átomo de hidrogênio em um campo eletromagnético + interação spin-órbita + correção relativística

- termo de acoplamento eletromagnético mínimo

$$\vec{p} \longrightarrow \vec{p} + \frac{e\vec{A}}{c} \quad (\text{elétron}) \implies H = \frac{1}{2m}\left(\vec{p} + \frac{e\vec{A}}{c}\right)^2 - e\varphi = H(\vec{x}, \vec{p}, t)$$

eq. de Hamilton

$$\begin{cases} \dot{x}_i = \dfrac{\partial H}{\partial p_i} = \dfrac{1}{m}\left(p_i + \dfrac{e}{c}A_i\right) = v_i \implies m\dot{v}_i = \dot{p}_i + \dfrac{e}{c}\dot{A}_i \\ \dot{p}_i = -\dfrac{\partial H}{\partial x_i} = \underbrace{-\dfrac{1}{m}\left(p_k + \dfrac{e}{c}A_k\right)}_{v_k} \dfrac{e}{c}\left(\dfrac{\partial A_k}{\partial x_i}\right) + e\dfrac{\partial \varphi}{\partial x_i} \end{cases}$$

$$\dot{A}_i = \frac{\partial A_i}{\partial t} + \underbrace{\frac{dx_k}{dt}}_{v_k}\frac{\partial A_i}{\partial x_k}$$

$$m\frac{dv_i}{dt} = -v_k\frac{e}{c}\left(\frac{\partial A_k}{\partial x_i}\right) + \underbrace{e\frac{\partial \varphi}{\partial x_i} + \frac{e}{c}\frac{\partial A_i}{\partial t}} + \frac{e}{c}v_k\frac{\partial A_i}{\partial x_k}$$

$$= e\underbrace{\left(\frac{\partial \varphi}{\partial x_i} + \frac{1}{c}\frac{\partial A_i}{\partial t}\right)}_{-\vec{E}} + \frac{e}{c}v_k\underbrace{\left(\frac{\partial A_i}{\partial x_k} - \frac{\partial A_k}{\partial x_i}\right)}_{(\nabla\times A)_j} = -\left[\vec{v}\times(\nabla\times\vec{A})\right]_i$$

$$\boxed{m\frac{d\vec{v}}{dt} = -e\vec{E} - e\frac{\vec{v}}{c}\times\vec{B} = \vec{F}}$$ (força de Lorentz)

• elétron s/spin em um campo coulombiano $(V = -e/r)$: $H = \frac{p^2}{2m} + V \Longrightarrow \boxed{\left(-\frac{\hbar^2}{2m} - e\varphi\right)\psi = i\hbar\frac{\partial\psi}{\partial t}}$ $(\vec{p} = -i\hbar\nabla)$ – (Schrödinger)

• elétron s/spin em um campo eletromagnético $\left(\vec{p} \to \vec{\pi} = \vec{p} + e\frac{\vec{A}}{c}\right)$: $H = \frac{\pi^2}{2m} - e\varphi = \frac{p^2}{2m} + \frac{e}{2mc}\left(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}\right) + \frac{e^2}{2mc^2}A^2 - e\varphi$

gauge de Coulomb $\Longrightarrow \vec{p}\cdot\vec{A}\,\psi = -i\hbar\frac{\partial}{\partial x_i}(A_i\psi) = -i\hbar\underbrace{\cancel{\left(\frac{\partial A_i}{\partial x_i}\right)}^{0}}_{\nabla\cdot\vec{A} = 0 \text{ (coulomb gauge)}}\psi - i\hbar A_i\frac{\partial\psi}{\partial x_i} = \vec{A}\cdot\vec{p}\,\varphi \Longrightarrow \vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p} = 2\vec{A}\cdot\vec{p}$

campo magnético uniforme : $\vec{A} = \frac{1}{2}\vec{B}\times\vec{r} \Longrightarrow \vec{A}\cdot\vec{p} = \frac{1}{2}(\vec{B}\times\vec{r})\cdot\vec{p} = \frac{1}{2}\vec{B}\cdot\overbrace{(\vec{r}\times\vec{p})}^{\vec{L}}$

$$H = \frac{p^2}{2m} + \left(\frac{e}{2mc}\right)\vec{L}\cdot\vec{B} + \frac{e^2}{2mc^2}A^2 - e\varphi \Longrightarrow \boxed{\left[-\frac{\hbar^2}{2m}\nabla^2 - e\varphi + \frac{e}{2mc}\vec{L}\cdot\vec{B} + \frac{e^2}{2mc^2}A^2\right]\psi = i\hbar\frac{\partial\psi}{\partial t}}$$

