left[p_x\ ,\ yp_x\right] = x\left[p_x\ ,\ p_y\right] + \left[p_x\ ,\ x\right]p_y - y\left[p_x\ ,\ p_x\right] - \left[p_x\ ,\ y\right]p_x \\
&=\; 0 - i\hbar p_y + 0 + 0 = -i\hbar p_y \quad ,
\end{aligned}$$

$$\begin{aligned}
\left[p_y\ ,\ L_z\right] \;&=\; \left[p_y\ ,\ xp_y - yp_x\right] \;= \\
&=\; \left[p_y\ ,\ xp_y\right] - \left[p_y\ ,\ yp_x\right] = x\left[p_y\ ,\ p_y\right] + \left[p_y\ ,\ x\right]p_y - y\left[p_y\ ,\ p_x\right] - \left[p_y\ ,\ y\right]p_x \\
&=\; 0 + 0 + 0 + i\hbar p_x = i\hbar p_x \quad ,
\end{aligned}$$

and

$$\begin{aligned}
\left[p_z\ ,\ L_z\right] \;&=\; \left[p_z\ ,\ xp_y - yp_x\right] \;= \\
&=\; \left[p_z\ ,\ xp_y\right] - \left[p_z\ ,\ yp_x\right] = x\left[p_z\ ,\ p_y\right] + \left[p_z\ ,\ x\right]p_y - y\left[p_z\ ,\ p_x\right] - \left[p_z\ ,\ y\right]p_x \\
&=\; 0 + 0 + 0 + 0 = 0 \quad .
\end{aligned}$$

b.

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

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

and

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

c.

$$\begin{aligned}
\left[p^2\ ,\ L_z\right] \;&=\; \left[p_x^2 + p_y^2 + p_z^2\ ,\ L_z\right] = \\
&=\; \left[p_x^2\ ,\ L_z\right] + \left[p_y^2\ ,\ L_z\right] + \left[p_z^2\ ,\ L_z\right] = -2i\hbar p_xp_y + 2i\hbar p_xp_y + 0 = 0 \quad .
\end{aligned}$$

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

$$\begin{aligned}
[V_C(r)\ ,\ L_z] &= [V_C(r)\ ,\ xp_y - yp_x] = \\
&= [V_C(r)\ ,\ xp_y] - [V_C(r)\ ,\ yp_x] \\
&= x\,[V_C(r)\ ,\ p_y] + [V_C(r)\ ,\ x]\,p_y - y\,[V_C(r)\ ,\ p_x] - [V_C(r)\ ,\ y]\,p_x \\
&= xi\hbar\frac{y}{r}\ \frac{dV_C(r)}{dr} + 0 - yi\hbar\frac{x}{r}\ \frac{dV_C(r)}{dr} + 0 = 0 \quad .
\end{aligned}$$

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 (23) 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,

$$\begin{aligned}
\left[L^2\ ,\ L_z\right] &= \left[L_x^2 + L_y^2 + L_z^2\ ,\ L_z\right] = \\
&= \left[L_x^2\ ,\ L_z\right] + \left[L_y^2\ ,\ L_z\right] + \left[L_z^2\ ,\ L_z\right] \\
&= -i\hbar L_xL_y - i\hbar L_yL_x + i\hbar L_yL_x + i\hbar L_xL_y + 0 = 0 \quad .
\end{aligned}$$

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 $|n,\ell,m\rangle$.

Exercício 17

Let us first recall that the radial part of the Schrödinger equation is given by ($\hbar = c = 1$)

$$\left\{-\frac{1}{2m}\left[\frac{d^2}{dr^2}-\frac{\ell\,(\ell+1)}{r^2}\right]+V(r)\right\}u_\ell(r) \;=\; Eu_\ell(r)=\frac{k^2}{2m}u_\ell(r)$$

For a free particle one has $V(r)=0$.
When we substitute $z=kr$, we obtain

$$-\frac{1}{2m}\left[\frac{k^2d^2}{dz^2}-\frac{k^2\ell\,(\ell+1)}{z^2}\right]u_\ell(z) \;=\; \frac{k^2}{2m}u_\ell(z)$$

or

$$-\left[\frac{d^2}{dz^2}-\frac{\ell\,(\ell+1)}{z^2}\right]u_\ell(z)=u_\ell(z) \quad\longrightarrow\quad \left\{-\frac{d^2}{dz^2}+\frac{\ell(\ell+1)}{z^2}-1\right\}u_\ell(z)=0$$

For $\ell=0$ and for $z\gg 1$ we obtain

$$\frac{d^2}{dz^2}u_\ell(z)=-u_\ell(z)$$

which is solved by

$$u_\ell(z)=\sin(z) \qquad\text{or}\qquad u_\ell(z)=\cos(z)$$

For $z\ll 1$ we obtain

$$\frac{d^2}{dz^2}u_\ell(z)=\frac{\ell(\ell+1)}{z^2}u_\ell(z)$$

which is solved by

$$u_\ell(z)=z^{\ell+1} \qquad\text{or}\qquad u_\ell(z)=z^{-\ell}$$

b.

$$\begin{aligned}
\frac{d^2}{dz^2}u_{\ell+1}(z) &= \frac{d^2}{dz^2}\left\{\frac{\ell+1}{z}-\frac{d}{dz}\right\}u_\ell(z)= \\
&= \frac{d}{dz}\left\{-\frac{\ell+1}{z^2}+\frac{\ell+1}{z}\frac{d}{dz}-\frac{d^2}{dz^2}\right\}u_\ell(z) \\
&= \frac{d}{dz}\left\{-\frac{\ell+1}{z^2}+\frac{\ell+1}{z}\frac{d}{dz}+1-\frac{\ell(\ell+1)}{z^2}\right\}u_\ell(z) \\
&= \frac{d}{dz}\left\{-\frac{(\ell+1)^2}{z^2}+\frac{\ell+1}{z}\frac{d}{dz}+1\right\}u_\ell(z)
\end{aligned}$$

$$= \left\{ 2\frac{(\ell+1)^2}{z^3} - \frac{(\ell+1)^2}{z^2}\frac{d}{dz} - \frac{\ell+1}{z^2}\frac{d}{dz} + \frac{\ell+1}{z}\frac{d^2}{dz^2} + \frac{d}{dz} \right\} u_\ell(z)$$
$$= \left\{ 2\frac{(\ell+1)^2}{z^3} - \frac{(\ell+1)^2}{z^2}\frac{d}{dz} - \frac{\ell+1}{z^2}\frac{d}{dz} + \frac{\ell+1}{z}\left(\frac{\ell(\ell+1)}{z^2} - 1\right) + \frac{d}{dz} \right\} u_\ell(z)$$
$$= \left\{ -\frac{(\ell+1)(\ell+2)}{z^2}\frac{d}{dz} + \frac{\ell+1}{z}\left(\frac{(\ell+1)(\ell+2)}{z^2} - 1\right) + \frac{d}{dz} \right\} u_\ell(z)$$
$$= \left(\frac{(\ell+1)(\ell+2)}{z^2} - 1\right)\left\{\frac{\ell+1}{z} - \frac{d}{dz}\right\} u_\ell(z) = \left(\frac{(\ell+1)(\ell+2)}{z^2} - 1\right) u_{\ell+1}(z)$$

c.

$$u_{\ell+1}(z) = z^{\ell+2}\left(-\frac{1}{z}\frac{d}{dz}\right)\frac{u_\ell(z)}{z^{\ell+1}} =$$
$$= -z^{\ell+1}\left\{-(\ell+1)\frac{u_\ell(z)}{z^{\ell+2}} + \frac{1}{z^{\ell+1}}\frac{d}{dz}u_\ell(z)\right\} = \left\{\frac{\ell+1}{z} - \frac{d}{dz}\right\} u_\ell(z)$$

d and **e**. The spherical Bessel and Neumann functions satisfy the following relations

$$\frac{d}{dz}\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} = \frac{\ell}{z}\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} - \left\{\begin{array}{c} j_{\ell+1}(z) \\ \\ n_{\ell+1}(z)\end{array}\right\} \quad , \tag{53}$$

which can be easily shown, starting from the definitions

$$\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} = z^\ell\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\} \quad . \tag{54}$$

We determine

$$\frac{d}{dz}\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} =$$

$$= \left(\frac{dz^\ell}{dz}\right)\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\} + z^\ell\frac{d}{dz}\left[\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\}\right]$$

$$= \frac{\ell}{z}z^\ell\left(-\frac{1}{z}\frac{d}{dz}\right)^\ell \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\} - z^{\ell+1}\left(-\frac{1}{z}\frac{d}{dz}\right)^{\ell+1} \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\}$$

$$= \frac{\ell}{z}\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} - \left\{\begin{array}{c} j_{\ell+1}(z) \\ \\ n_{\ell+1}(z)\end{array}\right\} \quad , \tag{55}$$

which proofs relation (53).

Now for $zj_\ell(z)$ and $zn_\ell(z)$ we have

$$\frac{d}{dz}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} = \left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} + z\frac{d}{dz}\left\{\begin{array}{c} j_\ell(z) \\ \\ n_\ell(z)\end{array}\right\} =$$

$$= \frac{1}{z}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} + \frac{\ell}{z}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} - \left\{\begin{array}{c} zj_{\ell+1}(z) \\ \\ zn_{\ell+1}(z)\end{array}\right\} = \frac{\ell+1}{z}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} - \left\{\begin{array}{c} zj_{\ell+1}(z) \\ \\ zn_{\ell+1}(z)\end{array}\right\}$$

Hence

$$\left\{\begin{array}{c} zj_{\ell+1}(z) \\ \\ zn_{\ell+1}(z)\end{array}\right\} = \frac{\ell+1}{z}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} - \frac{d}{dz}\left\{\begin{array}{c} zj_\ell(z) \\ \\ zn_\ell(z)\end{array}\right\} \tag{56}$$

which is the relation of alinea **b** for solutions $u_{\ell+1}$ and u_ℓ of equation (4) for respectively $\ell+1$ and ℓ. Consequently, when we show that $zj_0(z)$ and $zn_0(z)$ are solutions of equation (4) for $\ell = 0$, then we may use the relation of alinea **b** for higher values of ℓ.
Now

$$\left\{\begin{array}{c} zj_0(z) \\ \\ zn_0(z)\end{array}\right\} = zz^0\left(-\frac{1}{z}\frac{d}{dz}\right)^0 \frac{1}{z}\left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\} = \left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\}$$

which functions we have shown to be solutions of equation (4) for $\ell = 0$.

For $z \gg 1$ we use the results of alinea **a** to conlude that

$$\left\{\begin{array}{c} zj_{\ell+1}(z\uparrow\infty) \\ \\ zn_{\ell+1}(z\uparrow\infty)\end{array}\right\} \longrightarrow \text{linear combinations of } \left\{\begin{array}{c} \sin(z) \\ \\ -\cos(z)\end{array}\right\}$$

Actually, the results are

$$zj_\ell\left(z\uparrow\infty\right) \longrightarrow \sin\left(z-\ell\frac{\pi}{2}\right) \quad \text{and} \quad zn_\ell\left(z\uparrow\infty\right) \longrightarrow -\cos\left(z-\ell\frac{\pi}{2}\right)$$

For $z \ll 1$ we use the results of alinea **a** to conlude that

$$\left\{\begin{array}{c} zj_{\ell+1}(z\downarrow 0) \\ \\ zn_{\ell+1}(z\downarrow 0)\end{array}\right\} \longrightarrow \left\{\begin{array}{c} z^{\ell+1} \\ \\ -z^{-\ell}\end{array}\right\}$$

Actually, the results are

$$zj_\ell\left(z\downarrow 0\right) \longrightarrow \frac{(z)^{\ell+1}}{(2\ell+1)!!} \quad \text{and} \quad zn_\ell\left(z\downarrow 0\right) \longrightarrow -\frac{(2\ell-1)!!}{(z)^\ell}$$

where

$$(2\ell\pm 1)!! = (2\ell\pm 1)\,(2\ell\pm 1-2)\,(2\ell\pm 1-4)\ldots 1$$

Exercício 19

a. In the following we consider the Schrödinger equation for general values of the orbital angular momentum ℓ, given by

$$\frac{E}{\hbar\omega}u(r) = \frac{1}{\hbar\omega}\left[\frac{\hbar^2}{2\mu}\left\{-\frac{d^2u(r)}{dr^2}+\frac{\ell(\ell+1)}{r^2}u(r)\right\}+\tfrac{1}{2}\mu\omega^2r^2u(r)\right] \quad . \tag{57}$$

We perform the transformation of the Schrödinger equation (57) in two steps. First we consider the variable ρ, given by $\rho = \sqrt{\mu\omega/\hbar}\,r$, which casts the Schrödinger equation (57) into the form

$$\begin{aligned}\frac{E}{\hbar\omega}u(\rho) &= \frac{1}{\hbar\omega}\left[\frac{\hbar^2}{2\mu}\left\{-\frac{\mu\omega}{\hbar}\frac{d^2u(\rho)}{d\rho^2}+\frac{\mu\omega}{\hbar}\frac{\ell(\ell+1)}{\rho^2}u(\rho)\right\}+\tfrac{1}{2}\mu\omega^2\frac{\hbar\rho^2}{\mu\omega}u(\rho)\right]\\ &= \tfrac{1}{2}\left[-\frac{d^2u(\rho)}{d\rho^2}+\frac{\ell(\ell+1)}{\rho^2}u(\rho)+\rho^2u(\rho)\right] \quad .\end{aligned} \tag{58}$$

For small values of ρ we obtain for the leading terms in the Schrödinger equation (58) the relation (notice that $\rho \geq 0$, since r is always positive or 0):

$$-\frac{d^2u}{d\rho^2}+\frac{\ell(\ell+1)}{\rho^2}u = 0 \quad \text{for} \quad \rho \ll 1$$

which is solved by

$$u = \rho^{-\ell} \quad \text{and} \quad u = \rho^{\ell+1},$$

whereas, for large values of ρ, the leading terms in the Schrödinger equation (58) are given by

$$-\frac{d^2u}{d\rho^2}+\rho^2u = 0 \quad \text{for} \quad r \gg 1$$

which is solved by

$$u = e^{\pm\frac{1}{2}\rho^2}$$

according to

$$\frac{d^2u}{d\rho^2} = \pm e^{\pm\frac{1}{2}\rho^2}+\rho^2e^{\pm\frac{1}{2}\rho^2} = \rho^2e^{\pm\frac{1}{2}\rho^2} \quad \text{for} \quad \rho \gg 1$$

The boundary conditions at $\rho = 0$, namely $u(\rho = 0) = 0$, and for $\rho \longrightarrow \infty$, namely that $u(\rho \to \infty)$ tends rapidly to zero in order for the wave function to be integrable, leads to the choice

$$u(\rho) = \rho^{\ell+1}e^{-\frac{1}{2}\rho^2}P(\rho) \tag{59}$$

where the polynomial P has to be determined.
In order to do so, we determine the second derivative of the above expression:

$$\begin{aligned}\frac{d^2u}{d\rho^2} &= \frac{d}{d\rho}\frac{du}{d\rho}\\ &= \frac{d}{d\rho}\left[\left\{(\ell+1)\rho^\ell\right\}e^{-\frac{1}{2}\rho^2}P+\rho^{\ell+1}\left\{-\rho e^{-\frac{1}{2}\rho^2}\right\}P+\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\frac{dP}{d\rho}\right]\end{aligned}$$

$$
\begin{aligned}
&= \frac{d}{d\rho}\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\left[\frac{\ell+1}{\rho}P - \rho P + \frac{dP}{d\rho}\right] \\
&= \left\{(\ell+1)\rho^{\ell}\right\}e^{-\frac{1}{2}\rho^2}\left[\frac{\ell+1}{\rho}P - \rho P + \frac{dP}{d\rho}\right] + \\
&\quad +\rho^{\ell+1}\left\{-\rho e^{-\frac{1}{2}\rho^2}\right\}\left[\frac{\ell+1}{\rho}P - \rho P + \frac{dP}{d\rho}\right] + \\
&\quad +\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\left[-\frac{\ell+1}{\rho^2}P + \frac{\ell+1}{\rho}\frac{dP}{d\rho} - P - \rho\frac{dP}{d\rho} + \frac{d^2P}{d\rho^2}\right] \\
&= \rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\left\{\frac{\ell+1}{\rho}\left[\frac{\ell+1}{\rho}P - \rho P + \frac{dP}{d\rho}\right] + \right. \\
&\quad \left. -\rho\left[\frac{\ell+1}{\rho}P - \rho P + \frac{dP}{d\rho}\right] + \left[-\frac{\ell+1}{\rho^2}P + \frac{\ell+1}{\rho}\frac{dP}{d\rho} - P - \rho\frac{dP}{d\rho} + \frac{d^2P}{d\rho^2}\right]\right\} \\
&= \rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\left\{\left[\frac{(\ell+1)^2}{\rho^2} - (\ell+1) - (\ell+1) + \rho^2 - \frac{(\ell+1)}{\rho^2} - 1\right]P + \right. \\
&\quad \left. + \left[\frac{(\ell+1)}{\rho} - \rho + \frac{(\ell+1)}{\rho} - \rho\right]\frac{dP}{d\rho} + \frac{d^2P}{d\rho^2}\right\}
\end{aligned}
\tag{60}
$$

When this result is substituted into equation (58) we obtain

$$
\begin{aligned}
\frac{E}{\hbar\omega}\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}P &= \tfrac{1}{2}\left\{-\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\left(\left[\frac{(\ell+1)^2}{\rho^2} - (\ell+1) - (\ell+1) + \rho^2 - \frac{(\ell+1)}{\rho^2} - 1\right]P + \right.\right. \\
&\quad \left. + \left[\frac{(\ell+1)}{\rho} - \rho + \frac{(\ell+1)}{\rho} - \rho\right]\frac{dP}{d\rho} + \frac{d^2P}{d\rho^2}\right) + \\
&\quad \left. + \frac{\ell(\ell+1)}{\rho^2}\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}P + \rho^2\rho^{\ell+1}e^{-\frac{1}{2}\rho^2}P\right\} \\
&= \rho^{\ell+1}e^{-\frac{1}{2}\rho^2}\tfrac{1}{2}\left\{-\left(\left[\frac{(\ell+1)^2 - (\ell+1)}{\rho^2} - 2(\ell+1) + \rho^2 - 1\right]P + \right.\right. \\
&\quad \left.\left. + \left[\frac{2(\ell+1)}{\rho} - 2\rho\right]\frac{dP}{d\rho} + \frac{d^2P}{d\rho^2}\right) + \frac{\ell(\ell+1)}{\rho^2}P + \rho^2P\right\}
\end{aligned}
$$

Hence

$$
\begin{aligned}
\frac{2E}{\hbar\omega}P &= \left[\frac{-(\ell+1)^2 + (\ell+1) + \ell(\ell+1)}{\rho^2} + 2(\ell+1) - \rho^2 + 1 + \rho^2\right]P + \\
&\quad - \left[\frac{2(\ell+1)}{\rho} - 2\rho\right]\frac{dP}{d\rho} - \frac{d^2P}{d\rho^2}
\end{aligned}
$$

$$= \quad (2\ell + 3)\, P - \frac{2}{\rho}\left(\ell + 1 - \rho^2\right)\frac{dP}{d\rho} - \frac{d^2P}{d\rho^2}$$

or

$$-\rho\frac{d^2P(\rho)}{d\rho^2} - 2\left(\ell + 1 - \rho^2\right)\frac{dP(\rho)}{d\rho} + \left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)\rho P(\rho) = 0 \quad . \tag{61}$$

In the second step, we define $x = \rho^2$, hence

$$\frac{d}{d\rho} = \frac{dx}{d\rho}\frac{d}{dx} = 2\rho\frac{d}{dx} = 2\sqrt{x}\,\frac{d}{dx} \tag{62}$$

and

$$\frac{d^2}{d\rho^2} = 2\sqrt{x}\,\frac{d}{dx}\,2\sqrt{x}\,\frac{d}{dx} = 2\sqrt{x}\left(\frac{1}{\sqrt{x}}\frac{d}{dx} + 2\sqrt{x}\,\frac{d^2}{dx^2}\right) = 2\frac{d}{dx} + 4x\frac{d^2}{dx^2} \quad . \tag{63}$$

For equation (61) we then obtain

$$-\sqrt{x}\left(2\frac{d}{dx} + 4x\frac{d^2}{dx^2}\right)P(x) - 2\left(\ell + 1 - x\right)2\sqrt{x}\,\frac{dP(x)}{dx} + \left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)\sqrt{x}P(x) = 0$$

or

$$-4x\frac{d^2P(x)}{dx^2} - 2\left(2\ell + 3 - 2x\right)\frac{dP(x)}{dx} + \left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)P(x) = 0$$

or even

$$x\frac{d^2P(x)}{dx^2} + \left(\ell + \tfrac{3}{2} - x\right)\frac{dP(x)}{dx} - \tfrac{1}{4}\left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)P(x) = 0 \quad . \tag{64}$$

b. For general values of the orbital angular momentum ℓ, we obtained the result of equation (58) which for $\ell = 0$ reads

$$\frac{E}{\hbar\omega}u(\rho) \quad = \quad \tfrac{1}{2}\left[-\frac{d^2u(\rho)}{d\rho^2} + \rho^2u(\rho)\right]$$

Substitution of relation (63) gives

$$\frac{E}{\hbar\omega}u(x) \quad = \quad \tfrac{1}{2}\left[-2\frac{du(x)}{dx} - 4x\frac{d^2u(x)}{dx^2} + xu(x)\right] = -2xu'' - u' + \tfrac{1}{2}xu$$

c. For general values of the orbital angular momentum ℓ, we performed the substitution given in equation (59) which, for $\ell = 0$, $x = rho^2$ and $P = \phi$, reads

$$u(x) = \sqrt{x}\,e^{-\frac{1}{2}x}\phi(x)$$

and which lead to relation (64) which, for $\ell = 0$ and $P = \phi$, reads

$$x\frac{d^2\phi(x)}{dx^2} + \left(\tfrac{3}{2} - x\right)\frac{d\phi(x)}{dx} - \tfrac{1}{4}\left(3 - \frac{2E}{\hbar\omega}\right)\phi(x) = 0 \quad .$$

The substitution $s = \frac{E}{2\hbar\omega} - \frac{3}{4}$ gives

$$x\frac{d^2\phi(x)}{dx^2} + \left(\tfrac{3}{2} - x\right)\frac{d\phi(x)}{dx} + s\phi(x) = 0 \quad .$$

d.

$$\frac{d}{dx}{}_1F_1(a,b,x) =$$

$$= \frac{d}{dx}\left(1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!} + \frac{a(a+1)(a+2)(a+3)}{b(b+1)(b+2)(b+3)}\frac{x^4}{4!} + \cdots\right)$$

$$= \frac{a}{b} + \frac{a(a+1)}{b(b+1)}\frac{x}{1} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^2}{2!} + \frac{a(a+1)(a+2)(a+3)}{b(b+1)(b+2)(b+3)}\frac{x^3}{3!} + \cdots$$

$$= \frac{a}{b}\left(1 + \frac{(a+1)}{(b+1)}\frac{x}{1} + \frac{(a+1)(a+2)}{(b+1)(b+2)}\frac{x^2}{2!} + \frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)}\frac{x^3}{3!} + \cdots\right)$$

$$= \frac{a}{b}\,{}_1F_1(a+1,b+1,x)$$

Furthermore

$$(a+1)x\,{}_1F_1(a+2,b+2,x) =$$

$$= (a+1)x\left(1 + \frac{a+2}{b+2}x + \frac{(a+2)(a+3)}{(b+2)(b+3)}\frac{x^2}{2} + \frac{(a+2)(a+3)(a+4)}{(b+2)(b+3)(b+4)}\frac{x^3}{3!} + \cdots\right)$$

$$= (a+1)x + \frac{(a+1)(a+2)}{b+2}x^2 + \frac{(a+1)(a+2)(a+3)}{(b+2)(b+3)}\frac{x^3}{2} + $$

$$+ \frac{(a+1)(a+2)(a+3)(a+4)}{(b+2)(b+3)(b+4)}\frac{x^4}{3!} + \cdots \tag{65}$$

and

$$(b+1)(b-x)\,{}_1F_1(a+1,b+1,x) = b(b+1)\,{}_1F_1(a+1,b+1,x) - (b+1)x\,{}_1F_1(a+1,b+1,x)$$

