# 1 Formulari física quàntica I

## 1.1 Efecte fotoelèctric

$$K = h\nu - W, \quad W = h\nu_{\min} = \frac{hc}{\lambda_{\max}} = \frac{hc}{\lambda_{\text{llindar}}}$$

$$\frac{N_{\max}(e^-)}{A \cdot t} = \frac{I}{h\nu}$$

$\hbar c \approx 197\,\text{fm MeV}$ ($1\,\text{fm} = 10^{-15}\,\text{m}$).

## 1.2 Efecte Compton

$$\begin{cases} h\nu_i + mc^2 = h\nu_f + \sqrt{p^2c^2 + m^2c^4} \\ \vec{p}_{i,\gamma} + \vec{0} = \vec{p}_{f,\gamma} + \vec{p}_e \end{cases} \Rightarrow \Delta\lambda = \frac{h}{mc}(1 - \cos\theta)$$

## 1.3 Longitud d'ona de de Broglie

$$\lambda_{dB} = \frac{h}{p} = \frac{2\pi\hbar c}{pc} = \frac{2\pi\hbar c}{\sqrt{E^2 - m^2c^4}} = \frac{2\pi\hbar c}{K\sqrt{1 + \frac{2mc^2}{K}}}$$

Masses ($\text{MeV}/c^2$): $m_e = 0.51$, $m_n = 939.57$, $m_p = 938.27$.

## 1.4 Espèctre atòmic

$$\frac{1}{\lambda} = R_H z^2 \left( \frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

$R_H \equiv 1.097 \times 10^7\,\text{m}^{-1}$ (constant de Rydberg a l'hidrogen).
$n_f = 2$: sèrie de Balmer; $n_f = 3$: sèrie de Paschen.

## 1.5 Model de Bohr

$$r_n = 4\pi\varepsilon_0 \frac{n^2\hbar^2}{mze^2} = \frac{n^2}{z}a_0, \quad v_n = \frac{n\hbar}{mr_n}, \quad E_n = -\frac{R_y z^2}{n^2}$$

$a_0 \equiv 0.053 \times 10^{-9}\,\text{m}$ (radi de Bohr).
$R_y \equiv 13.6\,\text{eV} = 2\pi\hbar c \cdot R_H$ (constant de Rydberg).

## 1.6 Postulats de la quàntica

$$p_{a_i} = p(a_i, |b_j\rangle) = |\langle a_i | b_j \rangle|^2$$

$$H \Rightarrow |\varphi(t)\rangle = \sum \exp\left[ -\frac{iE_i}{\hbar}t \right] |E_i\rangle \langle E_i | \varphi(0) \rangle$$

$$(\Delta A)^2_\psi = \langle A^2 \rangle_\psi - \langle A \rangle^2_\psi$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle A \rangle_\psi = \frac{1}{i\hbar} \langle [A, H] \rangle_\psi \Rightarrow [A, H] = 0 \Rightarrow \langle A \rangle_{\psi(t)} \neq f(t)$$

## 1.7 Matrius de Pauli (spin 1/2)

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\sigma_i \sigma_j = \delta_{ij} \mathbb{1} + i\epsilon_{ijk}\sigma_k$$

$$\sigma_{\hat{n}} = \hat{n} \cdot \begin{pmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \end{pmatrix} = \begin{pmatrix} \cos\theta & e^{-i\phi}\sin\theta \\ e^{i\phi}\sin\theta & -\cos\theta \end{pmatrix}$$

$$|+\rangle_{\hat{n}} = \begin{pmatrix} \cos\frac{\theta}{2} e^{-i\frac{\varphi}{2}} \\ \sin\frac{\theta}{2} e^{i\frac{\varphi}{2}} \end{pmatrix}, \quad |-\rangle_{\hat{n}} = \begin{pmatrix} -\sin\frac{\theta}{2} e^{-i\frac{\varphi}{2}} \\ \cos\frac{\theta}{2} e^{i\frac{\varphi}{2}} \end{pmatrix}$$

$$\begin{aligned} &|+\rangle_x = (1,1)/\sqrt{2}, && |-\rangle_x = (1,-1)/\sqrt{2}, && \sigma_x |\pm\rangle = |\mp\rangle \\ &|+\rangle_y = (1,i)/\sqrt{2}, && |-\rangle_y = (i,1)/\sqrt{2}, && \sigma_y |\pm\rangle = \pm i |\mp\rangle \\ &|+\rangle_z = (1,0), && |-\rangle_z = (0,1), && \sigma_z |\pm\rangle = \pm |\pm\rangle \end{aligned}$$

