IX - SPIN DO ELÉTRON

Várias evidências de que o momento angular do e^- não era apenas orbital.

- Linhas espectrais não eram exatamente degeneradas, independentes de ℓ e m.
- Efeito Zeeman anômalo:

Tomando o átomo de H num campo $\mathbb{B} = B_0\hat{z}$; $\mathbb{A} = \frac{B_0}{2}(-y, x, 0)$

$$H = \frac{1}{2m_e}\left[\left(p_x + \frac{eB_0 y}{2}\right)^2 + \left(p_y - \frac{eB_0 x}{2}\right)^2 + p_z^2\right] + \frac{V_0}{r}$$ com B_0 pequeno,

$$H = H_0 + \frac{1}{2m_e}\left[eB_0(yp_x - xp_y)\right]$$

$$= H_0 - \frac{eB_0}{2m_e}L_z$$

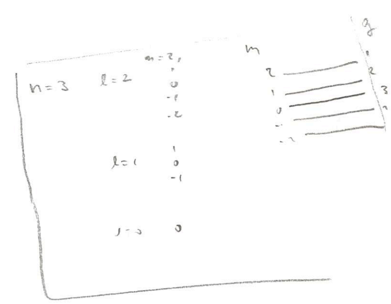
Definindo o momento magnético

$$\vec{M} = \frac{\mu_B}{\hbar}\vec{L} \quad ; \quad \mu_B = \frac{e\hbar}{2m_e} = \text{magneton de Bohr}$$

$$\boxed{\Delta H = -\vec{B}\cdot\vec{M}} \quad \text{ou} \quad \Delta H = -\frac{B_0\mu_B L_z}{\hbar}$$

Usando o C.C.O.C. H, L^2, L_z

$$E_{n,m} = -\frac{E_I}{n^2} - B_0\mu_B m$$



$n=2$, $\ell = 1, 0$

NÃO pert.   perturbados

Assim o nível $\underline{\ell=1} \longrightarrow \underset{(\text{impar})}{(2\ell+1)}$ sub-níveis $\equiv$ $m=-1$, $m=0$, $m=1$

Ocorria no entanto que o nível $\ell \longrightarrow$ nº PAR de subníveis. Esse efeito Zeeman "anômalo" ocorria com átomo de Z impar.

SPIN aparece naturalmente na teoria relativística. Aqui será introduzido como feito por PAULI.

Uhlenbeck e Goudsmit (1925): elétron tem momento angular intrínseco e mom. mag. intr. Evidências apontam para valores $\pm\hbar/2$ de S_z. O momento magnético associado ao spin é

fator giromagnético

$$\vec{M}_s = \frac{2\mu_B}{\hbar}\vec{S} \Rightarrow \text{produz } \Delta H' = -\vec{B}\cdot M_s = -\frac{2\mu_B}{\hbar}\cdot S_z = -\mu_B\sigma$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Espaço p/ descrever 1 elétron $= \mathcal{E}_r \otimes \mathcal{E}_s$

Operadores em $\mathcal{E}_r$ são os mesmos: $X, Y, Z, P_x, P_y, P_z, L_z, L^2$ etc

Operadores em $\mathcal{E}_s$ são $S^2, S_x, S_y, S_y, S_\pm$ etc, onde $\vec{S}$ é um op. de momento angular.

$$[S_x, S_y] = i\hbar S_z$$

Base em $\mathcal{E}_s$ $\quad |s,m\rangle$

$$S^2|s,m\rangle = \hbar^2 s(s+1)|s,m\rangle$$
$$S_z|s,m\rangle = m\hbar|s,m\rangle$$

s é inteiro ou semi-inteiro

$m: -s \longrightarrow +s$

Uma partícula tem sempre s fixo $\Rightarrow$ $\mathcal{E}_s$ é finito com $(2s+1)$ estados.

Para o elétron $s = 1/2$.

PROPRIEDADES DOS OPERADORES DO SPIN DO ELÉTRON

(REVISÃO)

$s = 1/2 \qquad s(s+1) = \frac{1}{2}\cdot\frac{3}{2} = 3/4$

$m = 1/2$ ou $-1/2 \rightarrow |+\rangle \quad |-\rangle$

$S^2|+\rangle = \frac{3\hbar^2}{4}|+\rangle \qquad (S^2) = \frac{3\hbar^2}{4}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$

$S^2|-\rangle = \frac{3\hbar^2}{4}|-\rangle \qquad (S_3) = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

$(\vec{S}) = \frac{\hbar}{2}\vec{\sigma} \qquad \sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \qquad \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$

$\sigma_+^2 = \sigma_-^2 = 0$

$$\begin{cases}\sigma_i^2 = 1\\ \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}\\ \sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k\end{cases}$$

$S_\pm = S_x \pm i S_y$

$S_+|+\rangle = 0 \qquad S_+|-\rangle = \hbar|+\rangle$

$S_-|-\rangle = 0 \qquad S_-|+\rangle = \hbar|-\rangle$

$$\boxed{\begin{array}{l} J_+|jm\rangle = \hbar\sqrt{j(j+1)-m(m+1)}\,|j,m+1\rangle \\ J_-|jm\rangle = \hbar\sqrt{j(j+1)-m(m-1)}\,|j,m-1\rangle \\ J_+|jj\rangle = 0 \ ; \quad J_-|j,-j\rangle = 0 \end{array}}$$

$(\sigma\cdot A)(\sigma\cdot B) = A\cdot B + i\sigma\cdot(A\times B)$ $\quad \begin{cases} A, B \text{ dois vetores ou} \\ A, B \text{ operadores vetoriais}\end{cases}$