The first term on the righthand side gives

$$b(b+1)\,{}_1F_1(a+1,b+1,x) =$$

$$= b(b+1)\left(1 + \frac{a+1}{b+1}x + \frac{(a+1)(a+2)}{(b+1)(b+2)}\frac{x^2}{2} + \frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)}\frac{x^3}{3!} + \cdots\right)$$

$$= b(b+1) + b(a+1)x + \frac{b(a+1)(a+2)}{(b+2)}\frac{x^2}{2} + \frac{b(a+1)(a+2)(a+3)}{(b+2)(b+3)}\frac{x^3}{3!} + \cdots \tag{66}$$

whereas the second term on the righthand side gives

$$-(b+1)x\,{}_1F_1(a+1,b+1,x)=$$

$$=-(b+1)x\left(1+\frac{a+1}{b+1}x+\frac{(a+1)(a+2)}{(b+1)(b+2)}\frac{x^2}{2}+\frac{(a+1)(a+2)(a+3)}{(b+1)(b+2)(b+3)}\frac{x^3}{3!}+\cdots\right)$$

$$=-(b+1)x-(a+1)x^2-\frac{(a+1)(a+2)}{(b+2)}\frac{x^3}{2}-\frac{(a+1)(a+2)(a+3)}{(b+2)(b+3)}\frac{x^4}{3!}+\cdots \qquad (67)$$

The sum of the zeroeth order in x terms from the results (65), (66) and (67) reads

$$b(b+1)$$

The sum of the first order in x terms from the results (65), (66) and (67) reads

$$(a+1)x+b(a+1)x-(b+1)x=a(b+1)x=b(b+1)\frac{a}{b}x$$

The sum of the second order in x terms from the results (65), (66) and (67) reads

$$\frac{(a+1)(a+2)}{b+2}x^2+\frac{b(a+1)(a+2)}{(b+2)}\frac{x^2}{2}-(a+1)x^2=a(a+1)\frac{x^2}{2}=b(b+1)\frac{a(a+1)}{b(b+1)}\frac{x^2}{2}$$

The sum of the third order in x terms from the results (65), (66) and (67) reads

$$\frac{(a+1)(a+2)(a+3)}{(b+2)(b+3)}\frac{x^3}{2}+\frac{b(a+1)(a+2)(a+3)}{(b+2)(b+3)}\frac{x^3}{3!}-\frac{(a+1)(a+2)}{(b+2)}\frac{x^3}{2}=$$

$$=\frac{a(a+1)(a+2)}{(b+2)}\frac{x^3}{3!}=b(b+1)\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!}$$

The sum of the n-th order in x terms from the results (65), (66) and (67) reads

$$\frac{(a+1)_n}{(b+2)_{n-1}}\frac{x^n}{(n-1)!}+\frac{b(a+1)_n}{(b+2)_{n-1}}\frac{x^n}{n!}-\frac{(a+1)_{n-1}}{(b+2)_{n-2}}\frac{x^n}{(n-1)!}=$$

$$=\frac{(a+1)_{n-1}}{(b+2)_{n-1}}\frac{x^n}{n!}\left(n(a+n)+b(a+n)-n(b+n)\right)$$

$$=a(b+n)\frac{(a+1)_{n-1}}{(b+2)_{n-1}}\frac{x^n}{n!}$$

$$=b(b+1)(b+n)\frac{a(a+1)_{n-1}}{b(b+1)(b+2)_{n-1}}\frac{x^n}{n!}$$

$$=b(b+1)(b+n)\frac{(a)_n}{(b)_n(b+n)}\frac{x^n}{n!}$$

$$=b(b+1)\frac{(a)_n}{(b)_n}\frac{x^n}{n!}$$

The latter results are based in some of the properties of the Pochhammer symbol $(p)_n$.

$$\begin{aligned}
(p)_n &= p(p+1)(p+2)\dots(p+n-1) \\
&= p(p+1)(p+2)\dots(p+1+(n-1)-1) = p(p+1)_{n-1} \\
(p+1)(p+2)_n &= (p+1)(p+2)\dots(p+2+(n-1)-1)(p+2+n-1) \\
&= (p+1)(p+2)\dots(p+1+n-1)(p+n+1) = (p+1)_n(p+n+1) \\
(p+1)_{n-1}(p+n) &= (p+1)(p+2)\dots(p+2+(n-1)-1)(p+1+n-1) = (p+1)_n
\end{aligned}$$

So, we find

$$\begin{aligned}
&(a+1)x\,{}_1F_1(a+2,b+2,x) + (b+1)(b-x)\,{}_1F_1(a+1,b+1,x) = \\
&\quad = b(b+1) + b(b+1)\frac{a}{b}x + b(b+1)\frac{a(a+1)}{b(b+1)}\frac{x^2}{2} + b(b+1)\frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!} \\
&\quad = b(b+1)\left(1 + \frac{a}{b}x + \frac{a(a+1)}{b(b+1)}\frac{x^2}{2} + \frac{a(a+1)(a+2)}{b(b+1)(b+2)}\frac{x^3}{3!} + \cdots\right) \\
&\quad = b(b+1){}_1F_1(a,b,x) \qquad (68)
\end{aligned}$$

e. By defining $b = \ell + \frac{3}{2}$ and $a = \frac{1}{4}\left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)$ we arrive for equation (64) at

$$x\frac{d^2P(x)}{dx^2} + (b-x)\frac{dP(x)}{dx} - aP(x) = 0 \quad , \qquad (69)$$

which is the famous Kummer's equation (see *e.g.* chapter 13 of the "*Handbook of Mathematical Functions*" by Milton Abramowitz and Irene A. Stegun).
In the following we show that this equation is solved by $P(x) = {}_1F_1(a,b,x)$.
First we deal with the first order derivative of P.

$$\frac{dP(x)}{dx} = \frac{d}{dx}{}_1F_1(a,b,x) = \frac{a}{b}{}_1F_1(a+1,b+1,x)$$

For the second order derivative of P we find, similarly

$$\frac{d^2P(x)}{dx^2} = \frac{a}{b}\frac{d}{dx}{}_1F_1(a+1,b+1,x) = \frac{a(a+1)}{b(b+1)}{}_1F_1(a+2,b+2,x)$$

By inserting those two results in the lefthand side of equation (69) we obtain

$$\begin{aligned}
&x\frac{d^2P(x)}{dx^2} + (b-x)\frac{dP(x)}{dx} - aP(x) = \\
&\quad = x\frac{a(a+1)}{b(b+1)}{}_1F_1(a+2,b+2,x) + (b-x)\frac{a}{b}{}_1F_1(a+1,b+1,x) - a{}_1F_1(a,b,x) \\
&\quad = \frac{a}{b(b+1)}\Big((a+1)x\,{}_1F_1(a+2,b+2,x) + (b+1)(b-x)\,{}_1F_1(a+1,b+1,x) + \\
&\qquad\qquad -b(b+1){}_1F_1(a+1,b+1,x)\Big)
\end{aligned}$$

which, when compared to relation (68), indeed vanishes as demanded by equation (69). We thus have shown that equation (69) is solved by ${}_1F_1(a,b,x)$.
By substituting back all the previous definitions, namely $x = \rho^2 = \mu\omega r^2$, $a = \frac{1}{4}\left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)$ and $b = \ell + \frac{3}{2}$, we obtain the solution for the Schrödinger equation (57):

$$u(r) = \left(\sqrt{\mu\omega}\, r\right)^{\ell+1} e^{-\frac{1}{2}\mu\omega r^2} {}_1F_1\left(-\frac{E}{2\hbar\omega} + \frac{1}{2}\left(\ell + \frac{3}{2}\right), \ell + \frac{3}{2}, \mu\omega r^2\right) \quad . \tag{70}$$

However, still some important detail has to be settled, which is explained in the following.
The n-th coefficient of $\frac{x^n}{n!}$ in the Taylor expansion of the Kummer function ${}_1F_1(a,b,x)$ is given by

$$\frac{(a)_n}{(n)_n} = \frac{a(a+1)(a+2)\cdots(a+n-2)(a+n-1)}{b(b+1)(b+2)\cdots(b+n-2)(b+n-1)}$$

For large n the ratios $(a+n-1)/(b+n-1)$, $(a+n-2)/(b+n-2)$, ... tend to 1 which implies that the coefficients of $\frac{x^n}{n!}$ all tend to a constant values for large n. We find then that the Kummer function tends to a constant times e^x and, consequently, the wave function tends to a constant times

$$\left(\sqrt{\mu\omega}\, r\right)^{\ell+1} e^{-\frac{1}{2}\mu\omega r^2} e^{\mu\omega r^2} = \left(\sqrt{\mu\omega}\, r\right)^{\ell+1} e^{+\frac{1}{2}\mu\omega r^2}$$

predicting a probability distribution which is large at large distances. Clearly, such distribution cannot describe at all the physical situation of a particle oscillating around the origin of the coordinate system. The latter system is expected to have a probability distribution which vanishes at large distances. Consequently, solution (70) does not correspond to the physical situation of a particle confined to a harmonic oscillator potential. But, there exists an exception to the rule that the Kummer function tends exponentially to infinity for large values of x, namely when a equals zero or a negative integer $-n$, because in those cases the Kummer polynomial is finite and thus the behaviour at large values of x is dominated by $e^{-\frac{1}{2}x}$. Below we show some examples.

$${}_1F_1(0,b,x) = 1 + \frac{0}{b}x + \frac{0(0+1)}{b(b+1)}\frac{x^2}{2} + \frac{0(0+1)(0+2)}{b(b+1)(b+2)}\frac{x^3}{3!} + \cdots = 1$$

$${}_1F_1(-1,b,x) = 1 + \frac{-1}{b}x + \frac{-1(-1+1)}{b(b+1)}\frac{x^2}{2} + \frac{-1(-1+1)(-1+2)}{b(b+1)(b+2)}\frac{x^3}{3!} + \cdots = 1 - \frac{x}{b}$$

This implies that for the expression $a = \frac{1}{4}\left(2\ell + 3 - \frac{2E}{\hbar\omega}\right)$ only negative integer or zero values are allowed. Hence

$$\frac{1}{4}\left(2\ell + 3 - \frac{2E}{\hbar\omega}\right) = -n \quad \text{for} \quad n = 0,\ 1,\ 2,\ 3,\ \ldots$$

We thus obtain the spectrum for the physically acceptable solutions of the Schrödinger equation (57):

$$E = \hbar\omega\left(2n + \ell + \frac{3}{2}\right) \quad \text{for} \quad (n,\ell) = 0,\ 1,\ 2,\ 3,\ \ldots$$

Exercício 20

a. The Schrödinger equation for $\ell = 0$ is given by $(2m = 1)$

$$\left(-\frac{d^2}{dr^2} + \lambda\delta(r-b) - k^2\right)u(r) = 0 \qquad \text{with} \qquad b > 0$$

The necessary boundary conditions for the wave function are

$$u(r \downarrow 0) = 0 \quad , \quad u(r \uparrow b) = u(r \downarrow b) \quad \text{and} \quad \left.\frac{du}{dr}\right|_{r\downarrow b} - \left.\frac{du}{dr}\right|_{r\uparrow b} = \lambda\, u(b)$$

The latter boundary condition can be found by integrating the differential equation in a small domain, $(b-\epsilon, b+\epsilon)$, around the delta-shell position $r = b$ and letting $\epsilon \downarrow 0$. One finds

$$\lim_{\epsilon\downarrow 0}\int_{b-\epsilon}^{b+\epsilon} dr \frac{d^2u(r)}{dr^2} = \lim_{\epsilon\downarrow 0}\left[\frac{du(r)}{dr}\right]_{b-\epsilon}^{b+\epsilon} = \lim_{\epsilon\downarrow 0}\left(\left.\frac{du(r)}{dr}\right|_{b+\epsilon} - \left.\frac{du(r)}{dr}\right|_{b-\epsilon}\right) = \left.\frac{du}{dr}\right|_{r\downarrow b} - \left.\frac{du}{dr}\right|_{r\uparrow b}$$

$$\lim_{\epsilon\downarrow 0}\int_{b-\epsilon}^{b+\epsilon} dr \lambda\delta(r-b)u(r) = \lim_{\epsilon\downarrow 0}\lambda u(r=b) = \lambda u(r=b)$$

$$\lim_{\epsilon\downarrow 0}\int_{b-\epsilon}^{b+\epsilon} dr\, k^2 u(r) = \int_b^b k^2 dr\, u(r) = 0$$

Putting things together, we find the third boundary condition.

b. For $r \neq b$ the wave equation reads

$$\left(-\frac{d^2}{dr^2} - k^2\right)u(r) = 0$$

which has solutions $\sin(kr)$ and $\cos(kr)$.
So, we select

$$u(r) = \begin{cases} A\sin(kr) + C\cos(kr) & \text{for} \quad 0 \leq r < b \\ B\sin(kr+\delta) & \text{for} \quad r > b \end{cases}$$

The boundary condition $u(r \downarrow 0) = 0$ results in $C = 0$.
The boundary condition $u(r \uparrow b) = u(r \downarrow b)$ results in

$$A\sin(kb) = B\sin(kb+\delta)$$

The boundary condition $\left.\frac{du}{dr}\right|_{r\downarrow b} - \left.\frac{du}{dr}\right|_{r\uparrow b} = \lambda\, u(b)$ results in

$$Bk\cos(kb+\delta) - Ak\cos(kb) = \lambda A\sin(kb)$$

We eliminate A and B by

$$\frac{k\cos(kb+\delta)}{\sin(kb+\delta)} = \frac{Bk\cos(kb+\delta)}{B\sin(kb+\delta)} = \frac{Ak\cos(kb) + \lambda A\sin(kb)}{A\sin(kb)} = k\text{cotg}(kb) + \lambda$$

We elaborate

$$\begin{aligned}\frac{k\left(\mathrm{cotg}(kb)\mathrm{cotg}(\delta)-1\right)}{\mathrm{cotg}(\delta)+\mathrm{cotg}(kb)} &= \frac{k\left(\cos(kb)\cos(\delta)-\sin(kb)\sin(\delta)\right)}{\sin(kb)\cos(\delta)+\cos(kb)\sin(\delta)}=\frac{k\cos(kb+\delta)}{\sin(kb+\delta)}\\ &= k\mathrm{cotg}(kb)+\lambda\end{aligned}$$

Hence

$$k\mathrm{cotg}(kb)\mathrm{cotg}(\delta)-k = k\mathrm{cotg}(kb)\mathrm{cotg}(\delta)+\lambda\mathrm{cotg}(\delta)+k\mathrm{cotg}^2(kb)+\lambda\mathrm{cotg}(kb)$$

and

$$\mathrm{cotg}(\delta) = -\mathrm{cotg}(kb)-\frac{k}{\lambda}\left(\mathrm{cotg}^2(kb)+1\right)=-\mathrm{cotg}(kb)-\frac{k}{\lambda\sin^2(kb)}$$

c. Already solved.

d.

$$S = e^{2i\delta}=\frac{e^{i\delta}}{e^{-i\delta}}=\frac{\cos(\delta)+i\sin(\delta)}{\cos(\delta)-i\sin(\delta)}=\frac{\mathrm{cotg}(\delta)+i}{\mathrm{cotg}(\delta)-i}$$

Hence

$$\begin{aligned}S &= \frac{-\mathrm{cotg}(kb)-\dfrac{k}{\lambda\sin^2(kb)}+i}{-\mathrm{cotg}(kb)-\dfrac{k}{\lambda\sin^2(kb)}-i}=\frac{k+\lambda\sin(kb)\left(\cos(kb)-i\sin(kb)\right)}{k+\lambda\sin(kb)\left(\cos(kb)+i\sin(kb)\right)}\\ &= \frac{k+\lambda\sin(kb)e^{-ikb}}{k+\lambda\sin(kb)e^{ikb}}\end{aligned}$$

and

$$\begin{aligned}|S-1|^2 &= \left|\frac{k+\lambda\sin(kb)\left(\cos(kb)-i\sin(kb)\right)}{k+\lambda\sin(kb)\left(\cos(kb)+i\sin(kb)\right)}-1\right|^2=\left|\frac{-2i\lambda\sin^2(kb)}{k+\lambda\sin(kb)\left(\cos(kb)+i\sin(kb)\right)}\right|^2\\ &= \frac{4\lambda^2\sin^4(kb)}{\left(k+\lambda\sin(kb)\cos(kb)\right)^2+\lambda^2\sin^4(kb)}=\frac{4\lambda^2}{\left(\dfrac{k}{\sin^2(kb)}+\lambda\mathrm{cotg}(kb)\right)^2+\lambda^2}\end{aligned}$$

Exercício 21

a.

$$\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}\begin{pmatrix}u(r_1)\\ u'(r_1)\end{pmatrix}=\begin{pmatrix}u(r_1)\\ u'(r_1)\end{pmatrix} = \mathcal{G}(r_1,r_1)\begin{pmatrix}u(r_1)\\ u'(r_1)\end{pmatrix}$$

Hence

$$\mathcal{G}(r_1,r_1)=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}=\mathbf{1}$$

Furthermore

$$\mathcal{G}\left(r_3, r_1\right)\begin{pmatrix} u\left(r_1\right) \\ u'\left(r_1\right) \end{pmatrix} = \begin{pmatrix} u\left(r_3\right) \\ u'\left(r_3\right) \end{pmatrix} = \mathcal{G}\left(r_3, r_2\right)\begin{pmatrix} u\left(r_2\right) \\ u'\left(r_2\right) \end{pmatrix} = \mathcal{G}\left(r_3, r_2\right)\mathcal{G}\left(r_2, r_1\right)\begin{pmatrix} u\left(r_1\right) \\ u'\left(r_1\right) \end{pmatrix}$$

Hence

$$\mathcal{G}\left(r_3, r_1\right) = \mathcal{G}\left(r_3, r_2\right)\mathcal{G}\left(r_2, r_1\right)$$

Finally

$$\begin{pmatrix} u\left(r_2\right) \\ u'\left(r_2\right) \end{pmatrix} = \mathcal{G}\left(r_2, r_1\right)\begin{pmatrix} u\left(r_1\right) \\ u'\left(r_1\right) \end{pmatrix}$$

$$\longrightarrow \quad \mathcal{G}^{-1}\left(r_2, r_1\right)\begin{pmatrix} u\left(r_2\right) \\ u'\left(r_2\right) \end{pmatrix} = \begin{pmatrix} u\left(r_1\right) \\ u'\left(r_1\right) \end{pmatrix} = \mathcal{G}\left(r_1, r_2\right)\begin{pmatrix} u\left(r_2\right) \\ u'\left(r_2\right) \end{pmatrix}$$

Hence

$$\mathcal{G}^{-1}\left(r_2, r_1\right) \quad = \quad \mathcal{G}\left(r_1, r_2\right)$$

b. The Schrödinger equation for $V = 0$ and $\ell = 0$ is given by $(2m = 1)$

$$\left(-\frac{d^2}{dr^2} - k^2\right)u(r) \quad = \quad 0$$

and is solved by $u(r) = A\sin(kr)$ which satisfies the boundary condition $u(r \downarrow 0) = 0$.
We obtain then

$$\begin{pmatrix} u\left(r\right) \\ u'\left(r\right) \end{pmatrix} \quad = \quad \begin{pmatrix} A\sin(kr) \\ Ak\cos(kr) \end{pmatrix}$$

We elaborate

$$\mathcal{G}\left(r_2, r_1\right)\begin{pmatrix} u\left(r_1\right) \\ u'\left(r_1\right) \end{pmatrix} =$$

$$= \begin{pmatrix} \sin\left(kr_2\right) & -\frac{\cos\left(kr_2\right)}{k} \\ k\cos\left(kr_2\right) & \sin\left(kr_2\right) \end{pmatrix}\begin{pmatrix} \sin\left(kr_1\right) & \frac{\cos\left(kr_1\right)}{k} \\ -k\cos\left(kr_1\right) & \sin\left(kr_1\right) \end{pmatrix}\begin{pmatrix} A\sin\left(kr_1\right) \\ Ak\cos\left(kr_1\right) \end{pmatrix}$$

$$= \begin{pmatrix} \sin\left(kr_2\right) & -\frac{\cos\left(kr_2\right)}{k} \\ k\cos\left(kr_2\right) & \sin\left(kr_2\right) \end{pmatrix}\begin{pmatrix} \sin\left(kr_1\right)A\sin\left(kr_1\right) + \frac{\cos\left(kr_1\right)}{k}Ak\cos\left(kr_1\right) \\ -k\cos\left(kr_1\right)A\sin\left(kr_1\right) + \sin\left(kr_1\right)Ak\cos\left(kr_1\right) \end{pmatrix}$$

$$= \begin{pmatrix} \sin\left(kr_2\right) & -\frac{\cos\left(kr_2\right)}{k} \\ k\cos\left(kr_2\right) & \sin\left(kr_2\right) \end{pmatrix}\begin{pmatrix} A \\ 0 \end{pmatrix} = \begin{pmatrix} A\sin\left(kr_2\right) \\ Ak\cos\left(kr_2\right) \end{pmatrix} = \begin{pmatrix} u\left(r_2\right) \\ u'\left(r_2\right) \end{pmatrix}$$

c. From the boundary conditions (see exercise 20) we have

$$u(r\uparrow b)=u(r\downarrow b)\quad\text{and}\quad u'(r\downarrow b)-u'(r\uparrow b)=\lambda\,u(b)=\lambda\,u(r\uparrow b)$$

In matrix language

$$\left(\begin{array}{c} u(r\downarrow b)\\ \\ u'(r\downarrow b)\end{array}\right)=\left(\begin{array}{c} u(r\uparrow b)\\ \\ \lambda\,u(r\uparrow b)+u'(r\uparrow b)\end{array}\right)=\left(\begin{array}{cc} 1 & 0\\ \\ \lambda & 1\end{array}\right)\left(\begin{array}{c} u\,(r\uparrow b)\\ \\ u'\,(r\uparrow b)\end{array}\right)$$

Exercício 22

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

$$S_x=\left(\begin{array}{cc} x_{11} & x_{12}\\ x_{21} & x_{22}\end{array}\right)\quad,\quad S_y=\left(\begin{array}{cc} y_{11} & y_{12}\\ y_{21} & y_{22}\end{array}\right)\quad,\quad S_z=\left(\begin{array}{cc} z_{11} & z_{12}\\ z_{21} & z_{22}\end{array}\right)\quad .$$

We obtain then

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

from which we may conclude

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

Similarly

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

from which we may conclude

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

Also

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

from which we may conclude

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

Moreover,

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

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 $\left|+\frac{1}{2}\right\rangle$ and $\left|-\frac{1}{2}\right\rangle$ 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,

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

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 23a).