## 1.8 Matrius d'spin 1

$$J_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{aligned} |{+\hbar}\rangle_x &= (1, \sqrt{2}, 1)/2 \\ |{-\hbar}\rangle_x &= (1, -\sqrt{2}, 1)/2 \\ |0\rangle_x &= (1, 0, -1)/\sqrt{2} \end{aligned}$$

$$J_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \begin{aligned} |{+\hbar}\rangle_y &= (-1, -\sqrt{2}i, 1)/2 \\ |{-\hbar}\rangle_y &= (-1, \sqrt{2}i, 1)/2 \\ |0\rangle_y &= (1, 0, 1)/\sqrt{2} \end{aligned}$$

$$J_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \begin{aligned} |{+\hbar}\rangle_z &= (1, 0, 0) \\ |{-\hbar}\rangle_z &= (0, 0, 1) \\ |0\rangle_z &= (0, 1, 0) \end{aligned}$$

## 1.9 Matrius d'spin 1 al quadrat

$$J_x^2 = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \quad \begin{aligned} \left|\hbar^2\right\rangle &= (1, 0, 1)/\sqrt{2} \\ \left|\hbar^2\right\rangle &= (0, 1, 0) \\ |0\rangle &= (1, 0, -1)/\sqrt{2} \end{aligned}$$

$$J_y^2 = \frac{\hbar^2}{2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}, \quad \begin{aligned} \left|\hbar^2\right\rangle &= (1, 0, -1)/\sqrt{2} \\ \left|\hbar^2\right\rangle &= (0, 1, 0) \\ |0\rangle &= (1, 0, 1)/\sqrt{2} \end{aligned}$$

$$J_z^2 = \hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{aligned} \left|\hbar^2\right\rangle &= (1, 0, 0) \\ \left|\hbar^2\right\rangle &= (0, 0, 1) \\ |0\rangle &= (0, 1, 0) \end{aligned}$$

## 1.10 Trigonometria

$$\begin{aligned} \sin^2\theta &= \frac{1}{2}(1 - \cos 2\theta) & \cos\frac{\pi}{3} &= \sin\frac{\pi}{6} = \frac{1}{2} \\ \cos^2\theta &= \frac{1}{2}(1 + \cos 2\theta) & \cos\frac{\pi}{4} &= \sin\frac{\pi}{4} = \frac{1}{\sqrt{2}} \\ \sin(\theta \pm \phi) &= \sin\theta\cos\phi \pm \cos\theta\sin\phi & \cos\frac{\pi}{6} &= \sin\frac{\pi}{3} = \frac{\sqrt{3}}{2} \\ \cos(\theta \pm \phi) &= \cos\theta\cos\phi \mp \sin\theta\sin\phi \end{aligned}$$

## 1.11 Eigenstuff a 2 × 2 (RMT)

$$\begin{aligned} \begin{pmatrix} a & c - id \\ c + id & b \end{pmatrix} &= \frac{a+b}{2}\mathbb{1} + \frac{a-b}{2}\sigma_z + c\sigma_x + d\sigma_y \\ &= \varepsilon\mathbb{1} + \vec{v} \cdot \vec{\sigma} \\ &\Rightarrow \textit{vaps} : \lambda_\pm = \varepsilon \pm \|\vec{v}\| \end{aligned}$$