• elétron c/ spin em um campo eletromagnético : $H = \frac{1}{2m}\Big[\vec{\sigma}\cdot\underbrace{\left(\vec{p} + \frac{e}{c}\vec{A}\right)}_{\vec{\pi}}\Big]^2 - e\varphi$

$$\boxed{\begin{aligned} \vec{\sigma}\cdot\vec{p} &= \underbrace{\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}}_{\sigma_x}p_x + \underbrace{\begin{pmatrix}0 & -i\\ +i & 0\end{pmatrix}}_{\sigma_y}p_y + \underbrace{\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}}_{\sigma_z}p_z \\ &= \begin{pmatrix}p_z & p_x - ip_y\\ p_x + ip_y & -p_z\end{pmatrix} \\ (\vec{\sigma}\cdot\vec{p})^2 &= |\vec{p}|^2 = \vec{p}\cdot\vec{p}\end{aligned}}$$

$$(\vec{\sigma}\cdot\vec{\pi})^2 = \pi^2 + i\,\vec{\sigma}\cdot(\vec{\pi}\times\vec{\pi}) = \pi^2 + \frac{e}{c}\vec{\sigma}\cdot\underbrace{(\vec{p}\times\vec{A})}_{-i\hbar(\nabla\times\vec{A})} + \frac{e}{c}\underbrace{\vec{\sigma}\cdot(\vec{A}\times\vec{p})}_{\vec{A}\cdot\cancel{(\vec{p}\times\vec{\sigma})}^{0}}$$

$$= p^2 + \frac{e}{c}\vec{L}\cdot\vec{B} + \frac{e^2}{2mc^2}A^2 + \frac{e\hbar}{c}\vec{\sigma}\cdot\vec{B}$$

$$H = \frac{p^2}{2m} + \frac{e}{2mc}\vec{L}\cdot\vec{B} + \frac{e}{2mc}\underbrace{\hbar\vec{\sigma}}_{2\vec{S}}\cdot B + \frac{e^2}{2mc^2}A^2 - e\varphi$$

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - e\varphi + \underbrace{\frac{e}{2mc}(\vec{L}+2\vec{S})\cdot\vec{B}}_{\text{termo paramagnético}} + \underbrace{\frac{e^2}{2mc^2}A^2}_{\text{termo diamagnético}}\right]\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = i\hbar\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}}_{\psi \to \text{ espinor de Pauli}}$$

- elétron c/ spin em um campo eletromagnético + interação spin-órbita + correção relativística

$$\left[\underbrace{-\frac{\hbar^2}{2m}\nabla^2 - e\varphi}_{(H_0)} + \underbrace{\left(\frac{e}{2mc}\right)^2\vec{L}\cdot\vec{S}}_{(V_{es})\text{(spin-órbita + correção relativ.)}} + \underbrace{\frac{e}{2mc}(\vec{L}+2\vec{S})\cdot\vec{B}}_{(V_m)\text{(paramagnetismo)}} + \underbrace{\frac{e^2}{2mc^2}\left|\frac{\vec{B}\times\vec{r}}{2}\right|^2}_{(V_d)\text{(diamagnetismo)}}\right]\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix} = i\hbar\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}}_{\psi}$$

$$\boxed{\begin{array}{ll} a_B = \frac{\hbar^2}{me^2} \sim 10^{-8}\,\text{cm} & 1\,\text{erg} \sim 10^{-7}\,\text{J} \\ \mu_B = \frac{e}{2mc}\hbar \sim 10^{-20}\,\text{erg/G} & \sim 10^{12}\,\text{eV} \end{array}}$$

<u>ordens de grandeza</u> : $E_0 \sim e^2/a_B \sim 10\,\text{eV}$

$$V_{es} \sim \frac{\mu_s\mu_e}{r^3} \sim \frac{\mu_B^2}{a_B^3} \sim \frac{10^{-40}}{10^{-24}} \sim 10^{-16}\,\text{erg} \sim 10^{-4}\,\text{eV} \Rightarrow \left|\frac{V_{es}}{E_0}\right| \sim 10^{-5}$$

$$V_m \sim \mu_B B \sim 10^{-20} B \sim 10^{-8} B(G)\,(\text{eV}) \Rightarrow \left|\frac{V_m}{E_0}\right| \sim 10^{-9} B(G) = 10^{-5} B(T)$$

$$V_d \sim \frac{e^2}{2mc^2}a_B^2 B^2 = \underbrace{\left(\frac{e\hbar}{2mc}\right)}_{\mu_B^2}\frac{a_B}{e^2}B^2 = \frac{\mu_B^2 B^2}{e^2/a_B} \sim \frac{V_m^2}{E_0} \Rightarrow \left|\frac{V_d}{E_0}\right| \sim 10^{-10}B^2(T)$$

$$\Rightarrow \begin{cases} \underline{B << 1\,T} \\ |V_{es}| >> |V_m| >> |V_d| \\ \\ B \sim 10\,T \\ |V_m| > V_{es} >> |V_d| \end{cases}$$