Exercício 23

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,

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

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

$$= \ yp_zzp_x - yp_zxp_z - zp_yzp_x + zp_yxp_z - zp_xyp_z + zp_xzp_y + xp_zyp_z - xp_zzp_y$$

$$= \ y(-i\hbar + zp_z)p_x - yxp_zp_z - z^2p_yp_x + zxp_yp_z - zyp_xp_z + z^2p_xp_y + xyp_zp_z - x(-i\hbar + zp_z)p_y$$

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

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

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

$$= \ zp_xxp_y - zp_xyp_x - xp_zxp_y + xp_zyp_x - xp_yzp_x + xp_yxp_z + yp_xzp_x - yp_xxp_z$$

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

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

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

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

$$= \ xp_yyp_z - xp_yzp_y - yp_xyp_z + yp_xzp_y - yp_zxp_y + yp_zyp_x + zp_yxp_y - zp_yyp_x$$

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

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

b:

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

$$
\begin{aligned}
&= L_x\left[\vec{L}\cdot\vec{S}\ ,\ L_x\right]+\left[\vec{L}\cdot\vec{S}\ ,\ L_x\right]L_x+L_y\left[\vec{L}\cdot\vec{S}\ ,\ L_y\right]+\left[\vec{L}\cdot\vec{S}\ ,\ L_y\right]L_y \\
&\qquad +L_z\left[\vec{L}\cdot\vec{S}\ ,\ L_z\right]+\left[\vec{L}\cdot\vec{S}\ ,\ L_z\right]L_z \\
&= L_x i\hbar\left[\vec{L}\times\vec{S}\right]_x+i\hbar\left[\vec{L}\times\vec{S}\right]_x L_x+L_y i\hbar\left[\vec{L}\times\vec{S}\right]_y+i\hbar\left[\vec{L}\times\vec{S}\right]_y L_y \\
&\qquad +L_z i\hbar\left[\vec{L}\times\vec{S}\right]_z+i\hbar\left[\vec{L}\times\vec{S}\right]_z L_z \\
&= L_x i\hbar\left[\vec{L}\times\vec{S}\right]_x+L_y i\hbar\left[\vec{L}\times\vec{S}\right]_y+L_z i\hbar\left[\vec{L}\times\vec{S}\right]_z \\
&\quad +i\hbar\left[\vec{L}\times\vec{S}\right]_x L_x+i\hbar\left[\vec{L}\times\vec{S}\right]_y L_y+i\hbar\left[\vec{L}\times\vec{S}\right]_z L_z \\
&= i\hbar\vec{L}\cdot\left[\vec{L}\times\vec{S}\right]\ +\ i\hbar\left[\vec{L}\times\vec{S}\right]\cdot\vec{L}\ =\ 0 \quad .
\end{aligned}
$$

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

$$
\begin{aligned}
\left[\vec{L}\cdot\vec{S}\ ,\ \vec{S}^{\,2}\right] &= \left[\vec{L}\cdot\vec{S}\ ,\ S_x^2+S_y^2+S_z^2\right] \\
&= \left[\vec{L}\cdot\vec{S}\ ,\ S_x^2\right]+\left[\vec{L}\cdot\vec{S}\ ,\ S_y^2\right]+\left[\vec{L}\cdot\vec{S}\ ,\ S_z^2\right] \\
&= S_x\left[\vec{L}\cdot\vec{S}\ ,\ S_x\right]+\left[\vec{L}\cdot\vec{S}\ ,\ S_x\right]S_x+S_y\left[\vec{L}\cdot\vec{S}\ ,\ S_y\right]+\left[\vec{L}\cdot\vec{S}\ ,\ S_y\right]S_y \\
&\qquad +S_z\left[\vec{L}\cdot\vec{S}\ ,\ S_z\right]+\left[\vec{L}\cdot\vec{S}\ ,\ S_z\right]S_z \\
&= -S_x i\hbar\left[\vec{L}\times\vec{S}\right]_x-i\hbar\left[\vec{L}\times\vec{S}\right]_x S_x-S_y i\hbar\left[\vec{L}\times\vec{S}\right]_y-i\hbar\left[\vec{L}\times\vec{S}\right]_y S_y \\
&\qquad -S_z i\hbar\left[\vec{L}\times\vec{S}\right]_z-i\hbar\left[\vec{L}\times\vec{S}\right]_z S_z \\
&= -S_x i\hbar\left[\vec{L}\times\vec{S}\right]_x-S_y i\hbar\left[\vec{L}\times\vec{S}\right]_y-S_z i\hbar\left[\vec{L}\times\vec{S}\right]_z \\
&\quad -i\hbar\left[\vec{L}\times\vec{S}\right]_x S_x-i\hbar\left[\vec{L}\times\vec{S}\right]_y S_y-i\hbar\left[\vec{L}\times\vec{S}\right]_z S_z \\
&= -\ i\hbar\vec{S}\cdot\left[\vec{L}\times\vec{S}\right]\ -\ i\hbar\left[\vec{L}\times\vec{S}\right]\cdot\vec{S}\ =\ 0 \quad .
\end{aligned}
$$

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

Exercício 26

a.

$$
\sum_{j=1}^{3}x_j\boldsymbol{e}_j=\vec{r}=\sum_{i=1}^{3}x'_i\boldsymbol{e}'_i=\sum_{i=1}^{3}x'_i\left\{\sum_{j=1}^{3}R_{ji}\boldsymbol{e}_j\right\}=\sum_{j=1}^{3}\left\{\sum_{i=1}^{3}R_{ji}x'_i\right\}\boldsymbol{e}_j
$$

Hence

$$
x_j=\sum_{i=1}^{3}R_{ji}x'_i
$$

Furthermore,

$$\sum_{j=1}^{3}\left[R^{-1}\right]_{ij}x_j=\sum_{j=1}^{3}\left[R^{-1}\right]_{ij}\left\{\sum_{k=1}^{3}R_{jk}x'_k\right\}=\sum_{k=1}^{3}\left\{\sum_{j=1}^{3}\left[R^{-1}\right]_{ij}R_{jk}\right\}x'_k$$
$$=\sum_{k=1}^{3}\left\{\left[R^{-1}R\right]_{ik}\right\}x'_k=\sum_{k=1}^{3}\delta_{ik}x'_k=x'_i$$

b.

$$\sum_{i=1}^{3}\left(x'_i\right)^2=\sum_{i=1}^{3}\left\{\sum_{j=1}^{3}\left[R^{-1}\right]_{ij}x_j\right\}\left\{\sum_{k=1}^{3}\left[R^{-1}\right]_{ik}x_k\right\}=\sum_{j=1}^{3}\sum_{k=1}^{3}\left\{\sum_{i=1}^{3}\left[R^{-1}\right]_{ij}\left[R^{-1}\right]_{ik}\right\}x_jx_k$$
$$=\sum_{j=1}^{3}\sum_{k=1}^{3}\left\{\sum_{i=1}^{3}\left[R^T\right]_{ij}\left[R^{-1}\right]_{ik}\right\}x_jx_k=\sum_{j=1}^{3}\sum_{k=1}^{3}\left\{\sum_{i=1}^{3}\left[R\right]_{ji}\left[R^{-1}\right]_{ik}\right\}x_jx_k$$
$$=\sum_{j=1}^{3}\sum_{k=1}^{3}\left\{\left[RR^{-1}\right]_{jk}\right\}x_jx_k=\sum_{j=1}^{3}\sum_{k=1}^{3}\delta_{jk}x_jx_k=\sum_{j=1}^{3}x_jx_j=\sum_{j=1}^{3}\left(x_j\right)^2$$

c. Since $r=r'$ one has $V(r')=V(r)$. Furthermore is it easy to show that $\sum_{i=1}^{3}\left(p'_i\right)^2=\sum_{j=1}^{3}\left(p_j\right)^2$.

d. In general one has for a Taylor expansion

$$\psi\left(x+\Delta x\ ,\ y+\Delta y\ ,\ z\right)=$$
$$=\psi\left(x,y,z\right)+\Delta x\left(\frac{\partial\psi}{\partial x}\right)+\Delta y\left(\frac{\partial\psi}{\partial y}\right)+\tfrac{1}{2}\Delta x^2\left(\frac{\partial^2\psi}{\partial x^2}\right)+\Delta x\Delta y\left(\frac{\partial^2\psi}{\partial x\partial y}\right)+\tfrac{1}{2}\Delta y^2\left(\frac{\partial^2\psi}{\partial y^2}\right)+\cdots$$

Hence, here we find

$$\psi\left(R_{ij}x_j\right)=\psi\left(R_{1j}x_j\ ,\ R_{2j}x_j\ ,\ R_{3j}x_j\right)=$$
$$=\psi\left(x-\tfrac{1}{2}\alpha^2x-\alpha y\ ,\ y-\tfrac{1}{2}\alpha^2y+\alpha x\ ,\ z\right)$$
$$=\psi\left(x,y,z\right)+\left(-\tfrac{1}{2}\alpha^2x-\alpha y\right)\left(\frac{\partial\psi}{\partial x}\right)+\left(-\tfrac{1}{2}\alpha^2y+\alpha x\right)\left(\frac{\partial\psi}{\partial y}\right)+\tfrac{1}{2}\left(-\tfrac{1}{2}\alpha^2x-\alpha y\right)^2\left(\frac{\partial^2\psi}{\partial x^2}\right)+$$
$$+\left(-\tfrac{1}{2}\alpha^2x-\alpha y\right)\left(-\tfrac{1}{2}\alpha^2y+\alpha x\right)\left(\frac{\partial^2\psi}{\partial x\partial y}\right)+\tfrac{1}{2}\left(-\tfrac{1}{2}\alpha^2y+\alpha x\right)^2\left(\frac{\partial^2\psi}{\partial y^2}\right)+\cdots$$
$$=\psi\left(x,y,z\right)+\left(-\tfrac{1}{2}\alpha^2x-\alpha y\right)\left(\frac{\partial\psi}{\partial x}\right)+\left(-\tfrac{1}{2}\alpha^2y+\alpha x\right)\left(\frac{\partial\psi}{\partial y}\right)+\tfrac{1}{2}\left(\alpha^2y^2\right)\left(\frac{\partial^2\psi}{\partial x^2}\right)+$$
$$+\left(-\alpha^2xy\right)\left(\frac{\partial^2\psi}{\partial x\partial y}\right)+\tfrac{1}{2}\left(\alpha^2x^2\right)\left(\frac{\partial^2\psi}{\partial y^2}\right)+\cdots$$
$$=\psi+\alpha\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\psi+\tfrac{1}{2}\alpha^2\left(-x\frac{\partial}{\partial x}-y\frac{\partial}{\partial y}+y^2\frac{\partial^2}{\partial x^2}-2xy\frac{\partial^2}{\partial x\partial y}+x^2\frac{\partial^2}{\partial y^2}\right)\psi+\cdots$$
$$=\psi+\alpha\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\psi+\tfrac{1}{2}\alpha^2\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\psi+\cdots$$
$$=\exp\left\{-\alpha\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)\right\}\ \psi=e^{-i\alpha L_z}\ \psi$$

for $L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$.

Exercício 27

a. The only non-zero matrix elements are

$$\begin{array}{lll} [A_1]_{23} = -\epsilon_{123} = -1 & [A_2]_{31} = -\epsilon_{231} = -1 & [A_3]_{12} = -\epsilon_{312} = -1 \\ [A_1]_{32} = -\epsilon_{132} = +1 & [A_2]_{13} = -\epsilon_{213} = +1 & [A_3]_{21} = -\epsilon_{321} = +1 \end{array}$$

Hence

$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \qquad A_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \qquad A_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

and

$$\vec{n}\cdot\vec{A} \equiv n_1A_1 + n_2A_2 + n_3A_3 = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix}$$

b. In general, one has

$$(\vec{n}\cdot\vec{A})^3 = (n_iA_i)(n_jA_j)(n_kA_k) = n_in_jn_kA_iA_jA_k.$$

We proceed by determining one matrix element of the resulting matrix. Using the property

$$\epsilon_{ijk}\epsilon_{ilm} = \epsilon_{1jk}\epsilon_{1lm} + \epsilon_{2jk}\epsilon_{2lm} + \epsilon_{3jk}\epsilon_{3lm} = \delta_{jl}\delta_{km} - \delta_{jm}\delta_{kl}.$$

of the Levi-Civita tensor, we find:

$$\begin{aligned} \{(\vec{n}\cdot\vec{A})^3\}_{ab} &= n_in_jn_k\{A_iA_jA_k\}_{ab} = n_in_jn_k(A_i)ac(A_j)_{cd}(A_k)_{db} \\ &= -n_in_jn_k\epsilon_{iac}\epsilon_{jcd}\epsilon_{kdb} = -n_in_jn_k\{\delta_{id}\delta_{aj} - \delta_{ij}\delta_{ad}\}\epsilon_{kdb} \\ &= -n_dn_an_k\epsilon_{kdb} + n^2n_k\epsilon_{kab} = 0 - n^2n_k(A_k)_{ab} \\ &= \{-n^2\vec{n}\cdot\vec{A}\}_{ab} \end{aligned}$$

The zero in the forelast step of the above derivation, comes from the deliberation that using the antisymmetry property of the Levi-Civita tensor, we have the following result for the contraction of two indices with a symmetric expression:

$$\epsilon_{ijk}n_jn_k = -\epsilon_{ikj}n_jn_k = -\epsilon_{ikj}n_kn_j = -\epsilon_{ijk}n_jn_k$$

where in the last step we used the fact that contracted indices are dummy and can consequently be represented by any symbol. So, we have obtained for the third power of the "innerproduct" the following:

$$(\vec{n}\cdot\vec{A})^3 = -n^2\vec{n}\cdot\vec{A}.$$

Using this relation repeatedly for the higher order powers of $\vec{n}\cdot\vec{A}$, we may also determine its exponential, *i.e.*

$$
\begin{aligned}
\exp\{\vec{n}\cdot\vec{A}\} &= \mathbf{1}+\vec{n}\cdot\vec{A}+\frac{1}{2!}(\vec{n}\cdot\vec{A})^2+\frac{1}{3!}(\vec{n}\cdot\vec{A})^3+\frac{1}{4!}(\vec{n}\cdot\vec{A})^4+\cdots \\
&= \mathbf{1}+\vec{n}\cdot\vec{A}+\frac{1}{2!}(\vec{n}\cdot\vec{A})^2+\frac{1}{3!}(-n^2\vec{n}\cdot\vec{A})+\frac{1}{4!}(-n^2(\vec{n}\cdot\vec{A})^2)+\cdots \\
&= \mathbf{1}+\{1-\frac{n^2}{3!}+\frac{n^4}{5!}-\frac{n^6}{7!}+\cdots\}(\vec{n}\cdot\vec{A})+ \\
&\quad +\{\frac{1}{2!}-\frac{n^2}{4!}+\frac{n^4}{6!}-\frac{n^6}{8!}+\cdots\}(\vec{n}\cdot\vec{A})^2 \\
&= \mathbf{1}+\{n-\frac{n^3}{3!}+\frac{n^5}{5!}-\frac{n^7}{7!}+\cdots\}(\hat{n}\cdot\vec{A})+ \\
&\quad +\{\frac{n^2}{2!}-\frac{n^4}{4!}+\frac{n^6}{6!}-\frac{n^8}{8!}+\cdots\}(\hat{n}\cdot\vec{A})^2.
\end{aligned}
$$

We recognize here the Taylor expansions for the cosine and sine functions. So, substituting these goniometric functions for their expansions, we obtain the following result:

$$\exp\{\vec{n}\cdot\vec{A}\} = \mathbf{1}+\sin(n)(\hat{n}\cdot\vec{A})+(1-\cos(n))(\hat{n}\cdot\vec{A})^2.$$

For the case $\vec{n}=\alpha\boldsymbol{e}_3$ we have

$$n=\alpha \qquad \text{and} \qquad \vec{n}\cdot\vec{A}=\alpha A_3=\alpha\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix}$$

Hence

$$
\begin{aligned}
\exp\left\{\alpha\boldsymbol{e}_3\cdot\vec{A}\right\} &= \begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix}+\sin(\alpha)\begin{pmatrix}0&-1&0\\1&0&0\\0&0&0\end{pmatrix}+(1-\cos(\alpha))\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&0\end{pmatrix} \\
&= \begin{pmatrix}\cos(\alpha)&-\sin(\alpha)&0\\\sin(\alpha)&\cos(\alpha)&0\\0&0&1\end{pmatrix}\equiv R(\hat{z},\alpha)
\end{aligned}
$$

c.

$$
\begin{aligned}
\{[A_i,A_j]\}_{kl} &= (A_iA_j)_{kl}-(A_jA_i)_{kl}=(A_i)_{km}(A_j)_{ml}-(A_j)_{km}(A_i)_{ml} \\
&= \epsilon_{ikm}\epsilon_{jml}-\epsilon_{jkm}\epsilon_{iml}=\epsilon_{mik}\epsilon_{mlj}-\epsilon_{mjk}\epsilon_{mli} \\
&= \delta_{il}\delta_{kj}-\delta_{ij}\delta_{kl}-(\delta_{jl}\delta_{ki}-\delta_{ji}\delta_{kl})=\delta_{il}\delta_{kj}-\delta_{jl}\delta_{ki} \\
&= \epsilon_{mij}\epsilon_{mlk}=-\epsilon_{ijm}\epsilon_{mkl}=\epsilon_{ijm}(A_m)_{kl} \\
&= (\epsilon_{ijm}A_m)_{kl}.
\end{aligned}
$$

So, for the commutator of the matrices $A_{1,2,3}$ we find:

$$[A_i, A_j] \;\; = \;\; \epsilon_{ijm} A_m$$

d and **e**. This was done in **b**.

Exercício 28

a.

$$\{(\vec{n}\cdot\vec{A})\vec{n}\}_i = (\vec{n}\cdot\vec{A})_{ij} n_j = (n_k A_k)_{ij} n_j = n_k (A_k)_{ij} n_j = -n_k \epsilon_{kij} n_j = 0,$$

or equivalently

$$(\vec{n}\cdot\vec{A})\vec{n} = 0$$

b.

$$\vec{n}\times\vec{v} \;\; = \;\; \begin{vmatrix} \boldsymbol{e}_1 & \boldsymbol{e}_2 & \boldsymbol{e}_3 \\ n_1 & n_2 & n_3 \\ n_2 - n_3 & n_3 - n_1 & n_1 - n_2 \end{vmatrix} = \begin{pmatrix} n_2\,(n_1 - n_2) - n_3\,(n_3 - n_1) \\ n_3\,(n_2 - n_3) - n_1\,(n_1 - n_2) \\ n_1\,(n_3 - n_1) - n_2\,(n_2 - n_3) \end{pmatrix}$$

$$= \;\; = \begin{pmatrix} (n_1 + n_2 + n_3)\,n_1 - (n_1^2 + n_2^2 + n_3^2) \\ (n_1 + n_2 + n_3)\,n_2 - (n_1^2 + n_2^2 + n_3^2) \\ (n_1 + n_2 + n_3)\,n_3 - (n_1^2 + n_2^2 + n_3^2) \end{pmatrix} = (n_1 + n_2 + n_3)\,\vec{n} - n^2 \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Hence

$$\vec{w} = \hat{n}\times\vec{v} \;\; = \;\; (n_1 + n_2 + n_3)\,\hat{n} - n \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

Furthermore

$$(\vec{n}\cdot\vec{A})\vec{v} = \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \begin{pmatrix} n_2 - n_3 \\ n_3 - n_1 \\ n_1 - n_2 \end{pmatrix}$$

$$= \begin{pmatrix} -n_3\,(n_3 - n_1) + n_2\,(n_3 - n_1) \\ n_3\,(n_2 - n_3) - n_1\,(n_1 - n_2) \\ -n_2\,(n_2 - n_3) + n_1\,(n_3 - n_1) \end{pmatrix} n\vec{w}$$

Hence $(\hat{n}\cdot\vec{A})\vec{v} = \vec{w}$.
Moreover

$$(\vec{n}\cdot\vec{A})\vec{w} = (\vec{n}\cdot\vec{A}) \left\{ (n_1 + n_2 + n_3)\,\hat{n} - n \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \right\} = 0 - n(\vec{n}\cdot\vec{A}) \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$= -n \begin{pmatrix} 0 & -n_3 & n_2 \\ n_3 & 0 & -n_1 \\ -n_2 & n_1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = -n \begin{pmatrix} -n_3+n_2 \\ n_3-n_1 \\ -n_2+n_1 \end{pmatrix} = -n\vec{v}$$

Hence $(\hat{n}\cdot\vec{A})\vec{w} = -\vec{v}$.
c.

$$\begin{aligned} \exp\{\vec{n}\cdot\vec{A}\}\vec{v} &= \mathbf{1}\vec{v} + \sin(n)(\hat{n}\cdot\vec{A})\vec{v} + (1-\cos(n))(\hat{n}\cdot\vec{A})^2\vec{v} \\ &= \vec{v} + \sin(n)\vec{w} - (1-\cos(n))\vec{v} = \cos(n)\vec{v} + \sin(n)\vec{w} \end{aligned}$$

and

$$\begin{aligned} \exp\{\vec{n}\cdot\vec{A}\}\vec{w} &= \mathbf{1}\vec{w} + \sin(n)(\hat{n}\cdot\vec{A})\vec{w} + (1-\cos(n))(\hat{n}\cdot\vec{A})^2\vec{w} \\ &= \vec{w} - \sin(n)\vec{v} - (1-\cos(n))\vec{w} = \cos(n)\vec{w} - \sin(n)\vec{v} \end{aligned}$$

Those transformations represent a transformation in the plane formed by the orthogonal vectors $\vec{v}$ and $\vec{w}$. Note that that plane is perpendicular to $\vec{n}$.

d. Any vector can be expressed in terms of the orthogonal set $\vec{n}$, $\vec{v}$ and $\vec{w}$. The component in the direction of $\vec{n}$ does not change, whereas the other two components rotate. Such transformation represents a rotation around the $\vec{n}$ axis with a rotation angle n.

Exercício 30

a. Notice that $\vec{L}$ are three differential operators which only act in the coordinates $\vec{r}$, not in the rotation angle α or the rotation axis $\hat{n}$, hence $\vec{L}$ commutes with $u_{ij}(\hat{n},\alpha)$ for $i,j=1,2$.

$$\psi'(\vec{r}\,) = \begin{pmatrix} u_{11}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_1(\vec{r}\,) + u_{12}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_2(\vec{r}\,) \\ u_{21}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_1(\vec{r}\,) + u_{22}(\hat{n},\alpha)e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_2(\vec{r}\,) \end{pmatrix} =$$

$$= \begin{pmatrix} u_{11}(\hat{n},\alpha) & u_{12}(\hat{n},\alpha) \\ u_{21}(\hat{n},\alpha) & u_{22}(\hat{n},\alpha) \end{pmatrix} \begin{pmatrix} e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_1(\vec{r}\,) \\ e^{-i\alpha\hat{n}\cdot\vec{L}}\psi_2(\vec{r}\,) \end{pmatrix} = \begin{pmatrix} u_{11}(\hat{n},\alpha) & u_{12}(\hat{n},\alpha) \\ u_{21}(\hat{n},\alpha) & u_{22}(\hat{n},\alpha) \end{pmatrix} e^{-i\alpha\hat{n}\cdot\vec{L}} \begin{pmatrix} \psi_1(\vec{r}\,) \\ \psi_2(\vec{r}\,) \end{pmatrix}$$

$$= e^{-i\alpha\hat{n}\cdot\vec{L}} \begin{pmatrix} u_{11}(\hat{n},\alpha) & u_{12}(\hat{n},\alpha) \\ u_{21}(\hat{n},\alpha) & u_{22}(\hat{n},\alpha) \end{pmatrix} \begin{pmatrix} \psi_1(\vec{r}\,) \\ \psi_2(\vec{r}\,) \end{pmatrix} = e^{-i\alpha\hat{n}\cdot\vec{L}}U(\hat{n},\alpha)\psi(\vec{r}\,)$$

b. Notice that $\vec{L}$ is Hermitian, *i.e.* $\vec{L}^\dagger = \vec{L}$ and, moreover, that $\hat{n}\cdot\vec{L}$ commutes with itself, hence $e^{i\alpha\hat{n}\cdot\vec{L}}e^{-i\alpha\hat{n}\cdot\vec{L}} = \mathbf{1}$.

$$\begin{aligned} &|\psi(\vec{r}\,)|^2 = |\psi'(\vec{r}\,)|^2 = \psi'(\vec{r}\,)^*\psi'(\vec{r}\,) = \\ &\quad = \psi(\vec{r}\,)^*U(\hat{n},\alpha)^\dagger e^{i\alpha\hat{n}\cdot\vec{L}}e^{-i\alpha\hat{n}\cdot\vec{L}}U(\hat{n},\alpha)\psi(\vec{r}\,) = \psi(\vec{r}\,)^*U(\hat{n},\alpha)^\dagger U(\hat{n},\alpha)\psi(\vec{r}\,) \end{aligned}$$

Consequently, $U(\hat{n},\alpha)^\dagger U(\hat{n},\alpha) = \mathbf{1}$.
Moreover,

$$\det(U)^2 = \det(U)\det(U) = \det(U)\det(U^\dagger) = \det(UU^\dagger) = 1 \quad\Longleftrightarrow\quad \det(U) = \pm 1$$

c. The most general form of a unitary matrix in two dimensions is given by

$$U(a,b) = \left(\begin{array}{cc} a^* & -b^* \\ b & a \end{array} \right)$$

where a and b represent arbitrary complex numbers.
Proof: Take an arbitrary 2×2 matrix

$$U = \left(\begin{array}{cc} A & B \\ C & D \end{array} \right)$$

Then

$$U^\dagger = \left(\begin{array}{cc} A^* & C^* \\ B^* & D^* \end{array} \right)$$

Hence

$$\mathbf{1} = UU^\dagger \quad = \quad \left(\begin{array}{cc} A & B \\ C & D \end{array} \right) \left(\begin{array}{cc} A^* & C^* \\ B^* & D^* \end{array} \right) = \left(\begin{array}{cc} AA^* + BB^* & AC^* + BD^* \\ CA^* + DB^* & CC^* + DD^* \end{array} \right)$$

with

$$AA^* + BB^* = 1 \quad , \quad AC^* + BD^* = 0 \quad , \quad CA^* + DB^* = 0 \quad \text{and} \quad CC^* + DD^* = 1$$

which is solved by $A = D^*$ and $B = -C^*$.
When, moreover this matrix has unit determinant, we have the condition

$$|a|^2 + |b|^2 = 1$$

A convenient paramatrization of unitary 2×2 matrices is by means of the *Cayley-Klein* parameters ξ_0, ξ_1, ξ_2 and ξ_3, which is a set of four real parameters related to the complex numbers a and b by

$$a = \xi_0 + i\xi_3 \quad \text{and} \quad b = \xi_2 - i\xi_1$$

When one substitutes a and b by the Cayley-Klein parameters, then one finds for a unitary 2×2 matrix the expression

$$U(\xi_0, \vec{\xi}) = \xi_0 \mathbf{1} - i\vec{\xi} \cdot \vec{\sigma}$$

where σ_1, σ_2 and σ_3 represent the Hermitean Pauli matrices.
The Pauli matrices satisfy the following relations.
For the product of two Pauli matrices one has

$$\sigma_i \sigma_j = \mathbf{1}\delta_{ij} + i\epsilon_{ijk}\sigma_k$$

for their commutator one has

$$\left[\sigma_i, \sigma_j\right] = 2i\epsilon_{ijk}\sigma_k$$

and for their anti-commutator

$$\left\{\sigma_i, \sigma_j\right\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\mathbf{1}$$