## 1.12 Moment angular (quàntica II)

$$J_\pm = J_x \pm J_-, \quad J_x = \frac{1}{2}(J_+ + J_-), \quad J_y = \frac{1}{2i}(J_+ - J_-)$$

$$[J_i, J_j] = i\hbar\epsilon_{ijk}J_k \qquad [J_z, J_\pm] = \pm\hbar J_\pm$$

$$[J_+, J_-] = 2\hbar J_z \qquad \left[J^2, J_{z,\pm}\right] = 0$$

$$J_\pm |j, m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}\, |j, m \pm 1\rangle$$

$$J^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$$

$$J_z |j, m\rangle = \hbar m |j, m\rangle$$

# 2 Formulari física quàntica I

## 2.1 Equació d'Schrödinger

$$\left[\frac{p^2}{2m}+V(x)\right]\psi_n(x)=E_n\psi_n(x), \quad p=-ih\frac{\partial}{\partial x}$$

## 2.2 Pou infinit

$$[0,L]\Rightarrow\begin{cases}\phi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) & x\in[0,L]\\ \phi_n(x)=0 & x\notin[0,L]\end{cases}$$

$$\left[-\frac{L}{2},\frac{L}{2}\right]\Rightarrow\begin{cases}\phi_n(x)=\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) & n \text{ senar}\\ \phi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) & n \text{ parell}\end{cases}$$

$$E_n=\frac{n^2\pi^2\hbar^2}{2mL^2}$$

## 2.3 Harmònics 1D

$$\text{Gaussiana: } \psi(x)=\frac{1}{(2\pi\sigma_x^2)^{1/4}}\exp\left[-\frac{x^2}{4\sigma_x^2}\right]$$

$$\boxed{\phi_n(x)=C_nH_n(\tilde{x})\exp\left[-\frac{\tilde{x}^2}{2}\right]}$$

$$\tilde{x}=\frac{x}{a_0},\quad a_0=\sqrt{\frac{\hbar}{m\omega}},\quad C_n=\left(\frac{1}{\pi a_0^2}\right)^{1/4}\left(\frac{1}{2^n n!}\right)^{1/2}$$

$$\begin{aligned}H_0(\tilde{x})&=1 & H_2(\tilde{x})&=4\tilde{x}^2-2\\ H_1(\tilde{x})&=2\tilde{x} & H_3(\tilde{x})&=8\tilde{x}^3-12\tilde{x}\end{aligned}$$

$$E_n=\hbar\omega\left(n+\frac{1}{2}\right),\quad p(E=E_n)_\psi=|\alpha_n|^2$$

## 2.4 Potencials centrals

$$\boxed{\phi_{nlm}(r,\theta,\varphi)=R_n^l(r)Y_l^m(\theta,\varphi)},\quad \begin{cases}l=0,1,\cdots,n-1\\ m=-l,-l-1,\cdots,l\end{cases}$$

$$\begin{aligned}\hat{H}\left|\phi_{nlm}\right\rangle&=-R_y/n^2\left|\phi_{nlm}\right\rangle,\quad R_y=13.6\,\text{eV}\\ \hat{L}^2\left|\phi_{nlm}\right\rangle&=\hbar^2 l(l+1)\left|\phi_{nlm}\right\rangle\\ \hat{L_z}\left|\phi_{nlm}\right\rangle&=\hbar m\left|\phi_{nlm}\right\rangle\\ E_n&=-\frac{m}{2\hbar^2}\left(\frac{ze^2}{4\pi\varepsilon_0 n}\right)^2\quad\text{(en general)}\end{aligned}$$

### Harmònics 3D

$$\begin{aligned}Y_0^0&=\sqrt{\frac{1}{4\pi}} & Y_2^0&=\sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)\\ Y_1^0&=\sqrt{\frac{3}{4\pi}}\cos\theta & Y_2^{\pm1}&=\mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\varphi}\\ Y_1^{\pm1}&=\mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\varphi} & Y_2^{\pm2}&=\sqrt{\frac{15}{32\pi}}\sin^2\theta e^{\pm2i\varphi}\end{aligned}$$