When, moreover the matrix $U(\xi_0, \vec{\xi})$ is unimodular, we have the condition

$$(\xi_0)^2 + (\xi_1)^2 + (\xi_2)^2 + (\xi_3)^2 = 1$$

This way we obtain three free parameters for the characterization of a 2×2 unimodular and unitary matrix.
Let us combine three parameters n_1, n_2 and n_3 into a vector $\vec{n}$ given by

$$\vec{n} = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} \quad \text{with} \quad \alpha = \sqrt{(n_1)^2 + (n_2)^2 + (n_3)^2}$$

By means of those parameters, one might select for the Cayley-Klein parameters the following parametrization

$$\xi_0 = \cos\left(\frac{\alpha}{2}\right) \quad \text{and} \quad \vec{\xi} = \hat{n}\sin\left(\frac{\alpha}{2}\right)$$

where $\hat{n}$ is defined by

$$\hat{n} = \begin{pmatrix} \hat{n}_1 \\ \hat{n}_2 \\ \hat{n}_3 \end{pmatrix} = \frac{1}{\alpha}\begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

This way we find for an arbitrary unimodular unitary 2×2 matrix the following general expression:

$$U(\hat{n}, \alpha) = \mathbf{1}\cos\left(\frac{\alpha}{2}\right) - i(\hat{n}\cdot\sigma)\sin\left(\frac{\alpha}{2}\right)$$

d. Noticing moreover that $(\hat{n}\cdot\vec{\sigma})^2 = \mathbf{1}$, it is easy to show that $U(\hat{n}, \alpha)$ may also be written in the form

$$U(\hat{n}, \alpha) = \exp\left\{-\frac{i}{2}\alpha\hat{n}\cdot\vec{\sigma}\right\}$$

as follows.
First we notice

$$(\vec{n}\cdot\vec{\sigma})^2 = \left(\sum_{i=1}^{i=3} n_i\sigma_i\right)^2 \quad = \quad \sum_{i=1}^{3} n_i\sigma_i \sum_{j=1}^{3} n_j\sigma_i = \sum_{i=1}^{3}\sum_{j=1}^{3} n_i n_j \left\{\mathbf{1}\delta_{ij} + i\epsilon_{ijk}\sigma_k\right\} = n^2\mathbf{1} + 0$$

Hence

$$(\hat{n}\cdot\vec{\sigma})^2 = \mathbf{1}$$

and

$$(\hat{n}\cdot\vec{\sigma})^3 = (\hat{n}\cdot\vec{\sigma})\ , \quad (\hat{n}\cdot\vec{\sigma})^4 = (\hat{n}\cdot\vec{\sigma})^2 = 1\ , \quad (\hat{n}\cdot\vec{\sigma})^5 = (\hat{n}\cdot\vec{\sigma})^3 = (\hat{n}\cdot\vec{\sigma})\ , \quad \ldots$$

So we find

$$
\begin{aligned}
U(\vec{n}) &= \mathbf{1}\cos\left(\frac{\alpha}{2}\right) - i(\hat{n}\cdot\sigma)\sin\left(\frac{\alpha}{2}\right) = \\
&= \mathbf{1}\left(1 - \tfrac{1}{2!}\left(\frac{\alpha}{2}\right)^2 + \tfrac{1}{4!}\left(\frac{\alpha}{2}\right)^4 + \dots\right) - i(\hat{n}\cdot\sigma)\left(\left(\frac{\alpha}{2}\right) - \tfrac{1}{3!}\left(\frac{\alpha}{2}\right)^3 + \dots\right) \\
&= \mathbf{1} + \left(-i\frac{\alpha}{2}(\hat{n}\cdot\sigma)\right) + \tfrac{1}{2!}\left(-i\frac{\alpha}{2}(\hat{n}\cdot\sigma)\right)^2 + \tfrac{1}{3!}\left(-i\frac{\alpha}{2}(\hat{n}\cdot\sigma)\right)^3 + \tfrac{1}{4!}\left(-i\frac{\alpha}{2}(\hat{n}\cdot\sigma)\right)^4 + \dots \\
&= e^{-\frac{i}{2}\alpha\hat{n}\cdot\sigma}
\end{aligned}
$$

Consequently, since $\vec{L}$ and σ commute, we find

$$
e^{-i\alpha\hat{n}\cdot\vec{L}}\,U(\hat{n},\alpha) \;=\; e^{-i\alpha\hat{n}\cdot\left(\vec{L}+\frac{\sigma}{2}\right)}
$$

e. The eigenvalues of $S_z = \frac{\vec{\sigma_3}}{2}$ are trivial

$$
\frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{1}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}
$$

The system describes a particle with spin 1/2.

Exercício 31

a. Let us first study the action of $L_\pm$ at $Y_{1,m}(\hat{r})$.

$$
L_\pm Y_{1,m}(\hat{r}) \;=\; \sqrt{1(1+1)-m(m\pm 1)}\,Y_{1,m\pm 1}(\hat{r}) = \sqrt{2-m(m\pm 1)}\,Y_{1,m\pm 1}(\hat{r})
$$

Hence

$$
\begin{array}{l}
L_+Y_{1,+1}(\hat{r}) = 0 \quad , \quad L_+Y_{1,0}(\hat{r}) = \sqrt{2}Y_{1,+1}(\hat{r}) \quad \text{and} \quad L_+Y_{1,-1}(\hat{r}) = \sqrt{2}Y_{1,0}(\hat{r}) \\
L_-Y_{1,+1}(\hat{r}) = \sqrt{2}Y_{1,0}(\hat{r}) \quad , \quad L_-Y_{1,0}(\hat{r}) = \sqrt{2}Y_{1,-1}(\hat{r}) \quad \text{and} \quad L_-Y_{1,-1}(\hat{r}) = 0
\end{array}
$$

So we have then

$$
L_x\sigma_1 + L_y\sigma_2 = L_x\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + L_y\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & L_x - iL_y \\ L_x + iL_y & 0 \end{pmatrix} = \begin{pmatrix} 0 & L_- \\ L_+ & 0 \end{pmatrix}
$$

Consequently

$$
L_x\sigma_1 + L_y\sigma_2\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 & L_- \\ L_+ & 0 \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} L_-\psi_2 \\ L_+\psi_1 \end{pmatrix}
$$

Furthermore

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

So

$$L_z\sigma_3\begin{pmatrix}\psi_1\\ \\ \psi_2\end{pmatrix}=\begin{pmatrix}L_z & 0\\ 0 & -L_z\end{pmatrix}\begin{pmatrix}\psi_1\\ \\ \psi_2\end{pmatrix}=\begin{pmatrix}L_z\psi_1\\ \\ -L_z\psi_2\end{pmatrix}$$

b. First, we determine J^2.

$$J^2=\left(\vec{L}+\frac{\vec{\sigma}}{2}\right)^2=L^2+\vec{L}\cdot\sigma+\tfrac{1}{4}\sigma^2=L^2+L_x\sigma_1+L_y\sigma_2+L_y\sigma_3+\tfrac{3}{4}\mathbf{1}=$$
$$=L^2+\begin{pmatrix}0 & L_-\\ L_+ & 0\end{pmatrix}+\begin{pmatrix}L_z & 0\\ 0 & -L_z\end{pmatrix}+\tfrac{3}{4}\mathbf{1}=\begin{pmatrix}L^2+L_z+\frac{3}{4} & L_-\\ L_+ & L^2-L_z+\frac{3}{4}\end{pmatrix}$$

For $Y_{1,m}(\hat{r})$ one has, moreover, $L^2Y_{1,m}(\hat{r})=2Y_{1,m}(\hat{r})$.
We obtain

$$J^2\begin{pmatrix}Y_{1,m}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}2+L_z+\frac{3}{4} & L_-\\ \\ L_+ & 2-L_z+\frac{3}{4}\end{pmatrix}\begin{pmatrix}Y_{1,m}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}\left(\frac{11}{4}+L_z\right)Y_{1,m}(\hat{r})\\ \\ L_+Y_{1,m}(\hat{r})\end{pmatrix}$$

and

$$J^2\begin{pmatrix}0\\ \\ Y_{1,m}(\hat{r})\end{pmatrix}=\begin{pmatrix}2+L_z+\frac{3}{4} & L_-\\ \\ L_+ & 2-L_z+\frac{3}{4}\end{pmatrix}\begin{pmatrix}0\\ \\ Y_{1,m}(\hat{r})\end{pmatrix}=\begin{pmatrix}L_-Y_{1,m}(\hat{r})\\ \\ \left(\frac{11}{4}-L_z\right)Y_{1,m}(\hat{r})\end{pmatrix}$$

c. First, we determine J_z.

$$J_z=L_z+\tfrac{1}{2}\sigma_3=\begin{pmatrix}L_z+\frac{1}{2} & 0\\ \\ 0 & L_z-\frac{1}{2}\end{pmatrix}$$

$$J^2\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}\left(\frac{11}{4}+L_z\right)Y_{1,+1}(\hat{r})\\ \\ L_+Y_{1,+1}(\hat{r})\end{pmatrix}=\begin{pmatrix}\frac{15}{4}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\tfrac{3}{2}\left(\tfrac{3}{2}+1\right)\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}$$

$$J_z\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}L_z+\frac{1}{2} & 0\\ \\ 0 & L_z-\frac{1}{2}\end{pmatrix}\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}\left(1+\frac{1}{2}\right)Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\tfrac{3}{2}\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}$$

Next, we determine J_-.

$$J_-=L_-+\tfrac{1}{2}\left(\sigma_1-i\sigma_2\right)=L_-+\tfrac{1}{2}\left\{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}-i\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\right\}=\begin{pmatrix}L_- & 0\\ 1 & L_-\end{pmatrix}$$

Hence

$$J_-\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}L_- & 0\\ \\ 1 & L_-\end{pmatrix}\begin{pmatrix}Y_{1,+1}(\hat{r})\\ \\ 0\end{pmatrix}=\begin{pmatrix}L_-Y_{1,+1}(\hat{r})\\ \\ Y_{1,+1}(\hat{r})\end{pmatrix}=\begin{pmatrix}\sqrt{2}Y_{1,0}(\hat{r})\\ \\ Y_{1,+1}(\hat{r})\end{pmatrix}$$

We determine

$$J^2 \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 2 + L_z + \frac{3}{4} & L_- \\ L_+ & 2 - L_z + \frac{3}{4} \end{pmatrix} \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} \left(\frac{11}{4} + L_z\right)\sqrt{2}Y_{1,0}(\hat{r}) + L_- Y_{1,+1}(\hat{r}) \\ L_+\sqrt{2}Y_{1,0}(\hat{r}) + \left(\frac{11}{4} - L_z\right) Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} \frac{15}{4}\sqrt{2}Y_{1,0}(\hat{r}) \\ \frac{15}{4}\sqrt{2}Y_{1,+1}(\hat{r}) \end{pmatrix} = \frac{3}{2}\left(\frac{3}{2}+1\right) \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix}$$

and

$$J_z \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} Lz + \frac{1}{2} & 0 \\ 0 & Lz - \frac{1}{2} \end{pmatrix} \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} \left(Lz + \frac{1}{2}\right)\sqrt{2}Y_{1,0}(\hat{r}) \\ \left(Lz - \frac{1}{2}\right) Y_{1,+1}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2}\sqrt{2}Y_{1,0}(\hat{r}) \\ \frac{1}{2}Y_{1,+1}(\hat{r}) \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix}$$

Furthermore

$$(J_-)^2 \begin{pmatrix} Y_{1,+1}(\hat{r}) \\ 0 \end{pmatrix} = J_- \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} L_- & 0 \\ 1 & L_- \end{pmatrix} \begin{pmatrix} \sqrt{2}Y_{1,0}(\hat{r}) \\ Y_{1,+1}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} \sqrt{2}L_- Y_{1,0}(\hat{r}) \\ \sqrt{2}Y_{1,0}(\hat{r}) + L_- Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

We determine

$$J^2 \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 2 + L_z + \frac{3}{4} & L_- \\ L_+ & 2 - L_z + \frac{3}{4} \end{pmatrix} \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} 2\left(\frac{11}{4} + L_z\right) Y_{1,-1}(\hat{r}) + 2\sqrt{2}L_- Y_{1,0}(\hat{r}) \\ 2L_+ Y_{1,-1}(\hat{r}) + 2\sqrt{2}\left(\frac{11}{4} - L_z\right) Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} \frac{15}{4}2Y_{1,-1}(\hat{r}) \\ \frac{15}{4}2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix} = \frac{3}{2}\left(\frac{3}{2}+1\right) \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

and

$$J_z \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} Lz + \frac{1}{2} & 0 \\ 0 & Lz - \frac{1}{2} \end{pmatrix} \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} \left(Lz + \frac{1}{2}\right) 2Y_{1,-1}(\hat{r}) \\ \left(Lz - \frac{1}{2}\right) 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

$$= -\frac{1}{2} \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

Finally

$$(J_-)^3 \begin{pmatrix} Y_{1,+1}(\hat{r}) \\ 0 \end{pmatrix} = J_- \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} L_- & 0 \\ 1 & L_- \end{pmatrix} \begin{pmatrix} 2Y_{1,-1}(\hat{r}) \\ 2\sqrt{2}Y_{1,0}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} 2L_-Y_{1,-1}(\hat{r}) \\ 2Y_{1,-1}(\hat{r}) + 2\sqrt{2}L_-Y_{1,0}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix}$$

We determine

$$J^2 \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 2 + L_z + \frac{3}{4} & L_- \\ L_+ & 2 - L_z + \frac{3}{4} \end{pmatrix} \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 6L_-Y_{1,-1}(\hat{r}) \\ 6\left(\frac{11}{4} - L_z\right) Y_{1,-1}(\hat{r}) \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ \frac{15}{4}6Y_{1,-1}(\hat{r}) \end{pmatrix} = \frac{3}{2}\left(\frac{3}{2} + 1\right) \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix}$$

and

$$J_z \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} L_z + \frac{1}{2} & 0 \\ 0 & L_z - \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 0 \\ \left(L_z - \frac{1}{2}\right) 6Y_{1,-1}(\hat{r}) \end{pmatrix}$$

$$= -\frac{3}{2} \begin{pmatrix} 0 \\ 6Y_{1,-1}(\hat{r}) \end{pmatrix}$$

We found

normalized state	operator	j	j_z
$\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}} = \begin{pmatrix} Y_{1,+1}(\hat{r}) \\ 0 \end{pmatrix}$		$\frac{3}{2}$	$+\frac{3}{2}$
$\mathcal{Y}_{\frac{3}{2},+\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0}(\hat{r}) \\ \sqrt{\frac{1}{3}}Y_{1,+1}(\hat{r}) \end{pmatrix}$	$\propto J_-\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$	$\frac{3}{2}$	$+\frac{1}{2}$
$\mathcal{Y}_{\frac{3}{2},-\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{1}{3}}Y_{1,-1}(\hat{r}) \\ \sqrt{\frac{2}{3}}Y_{1,0}(\hat{r}) \end{pmatrix}$	$\propto (J_-)^2\,\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$	$\frac{3}{2}$	$-\frac{1}{2}$
$\mathcal{Y}_{\frac{3}{2},-\frac{3}{2}} = \begin{pmatrix} 0 \\ Y_{1,-1}(\hat{r}) \end{pmatrix}$	$\propto (J_-)^3\,\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}}$	$\frac{3}{2}$	$-\frac{3}{2}$

So, out of the six states we have classified four linear combinations as eigenstates of J^2 with $j = \frac{3}{2}$. There are two more linear combinations, orthogonal to the two states with $j_z = \pm\frac{1}{2}$, which are

$$\mathcal{Y}_{\frac{1}{2},+\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{1}{3}}Y_{1,0}(\hat{r}) \\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r}) \end{pmatrix} \quad \text{and} \quad \mathcal{Y}_{\frac{1}{2},-\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r}) \\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r}) \end{pmatrix}$$

We determine

$$J^2\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}=\begin{pmatrix}2+L_z+\frac{3}{4} & L_-\\ L_+ & 2-L_z+\frac{3}{4}\end{pmatrix}\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}$$

$$=\begin{pmatrix}\sqrt{\frac{1}{3}}\left(\frac{11}{4}+L_z\right)Y_{1,0}(\hat{r})-\sqrt{\frac{2}{3}}L_-Y_{1,+1}(\hat{r})\\ \sqrt{\frac{1}{3}}L_+Y_{1,0}(\hat{r})-\sqrt{\frac{2}{3}}\left(\frac{11}{4}-L_z\right)Y_{1,+1}(\hat{r})\end{pmatrix}=\begin{pmatrix}\frac{3}{4}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\frac{3}{4}\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}=\frac{1}{2}\left(\frac{1}{2}+1\right)\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}$$

$$J^2\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}=\begin{pmatrix}2+L_z+\frac{3}{4} & L_-\\ L_+ & 2-L_z+\frac{3}{4}\end{pmatrix}\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}$$

$$=\begin{pmatrix}\sqrt{\frac{2}{3}}\left(\frac{11}{4}+L_z\right)Y_{1,-1}(\hat{r})-\sqrt{\frac{1}{3}}L_-Y_{1,0}(\hat{r})\\ \sqrt{\frac{2}{3}}L_+Y_{1,-1}(\hat{r})-\sqrt{\frac{1}{3}}\left(\frac{11}{4}-L_z\right)Y_{1,0}(\hat{r})\end{pmatrix}=\begin{pmatrix}\frac{3}{4}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\frac{3}{4}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}=\frac{1}{2}\left(\frac{1}{2}+1\right)\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}$$

and

$$J_Z\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}=\begin{pmatrix}L_Z+\frac{1}{2} & 0\\ 0 & L_Z-\frac{1}{2}\end{pmatrix}\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}$$

$$=\begin{pmatrix}\sqrt{\frac{1}{3}}\left(L_Z+\frac{1}{2}\right)Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}\left(L_Z-\frac{1}{2}\right)Y_{1,+1}(\hat{r})\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}$$

$$J_Z\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}=\begin{pmatrix}L_Z+\frac{1}{2} & 0\\ 0 & L_Z-\frac{1}{2}\end{pmatrix}\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}$$

$$=\begin{pmatrix}\sqrt{\frac{2}{3}}\left(L_Z+\frac{1}{2}\right)Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}\left(L_Z-\frac{1}{2}\right)Y_{1,0}(\hat{r})\end{pmatrix}=-\frac{1}{2}\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}$$

So, we found two linear combinations which are eigenstates of J^2 with $j=\frac{1}{2}$.

normalized state	j	j_z
$\mathcal{Y}_{\frac{1}{2},+\frac{1}{2}}=\begin{pmatrix}\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\\ -\sqrt{\frac{2}{3}}Y_{1,+1}(\hat{r})\end{pmatrix}$	$\frac{1}{2}$	$+\frac{1}{2}$
$\mathcal{Y}_{\frac{1}{2},-\frac{1}{2}}=\begin{pmatrix}\sqrt{\frac{2}{3}}Y_{1,-1}(\hat{r})\\ -\sqrt{\frac{1}{3}}Y_{1,0}(\hat{r})\end{pmatrix}$	$\frac{1}{2}$	$-\frac{1}{2}$

Exercício 32

a.

$$L^2 = L^2\mathbf{1} = \begin{pmatrix} L^2 & 0 \\ 0 & L^2 \end{pmatrix}$$

Hence

$$L^2 \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \begin{pmatrix} L^2 & 0 \\ 0 & L^2 \end{pmatrix} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \begin{pmatrix} L^2 Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$
$$= \begin{pmatrix} 1(1+1)Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = 2 \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$

and

$$L^2 \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \begin{pmatrix} L^2 & 0 \\ 0 & L^2 \end{pmatrix} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 0 \\ L^2 Y_{1,m}(\hat{r}) \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ 1(1+1)Y_{1,m}(\hat{r}) \end{pmatrix} = 2 \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix}$$

$$L_z = L_z\mathbf{1} = \begin{pmatrix} L_z & 0 \\ 0 & L_z \end{pmatrix}$$

Hence

$$L_z \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \begin{pmatrix} L_z & 0 \\ 0 & L_z \end{pmatrix} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \begin{pmatrix} L_z Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$
$$= \begin{pmatrix} mY_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = m \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$

and

$$L_z \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \begin{pmatrix} L_z & 0 \\ 0 & L_z \end{pmatrix} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \begin{pmatrix} 0 \\ L_z Y_{1,m}(\hat{r}) \end{pmatrix}$$
$$= \begin{pmatrix} 0 \\ mY_{1,m}(\hat{r}) \end{pmatrix} = m \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix}$$

$$\left(\frac{\vec{\sigma}}{2}\right)^2 = \tfrac{3}{4}\mathbf{1}$$

Hence

$$\left(\frac{\vec{\sigma}}{2}\right)^2 \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \tfrac{3}{4}\mathbf{1} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \tfrac{3}{4} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$

and

$$\left(\frac{\vec{\sigma}}{2}\right)^2 \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \tfrac{3}{4}\mathbf{1} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \tfrac{3}{4} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix}$$

$$\frac{\sigma_z}{2} = \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Hence

$$\frac{\sigma_z}{2} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix} = \tfrac{1}{2} \begin{pmatrix} Y_{1,m}(\hat{r}) \\ 0 \end{pmatrix}$$

and

$$\frac{\sigma_z}{2} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \tfrac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix} = \tfrac{1}{2} \begin{pmatrix} 0 \\ -Y_{1,m}(\hat{r}) \end{pmatrix} = -\tfrac{1}{2} \begin{pmatrix} 0 \\ Y_{1,m}(\hat{r}) \end{pmatrix}$$

b.

$$\begin{aligned}
\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = +1\rangle &= \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} \\
\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle &= \begin{pmatrix} Y_{1,0} \\ 0 \end{pmatrix} \\
\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = -1\rangle &= \begin{pmatrix} Y_{1,-1} \\ 0 \end{pmatrix} \\
\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = +1\rangle &= \begin{pmatrix} 0 \\ Y_{1,+1} \end{pmatrix} \\
\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle &= \begin{pmatrix} 0 \\ Y_{1,0} \end{pmatrix} \\
\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = -1\rangle &= \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix}
\end{aligned}$$

c. All six states in alinea **a** are eigenstates of $\boldsymbol{L^2}$ with the same eigenvalue **2**. Consequently, all linear combinations are also eigenstates of $\boldsymbol{L^2}$ with the same eigenvalue **2**.
All six states in alinea **a** are eigenstates of $\left(\frac{\vec{\boldsymbol{\sigma}}}{\mathbf{2}}\right)^{\mathbf{2}}$ with the same eigenvalue $\mathbf{\frac{3}{4}}$. Consequently, all linear combinations are also eigenstates of $\left(\frac{\vec{\boldsymbol{\sigma}}}{\mathbf{2}}\right)^{\mathbf{2}}$ with the same eigenvalue $\mathbf{\frac{3}{4}}$.
However, although all six states in alinea **a** are eigenstates of $\boldsymbol{L_z}$, they do not have the same eigenvalue. As a consequence linear combinations cannot always be eigenstates of $\boldsymbol{L_z}$. For example

$$L_z \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix} = \begin{pmatrix} L_z & 0 \\ 0 & L_z \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{2}{3}}L_zY_{1,0} \\ \sqrt{\frac{1}{3}}L_zY_{1,+1} \end{pmatrix} = \begin{pmatrix} 0 \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix}$$

Hence, this state is not an eigenstate of $\boldsymbol{L_z}$.
Similarly, although all six states in alinea **a** are eigenstates of $\frac{\boldsymbol{\sigma_z}}{\mathbf{2}}$, they do not have the same eigenvalue. As a consequence linear combinations cannot always be eigenstates of $\frac{\boldsymbol{\sigma_z}}{\mathbf{2}}$. For example

$$\frac{\sigma_z}{2} \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ -\sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix}$$

Hence, this state is not an eigenstate of $\frac{\boldsymbol{\sigma_z}}{\mathbf{2}}$.
Next, we determine J^2.

$$J^2 = \left(\vec{L} + \frac{\vec{\sigma}}{2}\right)^2 = L^2 + \vec{L}\cdot\sigma + \tfrac{1}{4}\sigma^2 = L^2 + L_x\sigma_1 + L_y\sigma_2 + L_y\sigma_3 + \tfrac{3}{4}\mathbf{1} =$$
$$= L^2 + \begin{pmatrix} 0 & L_- \\ L_+ & 0 \end{pmatrix} + \begin{pmatrix} L_z & 0 \\ 0 & -L_z \end{pmatrix} + \tfrac{3}{4}\mathbf{1} = \begin{pmatrix} L^2 + L_z + \frac{3}{4} & L_- \\ L_+ & L^2 - L_z + \frac{3}{4} \end{pmatrix}$$

For $Y_{1,m}$ one has, moreover, $L^2Y_{1,m} = 2Y_{1,m}$. Hence, for the present case one may write

$$J^2 = \begin{pmatrix} 2 + L_z + \frac{3}{4} & L_- \\ L_+ & 2 - L_z + \frac{3}{4} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix}$$

We obtain

$$J^2 \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} = \begin{pmatrix} \left(\frac{11}{4} + L_z\right) Y_{1,+1} \\ L_+Y_{1,+1}(\hat{r}) \end{pmatrix} = \begin{pmatrix} \frac{15}{4}Y_{1,+1} \\ 0 \end{pmatrix} = \tfrac{3}{2}\left(\tfrac{3}{2}+1\right) \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix}$$

$$J^2 \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix}$$

$$= \begin{pmatrix} \sqrt{\frac{2}{3}}\left(\frac{11}{4} + L_z\right) Y_{1,0} + \sqrt{\frac{1}{3}}L_-Y_{1,+1} \\ \sqrt{\frac{2}{3}}L_+Y_{1,0} + \sqrt{\frac{1}{3}}\left(\frac{11}{4} - L_z\right) Y_{1,+1} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{2}{3}}\frac{15}{4}Y_{1,0} \\ \sqrt{\frac{1}{3}}\frac{15}{4}\sqrt{2}Y_{1,+1} \end{pmatrix} = \tfrac{3}{2}\left(\tfrac{3}{2}+1\right) \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix}$$

$$J^2 \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix}$$

$$= \begin{pmatrix} \sqrt{\frac{1}{3}} \left(\frac{11}{4} + L_z\right) Y_{1,-1} + \sqrt{\frac{2}{3}} L_- Y_{1,0} \\ \sqrt{\frac{1}{3}} L_+ Y_{1,-1} + \sqrt{\frac{2}{3}} \left(\frac{11}{4} - L_z\right) Y_{1,0} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} \frac{15}{4} Y_{1,-1} \\ \sqrt{\frac{2}{3}} \frac{15}{4} Y_{1,0} \end{pmatrix} = \frac{3}{2}\left(\frac{3}{2}+1\right) \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix}$$

$$J^2 \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix} \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} = \begin{pmatrix} L_- Y_{1,-1} \\ \left(\frac{11}{4} - L_z\right) Y_{1,-1} \end{pmatrix}$$

$$= \begin{pmatrix} 0 \\ \frac{15}{4} Y_{1,-1} \end{pmatrix} = \frac{3}{2}\left(\frac{3}{2}+1\right) \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix}$$

Finally, we determine J_Z.

$$J_Z = L_Z + \tfrac{1}{2}\sigma_3 = \begin{pmatrix} L_Z + \frac{1}{2} & 0 \\ 0 & L_Z - \frac{1}{2} \end{pmatrix}$$

We obtain

$$J_Z \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} = \begin{pmatrix} L_Z + \frac{1}{2} & 0 \\ 0 & L_Z - \frac{1}{2} \end{pmatrix} \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix} = \begin{pmatrix} \left(L_Z + \frac{1}{2}\right) Y_{1,+1} \\ 0 \end{pmatrix} = \frac{3}{2} \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix}$$

$$J_Z \begin{pmatrix} \sqrt{\frac{2}{3}} Y_{1,0} \\ \sqrt{\frac{1}{3}} Y_{1,+1} \end{pmatrix} = \begin{pmatrix} L_Z + \frac{1}{2} & 0 \\ 0 & L_Z - \frac{1}{2} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{2}{3}} Y_{1,0} \\ \sqrt{\frac{1}{3}} Y_{1,+1} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{2}{3}} \left(L_Z + \frac{1}{2}\right) Y_{1,0} \\ \sqrt{\frac{1}{3}} \left(L_Z - \frac{1}{2}\right) Y_{1,+1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \sqrt{\frac{2}{3}} Y_{1,0} \\ \sqrt{\frac{1}{3}} Y_{1,+1} \end{pmatrix}$$

$$J_Z \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix} = \begin{pmatrix} L_Z + \frac{1}{2} & 0 \\ 0 & L_Z - \frac{1}{2} \end{pmatrix} \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{3}} \left(L_Z + \frac{1}{2}\right) Y_{1,-1} \\ \sqrt{\frac{2}{3}} \left(L_Z - \frac{1}{2}\right) Y_{1,0} \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} \sqrt{\frac{1}{3}} Y_{1,-1} \\ \sqrt{\frac{2}{3}} Y_{1,0} \end{pmatrix}$$

$$J_Z \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} = \begin{pmatrix} L_Z + \frac{1}{2} & 0 \\ 0 & L_Z - \frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix} = \begin{pmatrix} 0 \\ \left(L_Z - \frac{1}{2}\right) Y_{1,-1} \end{pmatrix} = -\frac{3}{2} \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix}$$

So, out of the six states we have classified four linear combinations as eigenstates of J^2 with $j = \frac{3}{2}$.

state	j	j_z
$\mathcal{Y}_{\frac{3}{2},+\frac{3}{2}} = \begin{pmatrix} Y_{1,+1} \\ 0 \end{pmatrix}$	$\frac{3}{2}$	$+\frac{3}{2}$
$\mathcal{Y}_{\frac{3}{2},+\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{2}{3}}Y_{1,0} \\ \sqrt{\frac{1}{3}}Y_{1,+1} \end{pmatrix}$	$\frac{3}{2}$	$+\frac{1}{2}$
$\mathcal{Y}_{\frac{3}{2},-\frac{1}{2}} = \begin{pmatrix} \sqrt{\frac{1}{3}}Y_{1,-1} \\ \sqrt{\frac{2}{3}}Y_{1,0} \end{pmatrix}$	$\frac{3}{2}$	$-\frac{1}{2}$
$\mathcal{Y}_{\frac{3}{2},-\frac{3}{2}} = \begin{pmatrix} 0 \\ Y_{1,-1} \end{pmatrix}$	$\frac{3}{2}$	$-\frac{3}{2}$

We determine furthermore

$$J^2 \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix} \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix}$$

$$= \begin{pmatrix} -\sqrt{\frac{1}{3}}\left(\frac{11}{4} + L_z\right)Y_{1,0} + \sqrt{\frac{2}{3}}L_-Y_{1,+1} \\ -\sqrt{\frac{1}{3}}L_+Y_{1,0} + \sqrt{\frac{2}{3}}\left(\frac{11}{4} - L_z\right)Y_{1,+1} \end{pmatrix} = \begin{pmatrix} -\frac{3}{4}\sqrt{\frac{1}{3}}Y_{1,0} \\ \frac{3}{4}\sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix} = \frac{1}{2}\left(\frac{1}{2}+1\right) \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix}$$

$$J^2 \begin{pmatrix} -\sqrt{\frac{2}{3}}Y_{1,-1} \\ \sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix} = \begin{pmatrix} \frac{11}{4} + L_z & L_- \\ L_+ & \frac{11}{4} - L_z \end{pmatrix} \begin{pmatrix} -\sqrt{\frac{2}{3}}Y_{1,-1} \\ \sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix}$$

$$= \begin{pmatrix} -\sqrt{\frac{2}{3}}\left(\frac{11}{4} + L_z\right)Y_{1,-1} + \sqrt{\frac{1}{3}}L_-Y_{1,0} \\ -\sqrt{\frac{2}{3}}L_+Y_{1,-1} + \sqrt{\frac{1}{3}}\left(\frac{11}{4} - L_z\right)Y_{1,0} \end{pmatrix} = \begin{pmatrix} -\frac{3}{4}\sqrt{\frac{2}{3}}Y_{1,-1} \\ \frac{3}{4}\sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix} = \frac{1}{2}\left(\frac{1}{2}+1\right) \begin{pmatrix} -\sqrt{\frac{2}{3}}Y_{1,-1} \\ \sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix}$$

and

$$J_z \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix} = \begin{pmatrix} Lz + \frac{1}{2} & 0 \\ 0 & Lz - \frac{1}{2} \end{pmatrix} \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix}$$

$$= \begin{pmatrix} -\sqrt{\frac{1}{3}}\left(Lz + \frac{1}{2}\right)Y_{1,0} \\ \sqrt{\frac{2}{3}}\left(Lz - \frac{1}{2}\right)Y_{1,+1} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -\sqrt{\frac{1}{3}}Y_{1,0} \\ \sqrt{\frac{2}{3}}Y_{1,+1} \end{pmatrix}$$

$$J_z \begin{pmatrix} -\sqrt{\frac{2}{3}}Y_{1,-1} \\ \sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix} = \begin{pmatrix} Lz + \frac{1}{2} & 0 \\ 0 & Lz - \frac{1}{2} \end{pmatrix} \begin{pmatrix} -\sqrt{\frac{2}{3}}Y_{1,-1} \\ \sqrt{\frac{1}{3}}Y_{1,0} \end{pmatrix}$$

$$= \begin{pmatrix} -\sqrt{\frac{2}{3}}\left(L_Z + \frac{1}{2}\right) Y_{1,-1} \\ \sqrt{\frac{1}{3}}\left(L_Z - \frac{1}{2}\right) Y_{1,0} \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} -\sqrt{\frac{2}{3}} Y_{1,-1} \\ \sqrt{\frac{1}{3}} Y_{1,0} \end{pmatrix}$$

So, we found two linear combinations which are eigenstates of J^2 with $j = \frac{1}{2}$.

normalized state	j	j_z
$\mathcal{Y}_{\frac{1}{2},+\frac{1}{2}} = \begin{pmatrix} -\sqrt{\frac{1}{3}} Y_{1,0} \\ \sqrt{\frac{2}{3}} Y_{1,+1} \end{pmatrix}$	$\frac{1}{2}$	$+\frac{1}{2}$
$\mathcal{Y}_{\frac{1}{2},-\frac{1}{2}} = \begin{pmatrix} -\sqrt{\frac{2}{3}} Y_{1,-1} \\ \sqrt{\frac{1}{3}} Y_{1,0} \end{pmatrix}$	$\frac{1}{2}$	$-\frac{1}{2}$

d.

$$\left|j = \tfrac{3}{2}, j_z = +\tfrac{3}{2}\right\rangle = \left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = +1\rangle$$
$$\left|j = \tfrac{3}{2}, j_z = +\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{2}{3}}\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle + \sqrt{\tfrac{1}{3}}\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = +1\rangle$$
$$\left|j = \tfrac{3}{2}, j_z = -\tfrac{1}{2}\right\rangle = \sqrt{\tfrac{1}{3}}\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = -1\rangle + \sqrt{\tfrac{2}{3}}\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle$$
$$\left|j = \tfrac{3}{2}, j_z = -\tfrac{3}{2}\right\rangle = \left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = -1\rangle$$
$$\left|j = \tfrac{1}{2}, j_z = +\tfrac{1}{2}\right\rangle = -\sqrt{\tfrac{1}{3}}\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle + \sqrt{\tfrac{2}{3}}\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = +1\rangle$$
$$\left|j = \tfrac{1}{2}, j_z = -\tfrac{1}{2}\right\rangle = -\sqrt{\tfrac{2}{3}}\left|s = \tfrac{1}{2}, s_z = +\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = -1\rangle + \sqrt{\tfrac{1}{3}}\left|s = \tfrac{1}{2}, s_z = -\tfrac{1}{2}\right\rangle \otimes |\ell = 1, \ell_z = 0\rangle$$

e. From the solutions of (**d**) we read the Clebsch-Gordan coefficients:

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ +1 & +\frac{1}{2} & +\frac{3}{2} \end{pmatrix} = 1$$

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ 0 & +\frac{1}{2} & +\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{2}{3}} \qquad \begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ +1 & -\frac{1}{2} & +\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{1}{3}}$$

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ -1 & +\frac{1}{2} & -\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{1}{3}} \qquad \begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ 0 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{2}{3}}$$

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{3}{2} \\ -1 & -\frac{1}{2} & -\frac{3}{2} \end{pmatrix} = 1$$

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 0 & +\frac{1}{2} & +\frac{1}{2} \end{pmatrix} = -\sqrt{\tfrac{1}{3}} \qquad \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ +1 & -\frac{1}{2} & +\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{2}{3}}$$

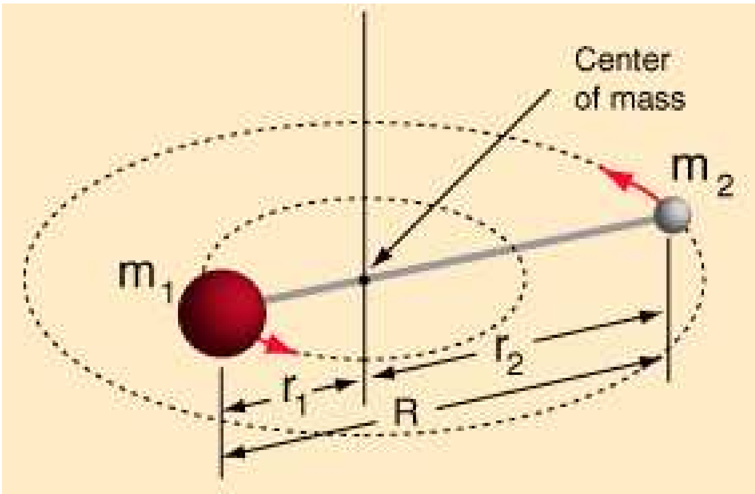
$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ -1 & +\frac{1}{2} & -\frac{1}{2} \end{pmatrix} = -\sqrt{\tfrac{2}{3}} \qquad \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{2} \\ 0 & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix} = \sqrt{\tfrac{1}{3}}$$

See also
http://en.wikipedia.org/wiki/Table_of_Clebsch-Gordan_coefficients#j1.3D2.2C_j2.3D1.2F2

Exercício 33

a. The two nuclei, with masses m_1 and m_2, are supposed to rotate around their common center of mass with a constant angular velocity ω. Let the common center of mass be the center of a coordinate system (x and y) of the plane in which the masses rotate. We indicate the position of mass m_1 by $\vec{r}_1$ and the position of mass m_2 by $\vec{r}_2$. Since, their common center of mass is in the origin of the coordinate system, one has

$$m_2\vec{r}_2 = -m_1\vec{r}_1 \quad \text{hence} \quad |\vec{r}_2| = \frac{m_1}{m_2}|\vec{r}_1| \quad .$$



The total moment of inertia is given by

$$\begin{aligned}
I &= m_1|\vec{r}_1|^2 + m_2|\vec{r}_2|^2 = m_1|\vec{r}_1|^2 + m_2\left\{\frac{m_1}{m_2}|\vec{r}_1|\right\}^2 = \\
&= \left\{m_1 + \frac{m_1^2}{m_2}\right\}|\vec{r}_1|^2 = \frac{m_1m_2}{m_1+m_2}\left(\frac{m_1+m_2}{m_2}\right)^2|\vec{r}_1|^2 \\
&= \frac{m_1m_2}{m_1+m_2}\left(|\vec{r}_1| + \frac{m_1}{m_2}|\vec{r}_1|\right)^2 = \frac{m_1m_2}{m_1+m_2}\left(|\vec{r}_1| + |\vec{r}_2|\right)^2 \\
&= \mu R^2 \quad \text{where} \quad R = |\vec{r}_1| + |\vec{r}_2| \quad .
\end{aligned}$$

Their velocities are given by

$$|\vec{v}_1| = \omega|\vec{r}_1| \quad \text{and} \quad |\vec{v}_2| = \omega|\vec{r}_2| = \omega\frac{m_1}{m_2}|\vec{r}_1| = \frac{m_1}{m_2}|\vec{v}_1| \quad ,$$

and are pointing in opposite directions, hence

$$\vec{v}_2 = -\frac{m_1}{m_2}\vec{v}_1 \quad .$$

Since the motion of each mass is circular, which implies that $\vec{r}$ and $\vec{v}$ are perpendicular, we have for the angular momentum

$$\begin{aligned}
\left|\vec{K}\right| &= \left|m_1\vec{r}_1 \times \vec{v}_1 + m_2\vec{r}_2 \times \vec{v}_2\right| = \\
&= \left|m_1\vec{r}_1 \times \vec{v}_1 + m_2\left\{-\frac{m_1}{m_2}\vec{r}_1\right\} \times \left\{-\frac{m_1}{m_2}\vec{v}_1\right\}\right| \\
&= \left\{m_1 + \frac{m_1^2}{m_2}\right\}\left|\vec{r}_1 \times \vec{v}_1\right| = \left\{m_1 + \frac{m_1^2}{m_2}\right\}\left|\vec{r}_1\right|\left|\vec{v}_1\right| = \left\{m_1 + \frac{m_1^2}{m_2}\right\}\left|\vec{r}_1\right|\omega\left|\vec{r}_1\right| \\
&= \left\{m_1 + \frac{m_1^2}{m_2}\right\}\omega\left|\vec{r}_1\right|^2 = \omega I \quad\Leftrightarrow\quad \omega = \frac{\left|\vec{K}\right|}{I} \quad .
\end{aligned}$$

The total rotational kinetic energy of this system is given by

$$\begin{aligned}
E &= \frac{1}{2}m_1\left|\vec{v}_1\right|^2 + \frac{1}{2}m_2\left|\vec{v}_2\right|^2 = \\
&= \frac{1}{2}m_1\left|\vec{v}_1\right|^2 + \frac{1}{2}m_2\left\{\frac{m_1}{m_2}\left|\vec{v}_1\right|\right\}^2 = \frac{1}{2}\left\{m_1 + \frac{m_1^2}{m_2}\right\}\left|\vec{v}_1\right|^2 \\
&= \frac{1}{2}\left\{m_1 + \frac{m_1^2}{m_2}\right\}\left\{\omega\left|\vec{r}_1\right|\right\}^2 = \frac{1}{2}I\omega^2 = \frac{1}{2}I\left\{\frac{\left|\vec{K}\right|}{I}\right\}^2 = \frac{\left|\vec{K}\right|^2}{2I} = \frac{\left|\vec{K}\right|^2}{2\mu R^2} \quad .
\end{aligned}$$

Hence for a rotational state we have something like

$$H\,\psi_K = \frac{\left|\vec{K}\right|^2}{2\mu R^2}\,\psi_K = \frac{\hbar^2 K(K+1)}{2\mu R^2}\,\psi_K \quad .$$

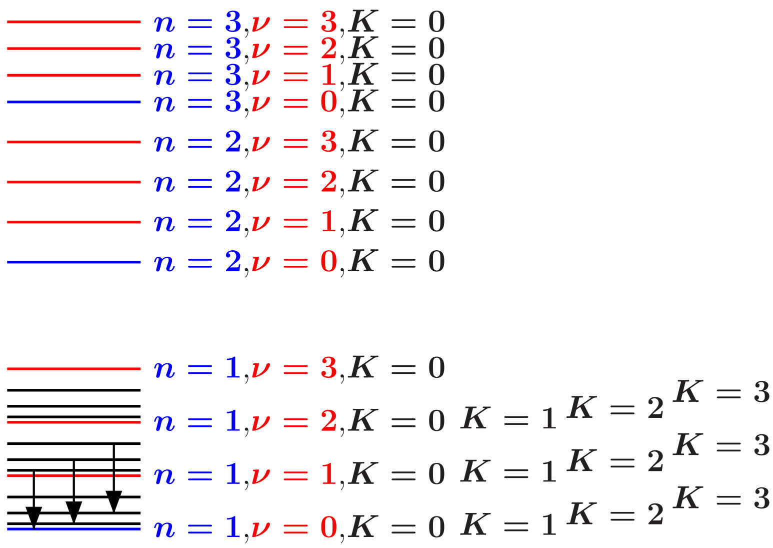
Transition go (to leading order = strong spectral lines) for $\Delta K = \pm 1$. Consequently, the emitted (or absorbed) photons have for $\Delta K = -1$ energy equal to

$$\begin{aligned}
\Delta E(\nu, K \to \nu - 1, K - 1) &= E_\nu + \frac{\hbar^2 K(K+1)}{2\mu R^2} - \left(E_{\nu-1} + \frac{\hbar^2 (K-1)K}{2\mu R^2}\right) = \\
&= \Delta E_{\nu\to\nu-1} + \frac{\hbar^2}{2\mu R^2}\left\{K(K+1) - (K-1)K\right\} = \Delta E_{\nu\to\nu-1} + \frac{\hbar^2 K}{\mu R^2} \quad .
\end{aligned}$$

We have no knowledge on $\Delta E_{\nu\to\nu-1} = E_\nu - E_{\nu-1}$, but we can study subsequent spectral lines. For example,

$$\begin{aligned}
&\Delta E(\nu, K+1 \to \nu - 1, K) - \Delta E(\nu, K \to \nu - 1, K - 1) = \\
&\left(\Delta E_{\nu\to\nu-1} + \frac{\hbar^2 (K+1)}{\mu R^2}\right) - \left(\Delta E_{\nu\to\nu-1} + \frac{\hbar^2 K}{\mu R^2}\right) = \frac{\hbar^2}{\mu R^2} \quad .
\end{aligned}$$

In the lectures it was explained how the levels for polar diatomic molecules are supposed to be ordered.



In the first place one has the electronic levels (n) of the outer electron(s). They have level spacings of the order of eV's. Then come the vibrational levels (ν) with spacings of tenths of eV's and finally the rotational levels (K) with hundredths of eV's.
Schematically this looks like depicted in the above figure, where we also depicted some of the possible transitions for the case $\Delta K = -1$.

From the wave lengths one may determine the energy differences ΔE between the various levels by using

$$\Delta E = hf = \frac{hc}{\lambda} \quad ,$$

where $hc = 1.239842$ eVμm.
We obtain

i	λ (μm)	ΔE (eV)	$\Delta E(i) - \Delta E(i-1)$ (eV)
1	120.3	0.01031	-
2	96.0	0.01292	0.00261
3	80.4	0.01542	0.00251
4	68.9	0.01800	0.00257
5	60.4	0.02053	0.00253

For the average difference $\Delta E(i) - \Delta E(i-1)$ we find 0.00256 eV.
When we assume that the above value corresponds to $\dfrac{\hbar^2}{\mu R^2}$, then we may estimate the distance of the H and the Cℓ nuclei.
We still need to determine μ.
In the tables we find masses 1.007825 and 34.96885 atomic units for H and Cℓ, respectively, and, furthermore, 931.494 MeV/c^2 for 1 atomic unit. Hence

$$\mu c^2 = \frac{1.007825 \times 34.96885}{1.007825 + 34.96885} \times 931.494 \text{ MeV} = 912.485 \text{ MeV} \quad .$$

We obtain then for the distance of the H and the Cℓ nuclei the value

$$R = \sqrt{\frac{\hbar^2 c^2}{\mu c^2 \times 0.00256 \text{ eV}}} \; = \; 1.29 \times 10^{-10} \text{ m} \quad .$$

Exercício 34

a. From exercise (33) we have learned that in the center-of-mass system of a two-body system

$$\vec{p}_2 = m_2 \vec{v}_2 = -m_2 \frac{m_1}{m_2} \vec{v}_1 = -m_1 \vec{v}_1 = -\vec{p}_1 \quad .$$

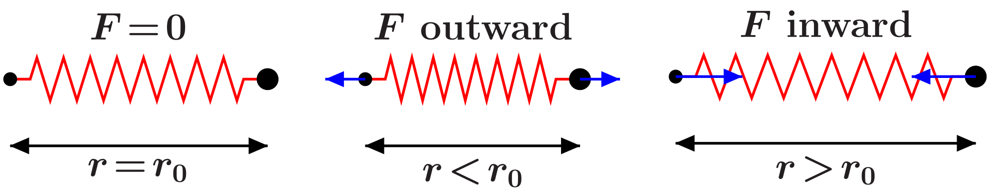
As a consequence, we obtain for the kinetic energy of a two-body system

$$E_{\mathbf{kin}} = \frac{1}{2} m_1 \left|\vec{v}_1\right|^2 + \frac{1}{2} m_2 \left|\vec{v}_2\right|^2 = \frac{\left|\vec{p}_1\right|^2}{2m_1} + \frac{\left|\vec{p}_2\right|^2}{2m_2} = \frac{1}{2} \frac{m_1 + m_2}{m_1 m_2} \left|\vec{p}_1\right|^2 = \frac{\left|\vec{p}_1\right|^2}{2\mu} \quad .$$

When we define $\vec{p} = \vec{p}_1 = -\vec{p}_2$, then we obtain thus

$$E_{\mathbf{kin}} = \frac{\left|\vec{p}\right|^2}{2\mu} = \frac{p^2}{2\mu} \quad .$$

For the potential energy of the spring we have the following results from classical mechanics and Hooke's law.



$$\boldsymbol{E_{\mathrm{pot}} = 0} \qquad \boldsymbol{E_{\mathrm{pot}} = \tfrac{1}{2} C (r_0 - r)^2} \qquad \boldsymbol{E_{\mathrm{pot}} = \tfrac{1}{2} C (r - r_0)^2}$$

With the substitution $x = r - r_0$, also defining $\omega = \sqrt{C/\mu}$ we find for the total energy

$$E_{\mathbf{tot}} = E_{\mathbf{kin}} + E_{\mathbf{pot}} = \frac{p^2}{2\mu} + \frac{1}{2} C x^2 = \frac{1}{2} \left\{ \frac{p^2}{\mu} + \mu \omega^2 x^2 \right\} \quad \longrightarrow \quad H = \frac{1}{2} \left\{ \frac{p^2}{\mu} + \mu \omega^2 x^2 \right\} \quad .$$