### Funcions d'ona radials

$$\begin{aligned}R_1^0&=2\left(\frac{1}{a_0}\right)^{3/2}\exp\left[-\frac{r}{a_0}\right]\\ R_2^1&=\frac{1}{\sqrt{3}}\left(\frac{1}{2a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\exp\left[-\frac{r}{2a_0}\right]\\ R_2^0&=2\left(\frac{1}{2a_0}\right)^{3/2}\left(1-\frac{r}{2a_0}\right)\exp\left[-\frac{r}{2a_0}\right]\\ R_3^2&=\frac{2\sqrt{2}}{27\sqrt{5}}\left(\frac{1}{3a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)^2\exp\left[-\frac{r}{3a_0}\right]\\ R_3^1&=\frac{4\sqrt{2}}{3}\left(\frac{1}{3a_0}\right)^{3/2}\left(\frac{r}{a_0}\right)\left(1-\frac{r}{6a_0}\right)\exp\left[-\frac{r}{3a_0}\right]\\ R_3^0&=2\left(\frac{1}{3a_0}\right)^{3/2}\left(1-\frac{2r}{3a_0}+\frac{2r^2}{27a_0^2}\right)\exp\left[-\frac{r}{3a_0}\right]\end{aligned}$$

### Àtom d'hidrogen

$$V(r)=-\frac{e^2}{4\pi\varepsilon_0 r}\quad\text{(energia potencial)}$$

### Probabilitats marginals

$$\rho(r,\theta,\varphi)\,\mathrm{d}V=\begin{cases}\rho(r)\,\mathrm{d}r\\ \rho(\theta)\,\mathrm{d}\theta\\ \rho(\varphi)\,\mathrm{d}\varphi\end{cases}\Rightarrow P[\zeta\le a]=\int_0^a\rho(\zeta)\,\mathrm{d}\zeta$$

on $\zeta$ pot ser $r,\theta,\varphi$. Recordem $(x,y,z)=(r\,\mathrm{s}\,\theta\,\mathrm{c}\,\varphi, r\,\mathrm{s}\,\theta\,\mathrm{s}\,\varphi, r\,\mathrm{c}\,\theta)$ i $\mathrm{d}V=r^2\,\mathrm{s}\,\theta\,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\varphi$.

$$\zeta=\zeta_{\max}\Leftrightarrow\frac{\mathrm{d}\rho(\zeta)}{\mathrm{d}\zeta}\equiv 0$$

## 2.5 Teoremes

$$\begin{aligned}\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}&=\frac{\langle p\rangle}{m},\quad \frac{\mathrm{d}\langle p\rangle}{\mathrm{d}t}=\left\langle\vec{F}(x)\right\rangle=-\left\langle\vec{\nabla}V(x)\right\rangle &&\text{(Ehrenfest)}\\ \frac{\mathrm{d}\langle\vec{r}\cdot\vec{p}\rangle}{\mathrm{d}t}&=\frac{\left\langle p^2\right\rangle}{m}-\left\langle\vec{r}\cdot\vec{\nabla}V(x)\right\rangle &&\text{(Virial)}\\ 2\langle K\rangle&=\frac{\left\langle p^2\right\rangle}{m}=\left\langle\vec{r}\cdot\vec{\nabla}V(x)\right\rangle &&\text{(Virial; estat estacionari)}\end{aligned}$$

## 2.6 Integrals i coses maques

$$\int_{-\infty}^{\infty}e^{-ax^2}x^2\,\mathrm{d}x=\frac{1}{2a}\sqrt{\frac{\pi}{a}},\quad \int_{-\infty}^{\infty}e^{-ax^2}x^4\,\mathrm{d}x=\frac{3}{4a^2}\sqrt{\frac{\pi}{a}}$$

$$\int_0^{\infty}e^{-ar}r^n\,\mathrm{d}r=\frac{n!}{(a)^{n+1}},\quad 0\le n$$

$$[A,f(B)]=f'(B)[A,B]$$

## 2.7 Trigonometria

$$\begin{aligned}\sin^2\theta&=\frac{1}{2}(1-\cos2\theta)\\ \cos^2\theta&=\frac{1}{2}(1+\cos2\theta)=\frac{3\cos^2\theta-1+\sin^2\theta}{2}\\ \sin(\theta\pm\phi)&=\sin\theta\cos\phi\pm\cos\theta\sin\phi\\ \cos(\theta\pm\phi)&=\cos\theta\cos\phi\mp\sin\theta\sin\phi\end{aligned}$$