---

b. We first define $\mathcal{N}_0 = \left[\frac{\mu\omega}{\pi\hbar}\right]^{1/4}$ and $\alpha = \mu\omega/\hbar$, to obtain for the wave function of equation (10), the expression

$$\psi_0(x) \; = \; \mathcal{N}_0 \, e^{-\frac{1}{2}\alpha x^2} \quad .$$

The second derivative follows readily

$$\frac{\partial^2}{\partial x^2} \, \psi_0(x) = \frac{\partial^2}{\partial x^2} \, \mathcal{N}_0 \, e^{-\frac{1}{2}\alpha x^2} =$$

$$= \mathcal{N}_0 \frac{\partial}{\partial x} \left\{ -\alpha x \, e^{-\frac{1}{2}\alpha x^2} \right\} = \mathcal{N}_0 \left\{ \left(\frac{\partial}{\partial x} (-\alpha x) \right) \, e^{-\frac{1}{2}\alpha x^2} - \alpha x \left(\frac{\partial}{\partial x} e^{-\frac{1}{2}\alpha x^2} \right) \right\}$$

$$= \mathcal{N}_0 \left\{ (-\alpha) \, e^{-\frac{1}{2}\alpha x^2} - \alpha x \left(-\alpha x \, e^{-\frac{1}{2}\alpha x^2} \right) \right\} = \mathcal{N}_0 \left\{ -\alpha + \alpha^2 x^2 \right\} \, e^{-\frac{1}{2}\alpha x^2}$$

$$\left\{ -\alpha + \alpha^2 x^2 \right\} \, \psi_0(x) \quad .$$

Consequently

$$\hbar^2 \frac{\partial^2}{\partial x^2}\, \psi_0(x) = \left\{ -\hbar\mu\omega + \mu^2\omega^2 x^2 \right\}\, \psi_0(x) \quad .$$

Or, also

$$\frac{1}{2\mu}\left(-\hbar^2 \frac{\partial^2}{\partial x^2} + (\mu\omega x)^2 \right)\, \psi_0(x) = \frac{1}{2\mu}\left\{ \hbar\mu\omega - \mu^2\omega^2 x^2 + (\mu\omega x)^2 \right\}\, \psi_0(x) = \frac{1}{2}\hbar\omega\, \psi_0(x) \quad .$$

---

c.
(i)

$$a\psi_0 = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right) \mathcal{N}_0\, e^{-\frac{1}{2}\alpha x^2} = \mathcal{N}_0 \sqrt{\frac{\mu\omega}{2\hbar}}\left(x e^{-\frac{1}{2}\alpha x^2} + \frac{1}{\alpha}\frac{\partial}{\partial x} e^{-\frac{1}{2}\alpha x^2} \right) =$$

$$= \mathcal{N}_0 \sqrt{\frac{\mu\omega}{2\hbar}}\left(x e^{-\frac{1}{2}\alpha x^2} + \frac{1}{\alpha}\left\{ -\alpha x e^{-\frac{1}{2}\alpha x^2} \right\} \right) = \mathcal{N}_0 \sqrt{\frac{\mu\omega}{2\hbar}}\left(x e^{-\frac{1}{2}\alpha x^2} - x e^{-\frac{1}{2}\alpha x^2} \right) = 0$$

(ii)

$$\hbar\omega\left(a^\dagger a + \frac{1}{2} \right) = \hbar\omega \sqrt{\frac{\mu\omega}{2\hbar}}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right) \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right) + \frac{1}{2}\hbar\omega =$$

$$= \hbar\omega \frac{\mu\omega}{2\hbar}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right)\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right) + \frac{1}{2}\hbar\omega$$

$$= \hbar\omega \frac{\mu\omega}{2\hbar}\left\{ x^2 + \frac{\hbar x}{\mu\omega}\frac{\partial}{\partial x} - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\, x - \left(\frac{\hbar}{\mu\omega} \right)^2 \frac{\partial^2}{\partial x^2} \right\} + \frac{1}{2}\hbar\omega$$

$$= \hbar\omega \frac{\mu\omega}{2\hbar}\left\{ x^2 + \frac{\hbar}{\mu\omega}\left[x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}\, x \right] - \left(\frac{\hbar}{\mu\omega} \right)^2 \frac{\partial^2}{\partial x^2} \right\} + \frac{1}{2}\hbar\omega$$

$$= \frac{\hbar\omega}{2}\left\{ \frac{\mu\omega}{\hbar}x^2 + \left[x\frac{\partial}{\partial x} - \left(\frac{\partial x}{\partial x} + x\frac{\partial}{\partial x} \right) \right] - \frac{\hbar}{\mu\omega}\frac{\partial^2}{\partial x^2} \right\} + \frac{1}{2}\hbar\omega$$

$$= \frac{\hbar\omega}{2}\left\{ \frac{\mu\omega}{\hbar}x^2 + \left[x\frac{\partial}{\partial x} - \left(1 + x\frac{\partial}{\partial x} \right) \right] - \frac{\hbar}{\mu\omega}\frac{\partial^2}{\partial x^2} \right\} + \frac{1}{2}\hbar\omega$$

$$= \frac{\hbar\omega}{2}\left\{ \frac{\mu\omega}{\hbar}x^2 - 1 - \frac{\hbar}{\mu\omega}\frac{\partial^2}{\partial x^2} \right\} + \frac{1}{2}\hbar\omega = \frac{1}{2}\mu\omega^2 x^2 - \frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2} = H$$

(iii)

$$\left[a\,,\; a^\dagger \right] = \left[\sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right)\;,\; \sqrt{\frac{\mu\omega}{2\hbar}}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x} \right) \right] =$$

$$= \frac{\mu\omega}{2\hbar}\left\{\left(x+\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right)\left(x-\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right)-\left(x-\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right)\left(x+\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right)\right\}$$

$$= \frac{\mu\omega}{2\hbar}\left\{\left(x^2-\frac{\hbar x}{\mu\omega}\frac{\partial}{\partial x}+\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}x-\left(\frac{\hbar}{\mu\omega}\right)^2\frac{\partial^2}{\partial x^2}\right)-\left(x^2+\frac{\hbar x}{\mu\omega}\frac{\partial}{\partial x}-\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}x-\left(\frac{\hbar}{\mu\omega}\right)^2\frac{\partial^2}{\partial x^2}\right)\right\}$$

$$= \frac{\mu\omega}{2\hbar}\left\{-2\frac{\hbar x}{\mu\omega}\frac{\partial}{\partial x}+2\frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}x\right\} = -x\frac{\partial}{\partial x}+\frac{\partial}{\partial x}x = -x\frac{\partial}{\partial x}+\left(\frac{\partial x}{\partial x}+x\frac{\partial}{\partial x}\right) = 1$$

(iv)

$$\left[H\ ,\ a^\dagger\right] = \left[\hbar\omega\left(a^\dagger a+\tfrac{1}{2}\right)\ ,\ a^\dagger\right] = \hbar\omega\left\{\left[a^\dagger a\ ,\ a^\dagger\right]+\left[\tfrac{1}{2}\ ,\ a^\dagger\right]\right\} =$$

$$= \hbar\omega\left[a^\dagger a\ ,\ a^\dagger\right] = \hbar\omega\left\{a^\dagger\left[a\ ,\ a^\dagger\right]+\left[a^\dagger\ ,\ a^\dagger\right]a\right\} = \hbar\omega a^\dagger\left[a\ ,\ a^\dagger\right] = \hbar\omega a^\dagger$$

(v)

$$[H\ ,\ a] = \left[\hbar\omega\left(a^\dagger a+\tfrac{1}{2}\right)\ ,\ a\right] = \hbar\omega\left\{\left[a^\dagger a\ ,\ a\right]+\left[\tfrac{1}{2}\ ,\ a\right]\right\} = \hbar\omega\left[a^\dagger a\ ,\ a\right] =$$

$$= \hbar\omega\left\{a^\dagger[a\ ,\ a]+\left[a^\dagger\ ,\ a\right]a\right\} = \hbar\omega\left[a^\dagger\ ,\ a\right]a = -\hbar\omega\left[a\ ,\ a^\dagger\right]a = -\hbar\omega a$$

---

d.

$$H\left(a^\dagger\psi\right) = \left\{Ha^\dagger\right\}\psi = \left\{Ha^\dagger-a^\dagger H+a^\dagger H\right\}\psi =$$

$$= \left\{\left[H\ ,\ a^\dagger\right]+a^\dagger H\right\}\psi = \left\{\hbar\omega a^\dagger+a^\dagger H\right\}\psi = \hbar\omega a^\dagger\psi+a^\dagger H\psi$$

$$= \hbar\omega a^\dagger\psi+a^\dagger E\psi = (E+\hbar\omega)\left(a^\dagger\psi\right)$$

Note that similarly

$$H(a\psi) = \{Ha\}\psi = \{[H\ ,\ a]+aH\}\psi =$$

$$= \{-\hbar\omega a+aE\}\psi = -\hbar\omega a\psi+aE\psi = (E-\hbar\omega)(a\psi)$$

Furthermore, since $a\psi_0 = 0$, it can be shown that ψ_0 is the ground state of the quantum harmonic oscillator. All other states can be created with $a^\dagger$. For example, we obtain all eigenstates of $H\psi_\nu = E_\nu\psi_\nu$, with $E_\nu = \left(\frac{1}{2}+\nu\right)\hbar\omega$, for $\nu = 0, 1, 2, ...$, by choosing $\psi_\nu \propto \left(a^\dagger\right)^\nu\psi_0$ (proportionality constants: X_1, X_2, X_3, ...).

eigenstate of H	eigenenergy
ψ_0	$\frac{1}{2}\hbar\omega$ (**b**)
$a^\dagger\psi_0 = X_1\psi_1$	$\frac{3}{2}\hbar\omega$ (**d**)
$\left(a^\dagger\right)^2\psi_0 = X_1 a^\dagger\psi_1 = X_1X_2\psi_2$	$\frac{5}{2}\hbar\omega$ (**d**)
$\vdots$	$\vdots$
$\left(a^\dagger\right)^\nu\psi_0 = X_1X_2\dots X_\nu\psi_\nu$	$\left(\frac{1}{2}+\nu\right)\hbar\omega$ (**d**)

Exercício 35

a. From the discussion regarding the solution of exercise (34d), we concluded that the eigenspectrum of H is given by $\frac{1}{2}\hbar\omega$, $\frac{3}{2}\hbar\omega$, $\frac{5}{2}\hbar\omega$, ..., whereas the respective eigenstates are given by $|0\rangle$, $|1\rangle$, $|2\rangle$, ... In a more compact notation

$$H|\nu\rangle = E_\nu|\nu\rangle \quad \text{with} \quad E_\nu = \left(\tfrac{1}{2}+\nu\right)\hbar\omega \quad ,$$

b.

$$\langle H\rangle \;=\; \langle\nu\,|H|\,\nu\rangle \;=\; \int_{-\infty}^{+\infty} dx\,\psi_\nu^*(x)\,H\,\psi_\nu(x) =$$

$$\int_{-\infty}^{+\infty} dx\,\psi_\nu^*(x)\,E_\nu\,\psi_\nu(x) = E_\nu\int_{-\infty}^{+\infty} dx\,\psi_\nu^*(x)\,\psi_\nu(x) = E_\nu\int_{-\infty}^{+\infty} dx\;|\psi_\nu(x)|^2 = E_\nu\,1 = E_\nu \quad .$$

Hence, in the case that the system is in the eigenstate $|\nu\rangle$, E_ν is the value we expect to find when the total energy of the system, given by $\langle H\rangle$, is measured.

---

c. Using the result of exercise (34d), we obtain

$$Ha^\dagger|\nu\rangle = \{E_\nu+\hbar\omega\}\,a^\dagger|\nu\rangle = \left\{\left(\tfrac{1}{2}+\nu\right)\hbar\omega+\hbar\omega\right\}a^\dagger|\nu\rangle = \left\{\tfrac{1}{2}+(\nu+1)\right\}\hbar\omega a^\dagger|\nu\rangle = E_{\nu+1}a^\dagger|\nu\rangle \quad ,$$

whereas, for $|\nu+1\rangle$ we also have $H|\nu+1\rangle = E_{\nu+1}|\nu+1\rangle$.
Now, since H has only one eigenstate for $E_{\nu+1}$, we must conclude that $a^\dagger|\nu\rangle$ and $|\nu+1\rangle$ are proportional.

The proportionality constant, say $X_{\nu+1}$, can be found by determining

$$\int_{-\infty}^{+\infty} dx\,\left\{a^\dagger\psi_\nu(x)\right\}^*\,a^\dagger\psi_\nu(x) = \int_{-\infty}^{+\infty} dx\,\left\{X_{\nu+1}\psi_{\nu+1}(x)\right\}^*\,X_{\nu+1}\psi_{\nu+1}(x) =$$

$$= X_{\nu+1}^*X_{\nu+1}\int_{-\infty}^{+\infty} dx\,\psi_{\nu+1}^*(x)\,\psi_{\nu+1}(x) = |X_{\nu+1}|^2\int_{-\infty}^{+\infty} dx\;|\psi_{\nu+1}(x)|^2 = |X_{\nu+1}|^2 \quad .$$

So, we determine X_1.
We start with ($\alpha = \mu\omega/\hbar$)

$$a^\dagger\psi_0 = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right)\mathcal{N}_0\, e^{-\frac{1}{2}\alpha x^2} =$$

$$= \mathcal{N}_0\sqrt{\frac{\mu\omega}{2\hbar}}\left(xe^{-\frac{1}{2}\alpha x^2} - \frac{1}{\alpha}\frac{\partial}{\partial x}e^{-\frac{1}{2}\alpha x^2}\right) = \mathcal{N}_0\sqrt{\frac{\mu\omega}{2\hbar}}\left(xe^{-\frac{1}{2}\alpha x^2} - \frac{1}{\alpha}\left\{-\alpha xe^{-\frac{1}{2}\alpha x^2}\right\}\right)$$

$$= \mathcal{N}_0\sqrt{\frac{\mu\omega}{2\hbar}}\left(xe^{-\frac{1}{2}\alpha x^2} + xe^{-\frac{1}{2}\alpha x^2}\right) = 2\mathcal{N}_0\sqrt{\frac{\mu\omega}{2\hbar}}xe^{-\frac{1}{2}\alpha x^2}$$

So, we must then determine

$$|X_1|^2 = \int_{-\infty}^{+\infty} dx\, \left\{a^\dagger\psi_0(x)\right\}^*\, a^\dagger\psi_0(x) = 2\,|\mathcal{N}_0|^2\,\frac{\mu\omega}{\hbar}\,\int_{-\infty}^{+\infty} dx\, x^2 e^{-\alpha x^2}$$

This integral may be looked up in the tables (Integral number 10 of the tables of integrals at http:-//www.sosmath.com/tables/integral/integ37/integ37.html maybe useful, note $\Gamma(n+1) = n\Gamma(n)$ en $\Gamma(1/2) = \sqrt{\pi}$.) We obtain then

$$|X_1|^2 = 2\left[\frac{\mu\omega}{\pi\hbar}\right]^{1/2}\frac{\mu\omega}{\hbar}\,\frac{\frac{1}{2}\sqrt{\pi}}{(\mu\omega/\hbar)^{3/2}} = 1 = 0+1 \quad .$$

This way, one can continue, for X_2 we must determine $a^\dagger\psi_1$ and its integral, etcetera. However, there exists a faster method.
First, we can make use of the general property

$$\int_{-\infty}^{+\infty} dx\, \left\{A^\dagger\phi_1(x)\right\}^*\, \phi_2(x) = \int_{-\infty}^{+\infty} dx\, \phi_1^*(x)\, A\, \phi_2(x) \quad .$$

Then, we may substitute

$$aa^\dagger = aa^\dagger - a^\dagger a + a^\dagger a = \left[a\ ,\ a^\dagger\right] + a^\dagger a = 1 + \left(\frac{H}{\hbar\omega} - \tfrac{1}{2}\right) = \frac{H}{\hbar\omega} + \tfrac{1}{2} \quad ,$$

whereas, moreover

$$\left(\frac{H}{\hbar\omega} + \tfrac{1}{2}\right)\,\psi_\nu = \left(\frac{E_\nu}{\hbar\omega} + \tfrac{1}{2}\right)\,\psi_\nu = \left(\frac{\left(\frac{1}{2}+\nu\right)\hbar\omega}{\hbar\omega} + \tfrac{1}{2}\right)\,\psi_\nu = (\nu+1)\,\psi_\nu \quad .$$

This way, we obtain

$$\int_{-\infty}^{+\infty} dx\, \left\{a^\dagger\psi_\nu(x)\right\}^*\, a^\dagger\psi_\nu(x) = \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, aa^\dagger\psi_\nu(x) = \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\,(\nu+1)\psi_\nu(x) = (\nu+1).$$

Which gives $|X_{\nu+1}|^2 = \nu + 1$.

---

d.

$$a + a^\dagger = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) + \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) = \sqrt{\frac{2\mu\omega}{\hbar}}\, x \quad .$$

Hence,

$$\langle \nu\, |x|\, \nu + m\rangle = \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x) \sqrt{\frac{\hbar}{2\mu\omega}}\left(a + a^\dagger\right) \psi_{\nu+m}(x) =$$

$$= \sqrt{\frac{\hbar}{2\mu\omega}}\left\{\int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, a\, \psi_{\nu+m}(x) + \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, a^\dagger\, \psi_{\nu+m}(x)\right\}$$

$$= \sqrt{\frac{\hbar}{2\mu\omega}}\left\{\int_{-\infty}^{+\infty} dx\, \left\{a^\dagger\, \psi_\nu(x)\right\}^*\, \psi_{\nu+m}(x) + \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, a^\dagger\, \psi_{\nu+m}(x)\right\}$$

$$= \sqrt{\frac{\hbar}{2\mu\omega}}\left\{\int_{-\infty}^{+\infty} dx\, \left\{X_{\nu+1}\, \psi_{\nu+1}(x)\right\}^*\, \psi_{\nu+m}(x) + \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, X_{\nu+m+1}\, \psi_{\nu+m+1}(x)\right\}$$

$$= \sqrt{\frac{\hbar}{2\mu\omega}}\left\{X_{\nu+1}^* \int_{-\infty}^{+\infty} dx\, \psi_{\nu+1}^*(x)\, \psi_{\nu+m}(x) + X_{\nu+m+1} \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, \psi_{\nu+m+1}(x)\right\}$$

$$= \sqrt{\frac{\hbar}{2\mu\omega}}\left\{X_{\nu+1}^*\, \delta_{\nu+1,\nu+m} + X_{\nu+m+1}\, \delta_{\nu,\nu+m+1}\right\} \quad .$$

The last step follows from the orthogonality relation of the normalized eigenfunctions of H, which reads

$$\int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, \psi_\mu(x) = \delta_{\nu,\mu} = \begin{cases} 1 & \text{for} \quad \nu = m \\ 0 & \text{for} \quad \nu \neq m \end{cases}$$

Now, $\delta_{\nu+1,\nu+m}$ is only non-zero for $\nu + 1 = \nu + m$ and in that case equal to 1, whereas $\delta_{\nu,\nu+m+1}$ is only non-zero for $\nu = \nu + m + 1$. In the former case $m = 1$, in the latter case $m = -1$. Electromagnetic transitions of vibrational molecular states are related to the x operator. Hence, transitions are favoured when $\Delta\nu = \pm 1$.

Exercício 36

a. In problem (35a) we have found for the Hamiltonian of such system

$$H = \frac{1}{2}\left\{\frac{p^2}{\mu} + \mu\omega^2 x^2\right\}$$

Furthermore, with the definitions of the annihilation and creation operators, respectively given by (see also equation 11)

$$a = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x + \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) \quad \text{and} \quad a^\dagger = \sqrt{\frac{\mu\omega}{2\hbar}}\left(x - \frac{\hbar}{\mu\omega}\frac{\partial}{\partial x}\right) \quad ,$$

we obtained

$$H = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right)$$

and, moreover

$$\left[H\ ,\ a^\dagger\right] = \hbar\omega\, a^\dagger \qquad \text{and} \qquad [H\ ,\ a] = -\hbar\omega\, a \quad ,$$

whereas, for the solutions of the Hamiltonian H, we found a ground state given by

$$\psi_0(x) \;=\; \left[\frac{\mu\omega}{\pi\hbar}\right]^{1/4} e^{-\frac{1}{2}\mu\omega x^2/\hbar} \quad ,$$

which solves the equation $H\psi_0 = \frac{1}{2}\hbar\omega\psi_0$, and, furthermore, radial excitations given by

$$\psi_\nu(x) \;=\; \left(a^\dagger\right)^\nu \psi_0(x) \quad \text{for} \quad \nu = 1, 2, 3, \dots \quad ,$$

which, using the identity

$$Ha^\dagger\psi \;=\; \left(1 + a^\dagger H\right)\psi$$

solve the equation $H\psi_\nu = \left(\nu + \frac{1}{2}\right)\hbar\omega\psi_\nu$.
So, we obtained for the eigenvalue spectrum of H the result

$$E_v \;=\; \hbar\omega\left(v + \tfrac{1}{2}\right) \quad , \qquad v = 0,\ 1,\ 2,\ 3,\ \dots \quad .$$

b. In exercise (35d) we found, by using the relation

$$a + a^\dagger \;=\; = \sqrt{\frac{2\mu\omega}{\hbar}}\, x \quad ,$$

the following result

$$\int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x)\, x\, \left(a + a^\dagger\right)\, \psi_{\nu+m}(x) =$$

$$= \int_{-\infty}^{+\infty} dx\, \psi_\nu^*(x) \sqrt{\frac{\hbar}{2\mu\omega}}\, \left(a + a^\dagger\right)\, \psi_{\nu+m}(x) = \sqrt{\frac{\hbar}{2\mu\omega}}\, \left\{X_{\nu+1}^*\, \delta_{\nu+1,\nu+m} + X_{\nu+m+1}\, \delta_{\nu,\nu+m+1}\right\} \quad ,$$

where the X_ν coefficients are determined in exercise (35c).
From the above result we may conclude that transitions occur for $\Delta\nu = \pm 1$ for a perfect harmonic oscillator.

c. In some branches of physics one uses the spectroscopic wavenumber $\tilde{\nu}$ to indicate the frequency of radiation. Its relation to energy is given by $E = hc\tilde{\nu}$. Hence, the unit cm^{-1} corresponds to an energy of

$$\begin{aligned} E \;&=\; hc\tilde{\nu} = \left(4.1356675 \times 10^{15}\ \text{eVs}\right)\left(2.99792458 \times 10^{10}\ \text{cm/s}\right)\left(1\ \text{cm}^{-1}\right) \\ &=\; 1.2398 \times 10^4\ \text{eV} \end{aligned}$$

We start by assuming that the very intense line in the vibration spectrum of HCl, with wave number $2886\ \text{cm}^{-1}$, stems form the transition from the first radial excitation, with $\nu = 1$, to the ground state, with $\nu = 0$. Hence

$$E_{\nu=1} - E_{\nu=0} \;=\; 2886\ \text{cm}^{-1}$$

For the other transitions we assume

$$E_{\nu=2} - E_{\nu=0} = 5668 \text{ cm}^{-1} \quad \text{and} \quad E_{\nu=3} - E_{\nu=0} = 8347 \text{ cm}^{-1}$$

From the formula, one has for the energy levels

$$E_\nu = \hbar\omega \left\{ \left(v + \tfrac{1}{2} \right) - a_1 \left(v + \tfrac{1}{2} \right)^2 \right\}$$

So, we find

$$\begin{aligned}
E_{\nu=0} &= \hbar\omega \left(\tfrac{1}{2} - a_1 \tfrac{1}{4} \right) \\
E_{\nu=1} &= \hbar\omega \left(\tfrac{3}{2} - a_1 \tfrac{9}{4} \right) \\
E_{\nu=2} &= \hbar\omega \left(\tfrac{5}{2} - a_1 \tfrac{25}{4} \right) \\
E_{\nu=3} &= \hbar\omega \left(\tfrac{7}{2} - a_1 \tfrac{49}{4} \right)
\end{aligned}$$

and

$$\begin{aligned}
E_{\nu=1} - E_{\nu=0} &= \hbar\omega\,(1 - 2a_1) \\
E_{\nu=2} - E_{\nu=0} &= \hbar\omega\,(2 - 6a_1) \\
E_{\nu=3} - E_{\nu=0} &= \hbar\omega\,(3 - 12a_1)
\end{aligned}$$

Let us start by eliminating a_1:

$$\begin{aligned}
3\,(E_{\nu=1} - E_{\nu=0}) - (E_{\nu=2} - E_{\nu=0}) &= \hbar\omega \\
2\,(E_{\nu=1} - E_{\nu=0}) - \tfrac{1}{3}\,(E_{\nu=3} - E_{\nu=0}) &= \hbar\omega
\end{aligned}$$

We determine

$$\begin{aligned}
3\,(E_{\nu=1} - E_{\nu=0}) - (E_{\nu=2} - E_{\nu=0}) &= 2990 \text{ cm}^{-1} \\
2\,(E_{\nu=1} - E_{\nu=0}) - \tfrac{1}{3}\,(E_{\nu=3} - E_{\nu=0}) &= 2990 \text{ cm}^{-1}
\end{aligned}$$

So, this appears to be consistent.
Now, we determine a_1:

$$\begin{aligned}
a_1 &= \tfrac{1}{2} \left\{ 1 - \frac{1}{\hbar\omega}\,(E_{\nu=1} - E_{\nu=0}) \right\} = 0.017391 \\
a_1 &= \tfrac{1}{6} \left\{ 2 - \frac{1}{\hbar\omega}\,(E_{\nu=2} - E_{\nu=0}) \right\} = 0.017391 \\
a_1 &= \tfrac{1}{12} \left\{ 3 - \frac{1}{\hbar\omega}\,(E_{\nu=3} - E_{\nu=0}) \right\} = 0.017363
\end{aligned}$$

which is also sufficiently consistent.
Consequently, we found

$$\hbar\omega = 2990 \text{ cm}^{-1} = 0.371 \text{ eV} \quad \text{and} \quad a_1 = 0.0174$$

In the literature we find for the vibration energy $\hbar\omega \approx 3000\ \mathrm{cm}^{-1}$
(see e.g. http://www.chem.ufl.edu/~itl/4411L_f00/hcl/hcl_il.html)

Exercício 37

Using the equation

$$\begin{pmatrix} h_c & \lambda V(r) \\ \lambda V(r) & h_s \end{pmatrix} \begin{pmatrix} u_c \\ u_s \end{pmatrix} = E \begin{pmatrix} u_c \\ u_s \end{pmatrix} ,$$

we arrive at a set of two differential equations

$$\left\{ \begin{array}{rcl} h_c u_c + \lambda V(r) u_s & = & E u_c \\ \lambda V(r) u_c + h_s u_s & = & E u_s \end{array} \right. .$$

The first boundary conditions can be found by integrating the differential equations in a small domain, $(a-\epsilon, a+\epsilon)$, around the delta-shell position at $r=a$ and letting $\epsilon \downarrow 0$. One finds

$$\lim_{\epsilon\downarrow 0} \int_{a-\epsilon}^{a+\epsilon} dr\, \frac{d^2u(r)}{dr^2} = \lim_{\epsilon\downarrow 0} \left[\frac{du(r)}{dr} \right]_{a-\epsilon}^{a+\epsilon} = \lim_{\epsilon\downarrow 0} \left(\left.\frac{du(r)}{dr}\right|_{a+\epsilon} - \left.\frac{du(r)}{dr}\right|_{a-\epsilon} \right) = \left.\frac{du}{dr}\right|_{r\downarrow a} - \left.\frac{du}{dr}\right|_{r\uparrow a}$$

$$\lim_{\epsilon\downarrow 0} \int_{a-\epsilon}^{a+\epsilon} dr\, \lambda\delta(r-a)u(r) = \lim_{\epsilon\downarrow 0} \lambda u(r=a) = \lambda u(r=a)$$

$$\lim_{\epsilon\downarrow 0} \int_{a-\epsilon}^{a+\epsilon} dr\ (E - M_1 - M2)\, u(r) = \int_{a}^{a} dr\ (E - M_1 - M2)\, u(r) = 0$$

Putting things together, we find the boundary condition

$$\left\{ \begin{array}{rcl} \frac{1}{2\mu_c}\left(- \left.\frac{d\, u_c(r)}{dr}\right|_{r\downarrow a} + \left.\frac{d\, u_c(r)}{dr}\right|_{r\uparrow a} \right) + \frac{\lambda}{2\mu_c a} u_s(a) & = & 0 \\ \frac{\lambda}{2\mu_c a} u_c(a) + \frac{1}{2\mu_s}\left(- \left.\frac{d\, u_s(r)}{dr}\right|_{r\downarrow a} + \left.\frac{d\, u_s(r)}{dr}\right|_{r\uparrow a} \right) & = & 0 \end{array} \right. .$$

The second boundary condition stems from the condition that the probability should be continuous.

Exercício 44

From the relation between the transition amplitude and the retarded wave functions we deduce for a local potential given by

$$\left\langle \vec{r} \left| V \right| \vec{r}\,' \right\rangle = V\left(\vec{r}\,'\right)\, \delta^{(3)}\left(\vec{r} - \vec{r}\,'\right)$$

the following

$$f\left(\vec{k}, \hat{r}\right) = -\sqrt{2\pi}\,\mu \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} V\left(\vec{r}\,'\right) \psi^{(+)}\left(\vec{k}, \vec{r}\,'\right)$$

$$
\begin{aligned}
&= -\sqrt{2\pi}\,\mu \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} \int d^3r''\, V\left(\vec{r}\,''\right)\, \delta^{(3)}\left(\vec{r}\,' - \vec{r}\,''\right)\, \psi^{(+)}\left(\vec{k},\vec{r}\,''\right) \\
&= -\sqrt{2\pi}\,\mu \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} \int d^3r''\, \left\langle \vec{r}\,' \left| V \right| \vec{r}\,'' \right\rangle \left\langle \vec{r}\,'' \middle| \psi^{(+)}\left(\vec{k}\right) \right\rangle \\
&= -\sqrt{2\pi}\,\mu \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} \left\langle \vec{r}\,' \left| V \right| \psi^{(+)}\left(\vec{k}\right) \right\rangle \quad .
\end{aligned}
$$

Next, we proceed by

$$
\begin{aligned}
f\left(\vec{k},\hat{r}\right) &= -\sqrt{2\pi}\,\mu \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} \int d^3k' \left\langle \vec{r}\,' \middle| \vec{k}\,' \right\rangle \left\langle \vec{k}\,' \left| V \right| \psi^{(+)}\left(\vec{k}\right) \right\rangle \\
&= -\sqrt{2\pi}\,\mu \int d^3k' \left\{ \int d^3r'\, e^{-ik\hat{r}\cdot\vec{r}\,'} \frac{e^{i\vec{k}\,'\cdot\vec{r}\,'}}{(2\pi)^{3/2}} \right\} \left\langle \vec{k}\,' \left| V \right| \psi^{(+)}\left(\vec{k}\right) \right\rangle \\
&= -\frac{\mu}{2\pi} \int d^3k' \left\{ \int d^3r'\, e^{i\left(\vec{k}\,' - k\hat{r}\right)\cdot\vec{r}\,'} \right\} \left\langle \vec{k}\,' \left| T\left(k^2 + i\epsilon\right) \right| \vec{k} \right\rangle \quad ,
\end{aligned}
$$

where the limit $\epsilon \downarrow 0$ is understood.
The integration in configuration space can, by the use of formula (19.68) of *Quantum Mechanics*, Eugen Merzbacher, 2nd edition (Wiley, NewYork), be handled as follows

$$
\begin{aligned}
\int d^3r'\, e^{i\left(\vec{k}\,' - k\hat{r}\right)\cdot\vec{r}\,'} &= (2\pi)^3\, \delta^{(3)}\left(\vec{k}\,' - k\hat{r}\right) \\
&= 2\pi^2 \sum_{\ell'=0}^{\infty} (2\ell'+1)\, P_{\ell'}\left(\hat{r}\cdot\hat{k}\,'\right) \frac{\delta(k-k')}{k^2} \quad .
\end{aligned}
$$

So, after calculating the matrix elements of the T-operator, one still has to perform integrations. Now, let us assume that the matrix elements of T have the following genuine form in the case of spherical symmetry

$$
\left\langle \vec{k} \left| T\left(k^2 + i\epsilon\right) \right| \vec{k}\,' \right\rangle = \sum_{\ell=0}^{\infty} (2\ell+1)\, P_\ell\left(\hat{k}\cdot\hat{k}\,'\right)\, T_\ell(k,k') \quad .
$$

By combining the above results, we obtain

$$
\begin{aligned}
f\left(\vec{k},\hat{r}\right) &= \\
&= -\pi\mu \sum_{\ell,\ell'=0}^{\infty} (2\ell+1)\,(2\ell'+1) \int d^3k'\, P_\ell\left(\hat{k}\cdot\hat{k}\,'\right)\, T_\ell(k,k')\, P_{\ell'}\left(\hat{r}\cdot\hat{k}\,'\right) \frac{\delta(k-k')}{k^2} \quad .
\end{aligned}
$$

Next, let us concentrate on the integration over the angles in k'-space, *i.e.*

$$
\int d\Omega_{k'}\, P_\ell\left(\hat{k}\cdot\hat{k}\,'\right)\, P_{\ell'}\left(\hat{r}\cdot\hat{k}\,'\right) \quad .
$$

Here, we may select the z-axis of the $\vec{k}\,'$-system in the direction of $\vec{k}$. But, that does not help much for the second term in the integrand. However, by the use of the addition theorem (see e.g.

formula 9.79 of *Quantum Mechanics*, Eugen Merzbacher, 2nd edition (Wiley, NewYork)) we find

$$\begin{aligned}
&\int d\Omega_{k'}\; P_\ell\left(\hat{k}\cdot\hat{k}'\right)\; P_{\ell'}\left(\hat{r}\cdot\hat{k}'\right) \; = \\
&= \int d\Omega_{k'}\; P_\ell\left(\hat{k}\cdot\hat{k}'\right)\; \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}\left(\hat{k}\cdot\hat{r}\right)\; Y_{\ell'_z}^{(\ell')}\left(\hat{k}\cdot\hat{k}'\right) \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}\left(\hat{k}\cdot\hat{r}\right) \int d\Omega_{k'}\; P_\ell\left(\Omega_{k'}\right)\; Y_{\ell'_z}^{(\ell')}\left(\Omega_{k'}\right) \quad .
\end{aligned}$$

Then, we substitute for $P_\ell\left(\Omega_{k'}\right)$ in the above expression formulas (9.78) and (9.65a) of *Quantum Mechanics*, Eugen Merzbacher, 2nd edition (Wiley, NewYork), to find

$$\begin{aligned}
&\int d\Omega_{k'}\; P_\ell\left(\hat{k}\cdot\hat{k}'\right)\; P_{\ell'}\left(\hat{r}\cdot\hat{k}'\right) \; = \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}\left(\hat{k}\cdot\hat{r}\right) \int d\Omega_{k'} \sqrt{\frac{4\pi}{2\ell+1}}\; Y_0^{(\ell)*}\left(\Omega_{k'}\right)\; Y_{\ell'_z}^{(\ell')}\left(\Omega_{k'}\right) \quad ,
\end{aligned}$$

which, after applying the orthogonality of spherical harmonics (see e.g. *Quantum Mechanics*, Eugen Merzbacher, 2nd edition (Wiley, NewYork) formula 9.69), leads to

$$\begin{aligned}
&\int d\Omega_{k'}\; P_\ell\left(\hat{k}\cdot\hat{k}'\right)\; P_{\ell'}\left(\hat{r}\cdot\hat{k}'\right) \; = \\
&= \frac{4\pi}{2\ell'+1} \sum_{\ell'_z=-\ell'}^{+\ell'} Y_{\ell'_z}^{(\ell')*}\left(\hat{k}\cdot\hat{r}\right) \sqrt{\frac{4\pi}{2\ell+1}}\; \delta_{\ell,\ell'}\; \delta_{0,\ell'_z} \\
&= \frac{4\pi}{2\ell'+1}\; Y_0^{(\ell')*}\left(\hat{k}\cdot\hat{r}\right) \sqrt{\frac{4\pi}{2\ell+1}}\; \delta_{\ell,\ell'} \; = \; \frac{4\pi}{2\ell+1}\; P_\ell\left(\hat{k}\cdot\hat{r}\right)\; \delta_{\ell,\ell'} \quad .
\end{aligned}$$

Combining everything, we find

$$\begin{aligned}
f\left(\vec{k},\hat{r}\right) &= -4\pi^2\mu \sum_{\ell=0}^{\infty}(2\ell+1)\; P_\ell\left(\hat{k}\cdot\hat{r}\right) \int_0^\infty dk'\; T_\ell(k,k')\; \delta(k-k') \\
&= -4\pi^2\mu \sum_{\ell=0}^{\infty}(2\ell+1)\; P_\ell\left(\hat{k}\cdot\hat{r}\right)\; T_\ell(k) \quad .
\end{aligned}$$

Exercício 46

Since the spectrum of H_c is discrete, it describes a system which is localized in a relatively small region, like a harmonic oscillator. Consequently, from the coupled Schrödinger equation we must eliminate ψ_c, since it vanishes at large distances and is thus *unobservable*. Formally, this can be done in a straightforward way. We then obtain

$$\psi_c\left(\vec{r}\,\right) \;=\; \left(E-H_c\right)^{-1} V_t\; \psi_f\left(\vec{r}\,\right)$$

and, furthermore, by substitution, the following Schrödinger equation for $\psi_f\left(\vec{r}\,\right)$

$$\left(E-H_f\right)\; \psi_f\left(\vec{r}\,\right) \;=\; V_t\; \left(E-H_c\right)^{-1} V_t\; \psi_f\left(\vec{r}\,\right) \quad .$$

By comparison of the above equation with the usual expressions for the scattering wave equations, we must conclude that the generalized potential, V, is here given by

$$V \ = \ V_t \ (E - H_c)^{-1} \ V_t \quad .$$

The relation between the scattering amplitude $f\left(\vec{k},\hat{r}\right)$, the partial wave scattering amplitude $T_\ell(k)$ and the potential V has been deduced in exercise (44) and is given by

$$\begin{aligned} f\left(\vec{k},\hat{r}\right) &= -4\pi^2\mu \sum_{\ell=0}^{\infty}(2\ell+1)\ P_\ell\left(\hat{k}\cdot\hat{r}\right) \int_0^\infty dk'\ T_\ell(k,k')\ \delta(k-k') \\ &= -4\pi^2\mu \sum_{\ell=0}^{\infty}(2\ell+1)\ P_\ell\left(\hat{k}\cdot\hat{r}\right)\ T_\ell(k) \quad . \end{aligned} \tag{71}$$

So, all we must do is determine $T_\ell(k)$. However, it is more straightforward to determine the off-shell scattering amplitude $T_\ell(k,k')$. The matrix elements of the T-operator are defined by the Lippmann-Schwinger equation

$$\begin{aligned} T\left(\vec{p}\,,\vec{p}\,'\,;E\right) \ &= \ V\left(\vec{p}\,,\vec{p}\,'\right) \ + \\ &+ \ \int d^3k' \int d^3k\, V\left(\vec{p}\,,\vec{k}\,'\right)\ G_f\left(\vec{k}\,'\,,\vec{k}\,;E\right)\ V\left(\vec{k}\,,\vec{p}\,'\right)\ + \\ &+ \ \int d^3k''' \int d^3k'' \int d^3k' \int d^3k\, V\left(\vec{p}\,,\vec{k}\,'''\right)\ G_f\left(\vec{k}\,'''\,,\vec{k}\,''\,;E\right)\ V\left(\vec{k}\,''\,,\vec{k}\,'\right)\ \times \\ &\quad \times G_f\left(\vec{k}\,'\,,\vec{k}\,;E\right)\ V\left(\vec{k}\,,\vec{p}\,'\right)\ +\ \dots \quad , \end{aligned} \tag{72}$$

where the Green's operator $G_f(E)$ corresponds to the self-adjoint free Hamiltonian H_f, according to

$$G_f\left(\vec{k}\,'\,,\vec{k}\,;E\right) \ = \ \left\langle \vec{k}\,' \left|(E-H_f)^{-1}\right| \vec{k}\,\right\rangle \ = \ \frac{2\mu}{2\mu E - k'^2}\left\langle \vec{k}\,' \,\middle|\, \vec{k}\,\right\rangle \quad . \tag{73}$$

It's relation to the retarded Green's function $G_+\left(\vec{r},\vec{r}\,'\right)$ is explained in section 4.3 of the lecture notes on scattering.

Substitution of relation (73) in expression (72) yields for the T-matrix elements the form

$$\begin{aligned} T\left(\vec{p}\,,\vec{p}\,'\,;E\right) \ &= \ V\left(\vec{p}\,,\vec{p}\,'\right) \ + \ \int d^3k\, V\left(\vec{p}\,,\vec{k}\,\right)\ \frac{2\mu}{2\mu E - k^2}\ V\left(\vec{k}\,,\vec{p}\,'\right)\ + \\ &+ \ \int d^3k' \int d^3k\, V\left(\vec{p}\,,\vec{k}\,'\right)\ \frac{2\mu}{2\mu E - k'^2}\ V\left(\vec{k}\,'\,,\vec{k}\,\right)\ \frac{2\mu}{2\mu E - k^2}\ V\left(\vec{k}\,,\vec{p}\,'\right)\ +\ \dots \quad . \end{aligned} \tag{74}$$

The first (Born) term in the expansion (74) takes the form

$$V\left(\vec{p}\,,\vec{p}\,'\right) \ = \ \left\langle \vec{p}\right| V \left|\vec{p}\,'\right\rangle \ = \ \left\langle \vec{p}\right| V_t\ \left(E(p) - H_c\right)^{-1}\ V_t \left|\vec{p}\,'\right\rangle \quad . \tag{75}$$

The total center-of-mass energy E and the linear momentum p are related by

$$E(p) \ = \ \frac{\vec{p}^{\,2}}{2\mu} \ + \ M_1 \ + \ M_2 \quad . \tag{76}$$

We denote the properly normalized eigensolutions of the operator H_c corresponding to the energy eigenvalue $E_{n\ell}$, by

$$\langle \vec{r}\,|n\ell m\rangle \;=\; Y^{(\ell)}_m(\hat{r})\;\mathcal{F}_{n\ell}(r) \quad , \quad \text{with } n=0,\,1,\,2,\,\ldots;\,\ell=0,\,1,\,2,\,\ldots;\,m=-\ell,\,\ldots,\,+\ell\,. \tag{77}$$

So, by letting the self-adjoint operator H_c act to the left in Eq. (75), we write

$$\begin{aligned}\langle\vec{p}|\,V\,\left|\vec{p}\,'\right\rangle &= \sum_{n\ell m}\langle\vec{p}|\,V_t\,|n\ell m\rangle\,\langle n\ell m|\,\left(E(p)-H_c\right)^{-1}\,V_t\,\left|\vec{p}\,'\right\rangle\\ &= \sum_{n\ell m}\langle\vec{p}|\,V_t\,\frac{|n\ell m\rangle\,\langle n\ell m|}{E(p)-E_{n\ell}}\,V_t\,\left|\vec{p}\,'\right\rangle \quad .\end{aligned} \tag{78}$$

Next, we insert several times unity to obtain

$$\begin{aligned}\langle\vec{p}|\,V\,\left|\vec{p}\,'\right\rangle &= \sum_{n\ell m}\int d^3r\int d^3r''\int d^3r'''\int d^3r'\\ &\times\frac{1}{E(p)-E_{n\ell}}\,\langle\vec{p}\,|\vec{r}\,\rangle\langle\vec{r}|\,V_t\,\left|\vec{r}\,''\right\rangle\left\langle\vec{r}\,''\,|n\ell m\right\rangle\left\langle n\ell m\left|\vec{r}\,'''\right.\right\rangle\left\langle\vec{r}\,'''\right|V_t\left|\vec{r}\,'\right\rangle\left\langle\vec{r}\,'\left|\vec{p}\,'\right.\right\rangle \quad .\end{aligned} \tag{79}$$

Two of the four integrations are trivial, since the local transition potential has the form

$$\langle\vec{r}|\,V_t\,\left|\vec{r}\,'\right\rangle \;=\; \frac{\lambda\bar{V}_t}{a^{3/2}}\,\delta\left(r-a\right)\;\delta^{(3)}\left(\vec{r}-\vec{r}\,'\right) \quad . \tag{80}$$

By inserting expression (80) into Eq. (79), also substituting $\langle\vec{r}\,|\vec{p}\,\rangle \;=\; e^{i\vec{p}\,\cdot\,\vec{r}}/(2\pi)^{3/2}$, we get

$$\begin{aligned}\langle\vec{p}|\,V\,\left|\vec{p}\,'\right\rangle &= \sum_{n\ell m}\int d^3r\int d^3r'\\ &\times\frac{1}{E(p)-E_{n\ell}}\,\frac{e^{-i\vec{p}\,\cdot\,\vec{r}}}{(2\pi)^{3/2}}\,\frac{\lambda\bar{V}_t}{a^{3/2}}\,\delta\left(r-a\right)\,\langle\vec{r}\,|n\ell m\rangle\,\left\langle n\ell m\left|\vec{r}\,'\right.\right\rangle\,\frac{\lambda\bar{V}_t}{a^{3/2}}\,\delta\left(r'-a\right)\,\frac{e^{i\vec{p}\,'\,\cdot\,\vec{r}\,'}}{(2\pi)^{3/2}} \quad .\end{aligned} \tag{81}$$

Next, we observe that the radial parts of the two remaining integrations are also trivial, because of the two delta functions. So we twice insert the expression for the confinement eigenfunctions of Eq. (77), to obtain

$$\begin{aligned}\langle\vec{p}|\,V\,\left|\vec{p}\,'\right\rangle &= \frac{1}{(2\pi)^3}\left(\frac{\lambda\bar{V}_t}{a^{3/2}}\right)^2\sum_{n\ell m}a^2\int d\Omega\,a^2\int d\Omega'\\ &\times\frac{1}{E(p)-E_{n\ell}}\,e^{-i\vec{p}\,\cdot\,a\hat{r}}\,Y^{(\ell)}_m(\hat{r})\;\mathcal{F}_{n\ell}(a)\,Y^{(\ell)\,*}_m(\hat{r}\,')\;\mathcal{F}^*_{n\ell}(a)\,e^{i\vec{p}\,'\,\cdot\,a\hat{r}\,'} \quad .\end{aligned} \tag{82}$$

For the integrations over the angles we introduce Bauer's formula, given by

$$e^{-i\vec{k}\,\cdot\,\vec{r}} \;=\; \sum_{\lambda,\mu}4\pi(-i)^\lambda j_\lambda(kr)Y^{(\lambda)\,*}_\mu(\hat{r})\,Y^{(\lambda)}_\mu\left(\hat{k}\right) \quad , \tag{83}$$

resulting in

$$\int d\Omega\left\{\begin{array}{c} e^{-i\vec{p}\,\cdot\,a\hat{r}}\;Y^{(\ell)}_m(\hat{r})\\ e^{i\vec{p}\,\cdot\,a\hat{r}}\;Y^{(\ell)\,*}_m(\hat{r}\,)\end{array}\right\} \;=\; 4\pi\;j_\ell(pa)\left\{\begin{array}{c}(-i)^\ell\;Y^{(\ell)}_m(\hat{p})\\ (i)^\ell\;Y^{(\ell)\,*}_m(\hat{p}\,)\end{array}\right\} \quad . \tag{84}$$

Substitution of the relations (84) into Eq. (82) leads to the expression

$$\langle \vec{p} |\, V \left| \vec{p}\,' \right\rangle \;=\; \frac{\lambda^2 \bar{V}_t^2 a}{\pi} \sum_{n\ell m} \frac{1}{E(p)-E_{n\ell}}\; Y_m^{(\ell)}\left(\hat{p}\right)\; Y_m^{(\ell)*}\left(\hat{p}\,'\right)\; j_\ell(pa)\; j_\ell(p'a)\; \left|\mathcal{F}_{n\ell}(a)\right|^2 \quad , \tag{85}$$

where the summation over the magnetic quantum number m can be performed by the use of the addition theorem, thus shaping the Born term (75) into its final form

$$\langle \vec{p} |\, V \left| \vec{p}\,' \right\rangle \;=\; \frac{\lambda^2 \bar{V}_t^2 a}{4\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1)\; P_\ell\left(\hat{p}\cdot\hat{p}\,'\right)\; j_\ell(pa)\; j_\ell(p'a) \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}} \quad . \tag{86}$$

For the second-order term, we start by substituting the result (86) into the second term of expansion (74), giving rise to the expression

$$\begin{aligned}
T^{(2)}\left(\vec{p}\,,\vec{p}\,'\,;E\right) \;=&\; \int d^3k\, \frac{\lambda^2 \bar{V}_t^2 a}{4\pi^2} \sum_{\ell=0}^{\infty} (2\ell+1)\; P_\ell\left(\hat{p}\cdot\hat{k}\right)\; j_\ell(pa)\; j_\ell(ka) \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}} \\
&\times \frac{2\mu}{2\mu E-k^2}\, \frac{\lambda^2 \bar{V}_t^2 a}{4\pi^2} \sum_{\ell'=0}^{\infty} (2\ell'+1)\; P_{\ell'}\left(\hat{k}\cdot\hat{p}\,'\right)\; j_{\ell'}(ka)\; j_{\ell'}(p'a) \sum_{n'=0}^{\infty} \frac{\left|\mathcal{F}_{n'\ell'}(a)\right|^2}{E(k)-E_{n'\ell'}} \\
=&\; \left(\frac{\lambda^2 \bar{V}_t^2 a}{4\pi^2}\right)^2 \sum_{\ell=0}^{\infty} (2\ell+1)\; j_\ell(pa) \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}} \sum_{\ell'=0}^{\infty} (2\ell'+1)\; j_{\ell'}(p'a) \\
&\times 2\mu \int d^3k\; P_\ell\left(\hat{p}\cdot\hat{k}\right)\; P_{\ell'}\left(\hat{k}\cdot\hat{p}\,'\right)\; \frac{j_\ell(ka)\; j_{\ell'}(ka)}{2\mu E-k^2} \sum_{n'=0}^{\infty} \frac{\left|\mathcal{F}_{n'\ell'}(a)\right|^2}{E(k)-E_{n'\ell'}} \quad .
\end{aligned} \tag{87}$$