## 2.8 Operadors sobre estats de Fock

$$x = \sqrt{\frac{\hbar}{2m\omega}}\big(a^\dagger + a\big), \quad p = i\sqrt{\frac{\hbar m\omega}{2}}\big(a^\dagger - a\big)$$

### Posició

$$\begin{aligned}
&x\left|0\right\rangle \to \left|1\right\rangle, && x^2\left|0\right\rangle \to \left|0\right\rangle + \sqrt{2}\left|2\right\rangle \\
&x\left|1\right\rangle \to \left|0\right\rangle + \sqrt{2}\left|3\right\rangle, && x^2\left|1\right\rangle \to 3\left|1\right\rangle + \sqrt{6}\left|3\right\rangle \\
&x\left|2\right\rangle \to \sqrt{2}\left|1\right\rangle + \sqrt{3}\left|3\right\rangle, && x^2\left|2\right\rangle \to \sqrt{2}\left|0\right\rangle + 5\left|2\right\rangle + 2\sqrt{3}\left|4\right\rangle \\
&x\left|3\right\rangle \to \sqrt{3}\left|2\right\rangle + \sqrt{4}\left|4\right\rangle, && x^2\left|3\right\rangle \to \sqrt{6}\left|1\right\rangle + 7\left|3\right\rangle + 2\sqrt{5}\left|5\right\rangle \\
&x\left|4\right\rangle \to \sqrt{4}\left|3\right\rangle + \sqrt{5}\left|5\right\rangle, && x^2\left|4\right\rangle \to 2\sqrt{3}\left|2\right\rangle + 9\left|4\right\rangle + \sqrt{30}\left|6\right\rangle \\
&x\left|5\right\rangle \to \sqrt{5}\left|4\right\rangle + \sqrt{6}\left|6\right\rangle, && x^2\left|5\right\rangle \to 2\sqrt{5}\left|3\right\rangle + 11\left|5\right\rangle + \sqrt{42}\left|7\right\rangle
\end{aligned}$$

### Moment

$$\begin{aligned}
&p\left|0\right\rangle \to \left|1\right\rangle, && p^2\left|0\right\rangle \to -\left|0\right\rangle + \sqrt{2}\left|2\right\rangle \\
&p\left|1\right\rangle \to -\left|0\right\rangle + \sqrt{2}\left|3\right\rangle, && p^2\left|1\right\rangle \to -3\left|1\right\rangle + \sqrt{6}\left|3\right\rangle \\
&p\left|2\right\rangle \to -\sqrt{2}\left|1\right\rangle + \sqrt{3}\left|3\right\rangle, && p^2\left|2\right\rangle \to \sqrt{2}\left|0\right\rangle - 5\left|2\right\rangle + 2\sqrt{3}\left|4\right\rangle \\
&p\left|3\right\rangle \to -\sqrt{3}\left|2\right\rangle + \sqrt{4}\left|4\right\rangle, && p^2\left|3\right\rangle \to \sqrt{6}\left|1\right\rangle - 7\left|3\right\rangle + 2\sqrt{5}\left|5\right\rangle \\
&p\left|4\right\rangle \to -\sqrt{4}\left|3\right\rangle + \sqrt{5}\left|5\right\rangle, && p^2\left|4\right\rangle \to 2\sqrt{3}\left|2\right\rangle - 9\left|4\right\rangle + \sqrt{30}\left|6\right\rangle \\
&p\left|5\right\rangle \to -\sqrt{5}\left|4\right\rangle + \sqrt{6}\left|6\right\rangle, && p^2\left|5\right\rangle \to 2\sqrt{5}\left|3\right\rangle - 11\left|5\right\rangle + \sqrt{42}\left|7\right\rangle
\end{aligned}$$