The details of the $\vec{k}$ integration are discussed furtheron. Since, as required by Eq. (92) below, $E(k)$ is quadratic in $\vec{k}$, we find for expression (87) the result

$$\begin{aligned}
T^{(2)}\left(\vec{p}\,,\vec{p}\,'\right) \;=&\; \left(\frac{\lambda^2 \bar{V}_t^2 a}{4\pi^2}\right)^2 \sum_{\ell=0}^{\infty} (2\ell+1)\; j_\ell(pa) \sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}} \sum_{\ell'=0}^{\infty} (2\ell'+1)\; j_{\ell'}(p'a) \\
&\times \left(-i\,\frac{4\pi^2 \mu p}{2\ell+1}\right)\; \delta_{\ell,\ell'}\; P_\ell\left(\hat{p}\cdot\hat{p}\,'\right)\; j_\ell(pa)\; h_\ell^{(1)}(pa) \sum_{n'=0}^{\infty} \frac{\left|\mathcal{F}_{n'\ell'}(a)\right|^2}{E(p)-E_{n'\ell'}} \\
=&\; -i\,\frac{\mu p}{\pi^2}\; \left(\lambda^2 \bar{V}_t^2 a\right)^2 \sum_{\ell=0}^{\infty} (2\ell+1)\;\; P_\ell\left(\hat{p}\cdot\hat{p}\,'\right)\; j_\ell^2(pa)\; h_\ell^{(1)}(pa)\; j_\ell(p'a) \left[\sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}}\right]^2 \quad .
\end{aligned} \tag{88}$$

Following steps similar to those in the foregoing, it is now straightforward to determine the higher-order contributions to the expansion (74). For the full T matrix to all orders, one ends up with the result

$$\begin{aligned}
T\left(\vec{p}\,,\vec{p}\,'\right) \;=&\; \\
=&\; \frac{1}{2\pi^2}\; \lambda^2 \bar{V}_t^2 a \sum_{\ell=0}^{\infty} (2\ell+1)\; P_\ell\left(\hat{p}\cdot\hat{p}\,'\right)\; \frac{j_\ell(pa)\; j_\ell(p'a) \displaystyle\sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}}}{1+2i\mu p\; \lambda^2 \bar{V}_t^2 a j_\ell(pa)\; h_\ell^{(1)}(pa) \displaystyle\sum_{n=0}^{\infty} \frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}}} \quad .
\end{aligned} \tag{89}$$

For radially symmetric interactions, it is useful to define the partial-wave matrix element T_ℓ of the on-shell ($\vec{p}\,' = \vec{p}$) T matrix, according to the relation

$$T\left(\vec{p}\,\right) \;=\; \sum_{\ell=0}^{\infty}(2\ell+1)\; P_\ell\left(\hat{p}\cdot\hat{p}\,'\,\right)\; T_\ell(p) \quad . \tag{90}$$

Hence, also using the result of Eq. (89), we find for the partial-wave scattering amplitude $S_\ell(p)$ the expression

$$\begin{aligned} S_\ell(p) \;&=\; 1 - 8i\pi^2\mu p\; T_\ell(p) \qquad\qquad (91)\\ &=\; \frac{1 - 2i\mu p\;\lambda^2\bar{V}_t^2 a j_\ell(pa)\; h_\ell^{(2)}(pa)\; \displaystyle\sum_{n=0}^{\infty}\frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}}}{1 + 2i\mu p\;\lambda^2\bar{V}_t^2 a j_\ell(pa)\; h_\ell^{(1)}(pa)\; \displaystyle\sum_{n=0}^{\infty}\frac{\left|\mathcal{F}_{n\ell}(a)\right|^2}{E(p)-E_{n\ell}}} \quad . \end{aligned}$$

Details of the $\vec{k}$ integration

Let us study the momentum-space integration

$$\begin{aligned} &\mathcal{I}_\ell\left(\vec{p}\,,\vec{p}\,'\,;\mu\,;f_\ell\right) \;= \qquad\qquad (92)\\ &= 2\mu\;\int d^3k\; P_\ell\left(\hat{p}\cdot\hat{k}\,\right)\; P_{\ell'}\left(\hat{k}\cdot\hat{p}\,'\right)\; \frac{j_\ell(ka)\; j_{\ell'}(ka)}{2\mu E - k^2}\; f_\ell\left(k^2\right)\\ &= 2\mu\;\int d\Omega_k\; P_\ell\left(\hat{p}\cdot\hat{k}\,\right)\; P_{\ell'}\left(\hat{k}\cdot\hat{p}\,'\right)\; \int_0^\infty k^2 dk\; \frac{j_\ell(ka)\; j_{\ell'}(ka)}{2\mu E - k^2} f_\ell\left(k^2\right) \quad , \end{aligned}$$

where f_ℓ represents an arbitrary well-behaved function of k^2. For the integration over the angles, we can employ the orthogonality of spherical harmonics. Hence, we must concentrate on the radial integration, i.e.,

$$\int_0^\infty k^2 dk\; \frac{j_\ell^2(ka)}{2\mu E - k^2}\; f_\ell\left(k^2\right) \quad . \tag{93}$$

We shall show below that the integration can easily be performed, yielding

$$\int_0^\infty k^2 dk\; \frac{j_\ell^2(ka)}{2\mu E - k^2}\; f_\ell\left(k^2\right) \;=\; \frac{1}{2}\int_{-\infty}^\infty k^2 dk\; \frac{j_\ell(ka)\; h_\ell^{(1)}(ka)}{2\mu E - k^2}\; f_\ell\left(k^2\right) \quad , \tag{94}$$

by using the following properties of the spherical Bessel and Hankel functions:

$$j_\ell\left(e^{\pi i}\; ka\right) \;=\; e^{\pi i\ell}\; j_\ell(ka) \quad \text{and} \quad h_\ell^{(1)}\left(e^{\pi i}\; ka\right) \;=\; e^{-\pi i\ell}\; h_\ell^{(2)}(ka) \quad . \tag{95}$$

For large imaginary part of the argument ka, the function $h_\ell^{(1)}(ka)$ tends to zero. Therefore, we can close the integration path in the complex k plane by a non-contributing semicircle in the upper half plane. If we then set $2\mu E \;=\; (p+i\epsilon)^2$, taking the limit $\epsilon\downarrow 0$ after the integration, the integral (94) can be simply computed with Cauchy's residue theorem, yielding

$$\begin{aligned} \int_0^\infty k^2 dk\; \frac{j_\ell^2(ka)}{2\mu E - k^2}\; f_\ell\left(k^2\right) \;&=\; \lim_{\epsilon\downarrow 0}\;\frac{1}{2}\oint k^2 dk\; \frac{j_\ell(ka)\; h_\ell^{(1)}(ka)}{(p+i\epsilon-k)(p+i\epsilon+k)}\; f_\ell\left(k^2\right)\\ &=\; -\frac{i\pi p}{2}\; j_\ell(pa)\; h_\ell^{(1)}(pa)\; f_\ell\left(p^2\right) \quad . \qquad (96) \end{aligned}$$

Putting everything together, we obtain for Eq. (92) the final result

$$\mathcal{I}_\ell\left(\vec{p}\,,\vec{p}\,'\,;\mu\,;f_\ell\right) \;=\; -i\,\frac{4\pi^2\mu p}{2\ell+1}\,\delta_{\ell,\ell'}\,P_\ell\left(\hat{p}\cdot\hat{p}\,'\,\right)\,j_\ell(pa)\,h_\ell^{(1)}(pa)\,f_\ell\left(p^2\right) \quad . \tag{97}$$

Exercício 47

a. We start with

$$-\nabla^2\,\frac{u(r)}{r}Y_\ell^m\left(\hat{r}\,\right) \;=\; Y_\ell^m\left(\hat{r}\,\right)\left\{-\frac{1}{r}\frac{d^2}{dr^2}r+\frac{\ell(\ell+1)}{r^2}\right\}\,\frac{u(r)}{r}$$

which for S wave ($\ell=0$) leads to

$$0=\left\{-\frac{1}{r}\frac{d^2}{dr^2}r+g\delta(a-r)-k^2\right\}\,\frac{u(r)}{r} \;=\; \frac{1}{r}\left\{-\frac{d^2}{dr^2}+g\delta(a-r)-k^2\right\}\,u(r)$$

The equation

$$\left\{-\frac{d^2}{dr^2}+g\delta(a-r)-k^2\right\}\,u(r) \;=\; 0$$

is for $r\neq a$ given by

$$\frac{d^2}{dr^2}\,u(r) \;=\; -k^2u(r)$$

which is solved by

$$u(r) \;\propto\; \sin(kr+\phi)$$

where ϕ depends on the boundary conditions.
For $r<a$ one has the boundary condition $u(r=0)=0$. Hence a suitable solution for $r<a$ is given by

$$u(r) \;=\; A\sin(kr)$$

For $r>a$ one defines the phase shift by $\phi=\delta$. Hence a suitable solution for $r>a$ is given by

$$u(r) \;=\; B\sin(kr+\delta)$$

Further boundary conditions are given by

$$u\left(r\uparrow a\right)=u\left(r\downarrow a\right) \qquad \text{and} \qquad \left(\frac{du}{dr}\right)_{r\,\uparrow\,a}-\left(\frac{du}{dr}\right)_{r\,\downarrow\,a}+gu\left(r=a\right)=0$$

which translates to the conditions

$$A\sin(ka)=B\sin(ka+\delta) \qquad \text{and} \qquad kA\cos(ka)-kB\cos(ka+\delta)+gA\sin(ka)=0$$

Hence

$$\frac{\sin(ka+\delta)}{\sin(ka)} \;=\frac{A}{B}=\; \frac{k\cos(ka+\delta)}{k\cos(ka)+g\sin(ka)}$$

or

$$\frac{\sin(ka)\cos(\delta)+\cos(ka)\sin(\delta)}{\sin(ka)} \quad = \quad \frac{k\left\{\cos(ka)\cos(\delta)-\sin(ka)\sin(\delta)\right\}}{k\cos(ka)+g\sin(ka)}$$

or

$$\mathrm{cotg}(\delta)+\mathrm{cotg}(ka) \quad = \quad \frac{k\left\{\mathrm{cotg}(ka)\mathrm{cotg}(\delta)-1\right\}}{k\mathrm{cotg}(ka)+g}$$

or

$$(k\mathrm{cotg}(ka)+g)\left(\mathrm{cotg}(\delta)+\mathrm{cotg}(ka)\right) \quad = \quad k\left\{\mathrm{cotg}(ka)\mathrm{cotg}(\delta)-1\right\}$$

or

$$g\mathrm{cotg}(\delta)+k\mathrm{cotg}^2(ka)+g\mathrm{cotg}(ka) \quad = \quad -k$$

Hence

$$\mathrm{cotg}(\delta) \quad = \quad -\mathrm{cotg}(ka)-\frac{k}{g}\left\{1+\mathrm{cotg}^2(ka)\right\}=-\mathrm{cotg}(ka)-\frac{k}{g\sin^2(ka)}$$

Furthermore

$$\frac{A}{B} \quad = \quad \frac{\sin(ka+\delta)}{\sin(\kappa a)}=\frac{\sin(ka)\cos(\delta)+\cos(ka)\sin(\delta)}{\sin(ka)}=\sin(\delta)\left\{\mathrm{cotg}(\delta)+\mathrm{cotg}(ka)\right\}$$

Now

$$\mathrm{cotg}(\delta)+\mathrm{cotg}(ka) \quad = \quad -\frac{k}{g\sin^2(ka)}$$

Furthermore

$$1+\mathrm{cotg}^2(\delta)=1+\left\{\mathrm{cotg}(ka)+\frac{k}{g}\left(1+\mathrm{cotg}^2(ka)\right)\right\}^2=$$

$$= \quad 1+\mathrm{cotg}^2(ka)+2\frac{k}{g}\mathrm{cotg}(ka)\left(1+\mathrm{cotg}^2(ka)\right)+\frac{k^2}{g^2}\left(1+\mathrm{cotg}^2(ka)\right)^2$$

$$= \quad \left\{1+2\frac{k}{g}\mathrm{cotg}(ka)+\frac{k^2}{g^2}\left(1+\mathrm{cotg}^2(ka)\right)\right\}\left(1+\mathrm{cotg}^2(ka)\right)$$

and

$$\sin^2(ka)\sqrt{1+\mathrm{cotg}^2(\delta)} \quad = \quad \sqrt{\sin^2(ka)+2\frac{k}{g}\sin(ka)\cos(ka)+\frac{k^2}{g^2}}$$

Hence

$$\frac{A}{B}=\sin(\delta)\left\{\mathrm{cotg}(\delta)+\mathrm{cotg}(ka)\right\}=\frac{\mathrm{cotg}(\delta)+\mathrm{cotg}(ka)}{\pm\sqrt{1+\mathrm{cotg}^2(\delta)}}=$$

$$=\frac{\pm k/g}{\sin^2(ka)\sqrt{1+\mathrm{cotg}^2(\delta)}}=\frac{\pm k/g}{\sqrt{\sin^2(ka)+2\frac{k}{g}\sin(ka)\cos(ka)+\frac{k^2}{g^2}}}$$

b. We start with the angular integration

$$
\begin{aligned}
f(k,\hat{r}) = -\frac{gm}{2\pi}\int d^3r'\, e^{i\left(\vec{k}-k\hat{r}\right)\cdot\vec{r}'}\delta(a-r') = \\
= -\frac{gm}{2\pi}\int_0^\infty (r')^2dr'\left\{\int_0^{2\pi}d\varphi\int_{-1}^{+1}d\cos(\vartheta)e^{i\left|\vec{k}-k\hat{r}\right|r'\cos(\vartheta)}\right\}\delta(a-r') \\
= -\frac{gm}{2\pi}\int_0^\infty (r')^2dr'\left\{2\pi\frac{e^{i\left|\vec{k}-k\hat{r}\right|r'}-e^{-i\left|\vec{k}-k\hat{r}\right|r'}}{i\left|\vec{k}-k\hat{r}\right|r'}\right\}\delta(a-r') \\
= -\frac{2gm}{\left|\vec{k}-k\hat{r}\right|}\int_0^\infty r'dr'\,\sin\left(\left|\vec{k}-k\hat{r}\right|r'\right)\,\delta(a-r') \\
= -\frac{2gm}{\left|\vec{k}-k\hat{r}\right|}\,a\sin\left(\left|\vec{k}-k\hat{r}\right|a\right)
\end{aligned}
$$

c. In the formalism of alinea (**a**):
For S-wave the scattering amplitude is given by

$$
f(k) \;=\; \frac{2m}{k}\,e^{i\delta}\,\sin(\delta) = \frac{2m}{k\,(\mathrm{cotg}(\delta)-i)}
$$

Now,

$$
\begin{aligned}
\mathrm{cotg}(\delta)-i &= -\mathrm{cotg}(ka)-\frac{k}{g\sin^2(ka)}-i = -\frac{e^{ika}}{\sin(ka)}-\frac{k}{g\sin^2(ka)} \\
&= -\frac{k+ge^{ika}\sin(ka)}{g\sin^2(ka)}
\end{aligned}
$$

So,

$$
f(k) = -\frac{2m}{k}\,\frac{g\sin^2(ka)}{k+ge^{ika}\sin(ka)} \qquad \text{limit }\ (g\downarrow 0) \qquad -\frac{2gm}{k^2}\,\sin^2(ka)
$$

d. In the formalism of alinea (**b**):
For S-wave the scattering amplitude is given by

$$
f(k) \;=\; \int\frac{d\Omega}{4\pi}\,f(k,\hat{r}) = -\int\frac{d\Omega}{4\pi}\,\frac{2gm}{\left|\vec{k}-k\hat{r}\right|}\,a\sin\left(\left|\vec{k}-k\hat{r}\right|a\right)
$$

Now

$$
\left|\vec{k}-k\hat{r}\right| \;=\; \sqrt{k^2-2k\vec{k}\cdot\hat{r}+k^2} = k\sqrt{2}\sqrt{1-\cos(\vartheta)}
$$

where ϑ is the angle between $\vec{k}$ and $\hat{r}$.
Hence

$$
f(k) \;=\; -\frac{1}{4\pi}\int_0^{2\pi}d\varphi\int_{-1}^{+1}d\cos(\vartheta)\frac{2gma}{k\sqrt{2}\sqrt{1-\cos(\vartheta)}}\,\sin\left(ka\sqrt{2}\sqrt{1-\cos(\vartheta)}\right)
$$

$$= -\frac{1}{2}\int_{-1}^{+1} d\cos(\vartheta)\frac{2gma}{k\sqrt{2}\sqrt{1-\cos(\vartheta)}} \sin\left(ka\sqrt{2}\sqrt{1-\cos(\vartheta)}\right)$$

We define the integration variable $\xi = \sqrt{1-\cos(\vartheta)}$.
Hence

$$\begin{array}{rll} \cos(\vartheta) = -1 & \text{corresponds to} & \xi = \sqrt{2} \\ \cos(\vartheta) = +1 & \text{corresponds to} & \xi = 0 \\ \text{and } \; d\cos(\vartheta) = -2\xi d\xi & & \end{array}$$

We obtain

$$\begin{aligned} f(k) &= -\int_0^{\sqrt{2}} \xi d\xi \frac{2gma}{\xi k\sqrt{2}} \sin\left(\xi ka\sqrt{2}\right) = -\frac{2gma}{k\sqrt{2}} \int_0^{\sqrt{2}} d\xi \sin\left(\xi ka\sqrt{2}\right) \\ &= -\frac{2gma}{k\sqrt{2}} \frac{1-\cos(2ka)}{ka\sqrt{2}} = -\frac{2gm}{k^2} \sin^2(ka) \end{aligned}$$

Exercício 50

a.

$$H\begin{pmatrix} 1 \\ \pm r \end{pmatrix} = \begin{pmatrix} A & \frac{B}{r} \\ Br & A \end{pmatrix}\begin{pmatrix} 1 \\ \pm r \end{pmatrix} = \begin{pmatrix} A \pm B \\ Br \pm Ar \end{pmatrix} = (A \pm B)\begin{pmatrix} 1 \\ \pm r \end{pmatrix} \quad .$$

Hence, the eigenvalues are given by $E_\pm = A \pm B$. For the normalization we determine

$$\phi_\pm^\dagger \phi_\pm = \frac{1}{1+|r|^2}\begin{pmatrix} 1 & \pm r^* \end{pmatrix}\begin{pmatrix} 1 \\ \pm r \end{pmatrix} = \frac{1}{1+|r|^2}(1 + r^* r) = 1 \quad .$$

b.

$$\begin{aligned} &\frac{1}{E_+ - E_-}\left\{(E_+ - H)\, e^{-iE_- t} - (E_- - H)\, e^{-iE_+ t}\right\}\psi(0) = \\ &= \frac{1}{E_+ - E_-}\left\{(E_+ - H)\, e^{-iE_- t} - (E_- - H)\, e^{-iE_+ t}\right\}(c_+\phi_+ + c_-\phi_-) \\ &= \frac{c_+}{E_+ - E_-}\left\{(E_+ - E_+)\, e^{-iE_- t} - (E_- - E_+)\, e^{-iE_+ t}\right\}\phi_+ + \\ &+ \frac{c_-}{E_+ - E_-}\left\{(E_+ - E_-)\, e^{-iE_- t} - (E_- - E_-)\, e^{-iE_+ t}\right\}\phi_- \\ &= c_+ e^{-iE_+ t}\phi_+ + c_- e^{-iE_- t}\phi_- = c_+ e^{-iHt}\phi_+ + c_- e^{-iHt}\phi_- \\ &= e^{-iHt}(c_+\phi_+ + c_-\phi_-) = e^{-iHt}\psi(0) \quad . \end{aligned}$$

c. First, we use

$$\langle\downarrow|H|\uparrow\rangle = \begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} A & \frac{B}{r} \\ Br & A \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \end{pmatrix}\begin{pmatrix} A \\ Br \end{pmatrix} = Br \quad .$$

Next, we use

$$\begin{aligned}
&\left\langle\downarrow\left|e^{-iHt}\right|\uparrow\right\rangle = \\
&= \frac{1}{E_+ - E_-}\left\{\left(\langle\downarrow|E_+|\uparrow\rangle - \langle\downarrow|H|\uparrow\rangle\right)e^{-iE_-t} - \left(\langle\downarrow|E_-|\uparrow\rangle - \langle\downarrow|H|\uparrow\rangle\right)e^{-iE_+t}\right\} \\
&= \frac{1}{E_+ - E_-}\left\{\left(E_+\langle\downarrow|\uparrow\rangle - Br\right)e^{-iE_-t} - \left(E_-\langle\downarrow|\uparrow\rangle - Br\right)e^{-iE_+t}\right\} \\
&= \frac{1}{E_+ - E_-}\left\{(0 - Br)\,e^{-iE_-t} - (0 - Br)\,e^{-iE_+t}\right\} \\
&= \frac{Br}{E_+ - E_-}\left\{-e^{-iE_-t} + e^{-iE_+t}\right\} = \frac{Br}{2B}\left\{-e^{-iE_-t} + e^{-iE_+t}\right\} \\
&= \frac{r}{2}\left\{-e^{-iE_-t} + e^{-iE_+t}\right\} \quad .
\end{aligned}$$

Furthermore

$$E_+ = A + B = M - \tfrac{1}{2}i\gamma_1 \quad \text{and} \quad E_- = A - B = M + \Delta M - \tfrac{1}{2}i\gamma_2 \quad .$$

Hence the transition amplitude equals

$$\begin{aligned}
&\left\langle\downarrow\left|e^{-iHt}\right|\uparrow\right\rangle = \\
&= \frac{r}{2}\left\{-e^{-i\left(M + \Delta M - \frac{1}{2}i\gamma_2\right)t} + e^{-i\left(M - \frac{1}{2}i\gamma_1\right)t}\right\} \\
&= \frac{r}{2}\left\{-e^{-i(M+\Delta M)t - \frac{1}{2}\gamma_2 t} + e^{-iMt - \frac{1}{2}\gamma_1 t}\right\} \\
&= \frac{r}{2}e^{-iMt}\left\{-e^{-i\Delta Mt - \frac{1}{2}\gamma_2 t} + e^{-\frac{1}{2}\gamma_1 t}\right\} \quad .
\end{aligned}$$

The decay rate is given by

$$\begin{aligned}
&\left|\left\langle\downarrow\left|e^{-iHt}\right|\uparrow\right\rangle\right|^2 = \\
&= \tfrac{1}{4}|r|^2\left\{-e^{-i\Delta Mt - \frac{1}{2}\gamma_2 t} + e^{-\frac{1}{2}\gamma_1 t}\right\}\left\{-e^{i\Delta Mt - \frac{1}{2}\gamma_2 t} + e^{-\frac{1}{2}\gamma_1 t}\right\} \\
&= \tfrac{1}{4}|r|^2\left\{e^{-\gamma_1 t} + e^{-\gamma_2 t} - e^{-i\Delta Mt - \frac{1}{2}(\gamma_1+\gamma_2)t} - e^{i\Delta Mt - \frac{1}{2}(\gamma_1+\gamma_2)t}\right\}
\end{aligned}$$

$$= \tfrac{1}{4}\,|r|^2 \left\{ e^{-\gamma_1 t} + e^{-\gamma_2 t} - e^{-\frac{1}{2}\,(\gamma_1+\gamma_2)\,t} \left(e^{i\Delta M t} + e^{-i\Delta M t} \right) \right\}$$

$$= \tfrac{1}{4}\,|r|^2 \left\{ e^{-\gamma_1 t} + e^{-\gamma_2 t} - 2e^{-\frac{1}{2}\,(\gamma_1+\gamma_2)\,t} \cos(\Delta M t) \right\} \quad .$$

d. From the inset of the figure we read

$$\Delta M T = 2\pi \quad \text{for} \quad T = 12.0 \times 10^{-10}\ \text{s} \quad .$$

Hence,

$$\Delta M = 2\pi/(12.0 \times 10^{-10}\ \text{s}) = 0.52 \times 10^{10}\ \text{s}^{-1} =$$

$$= 0.52 \times 10^{10}\ \text{s}^{-1} \times 0.66 \times 10^{-15}\ \text{eVs} = 3.5 \times 10^{-6}\ \text{eV} \quad .$$