Descrição NÃO-relativística de 1 partícula com spin 1/2

- OBSERVÁVEIS e ESPAÇO DE ESTADOS

C.C.O.C $\qquad X, Y, Z, S^2, S_3 \qquad$ etc

$\qquad\qquad P_x, P_y, P_z, S^2, S_3$

ESTADOS $\qquad |r, \varepsilon\rangle = |x, y, z, \varepsilon\rangle = |r\rangle \otimes |\varepsilon\rangle \qquad \varepsilon = +$ ou $-$

$X|r,\varepsilon\rangle = x|r,\varepsilon\rangle$

$S_3|r,\varepsilon\rangle = \frac{\hbar}{2}\varepsilon|r,\varepsilon\rangle$

$S^2|r,\varepsilon\rangle = \frac{3\hbar^2}{4}|r,\varepsilon\rangle$

ORTOGON. e COMPLETEZA

$$\langle \mathbf{r}', \varepsilon' | \mathbf{r}, \varepsilon \rangle = \delta(\mathbf{r}-\mathbf{r}')\, \delta_{\varepsilon\varepsilon'}$$

$$\sum_{\varepsilon} \int |\mathbf{r}, \varepsilon\rangle\langle \mathbf{r}, \varepsilon|\, d^3\mathbf{r} = 1$$

Um estado $|\psi\rangle$ qualquer nessa base $|\mathbf{r}, \varepsilon\rangle$ fica:

$$|\psi\rangle = \sum_{\varepsilon} \int d^3\mathbf{r}\, \langle \mathbf{r}, \varepsilon | \psi\rangle\, |\mathbf{r}, \varepsilon\rangle = \int \left[\psi_+(\mathbf{r})\, |\mathbf{r}+\rangle + \psi_-(\mathbf{r})\, |\mathbf{r}-\rangle\right] d^3 r$$

$$\langle \mathbf{r}, \varepsilon | \psi\rangle \equiv \psi_{\varepsilon}(\mathbf{r}) \longrightarrow \begin{cases} \langle \mathbf{r}, + | \psi\rangle = \psi_+(\mathbf{r}) \\ \langle \mathbf{r}, - | \psi\rangle = \psi_-(\mathbf{r}) \end{cases}$$

SPINOR $\quad [\psi](\mathbf{r}) = \begin{pmatrix} \psi_+(\mathbf{r}) \\ \psi_-(\mathbf{r}) \end{pmatrix}$

$$\langle \psi | = \sum_{\varepsilon} \int d^3\mathbf{r}\, \langle \psi | \mathbf{r}, \varepsilon\rangle\, \langle \mathbf{r}, \varepsilon |$$

$$[\psi]^{\dagger}(\mathbf{r}) = \left(\psi_+^*(\mathbf{r}) \quad \psi_-^*(\mathbf{r})\right)$$

$$\langle \psi | \varphi\rangle = \sum_{\varepsilon} \int d^3\mathbf{r}\, \langle \psi | \mathbf{r}, \varepsilon\rangle\langle \mathbf{r}, \varepsilon | \varphi\rangle$$

$$= \int d^3\mathbf{r} \left[\psi_+^*(\mathbf{r})\, \varphi_+(\mathbf{r}) + \psi_-^*(\mathbf{r})\, \varphi_-(\mathbf{r})\right]$$

$$= \int d^3\mathbf{r}\, [\psi]^{\dagger} [\varphi]$$

Se $|\Psi\rangle = |\varphi\rangle \otimes |\chi\rangle$

onde $|\chi\rangle = c_+ |+\rangle + c_- |-\rangle$; $|\Psi\rangle = c_+ |\varphi\rangle \otimes |+\rangle + c_- |\varphi\rangle \otimes |-\rangle$

$$[\Psi](\mathbf{r}) = \begin{pmatrix} c_+ \varphi(\mathbf{r}) \\ c_- \varphi(\mathbf{r}) \end{pmatrix} = \varphi(\mathbf{r}) \begin{pmatrix} c_+ \\ c_- \end{pmatrix}$$

OPERADORES → representados por matrizes 2×2 no espaço de spinores

Exemplos

(A)

$$|\Psi'\rangle = S_+ |\Psi\rangle \quad ; \quad [\Psi](\mathbf{r}) = \begin{bmatrix} \Psi^+ \\ \Psi^- \end{bmatrix}$$

$$= S_+ \left[\sum_{\varepsilon} \int d^3\mathbf{r} \, \langle \mathbf{r}, \varepsilon | \Psi \rangle \, |\mathbf{r}, \varepsilon\rangle \right]$$

$$= \hbar \int d^3\mathbf{r} \, \langle \mathbf{r}, - | \Psi \rangle \, |\mathbf{r}, +\rangle \equiv \hbar \int d^3\mathbf{r} \, \Psi_-(\mathbf{r}) \, |\mathbf{r}, +\rangle$$

$$\Rightarrow [\Psi'](\mathbf{r}) = \begin{pmatrix} \hbar \Psi_-(\mathbf{r}) \\ 0 \end{pmatrix}$$

$$(S_+) = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

(B)

$$|\Psi'\rangle = X |\Psi\rangle$$

$$= \sum_{\varepsilon} \int d^3\mathbf{r} \, x \, \langle \mathbf{r}, \varepsilon | \Psi \rangle \, |\mathbf{r}, \varepsilon\rangle$$

$$[\Psi'](\mathbf{r}) = \begin{pmatrix} x \Psi^+(\mathbf{r}) \\ x \Psi^-(\mathbf{r}) \end{pmatrix} \Rightarrow X = \begin{pmatrix} x & 0 \\ 0 & x \end{pmatrix}$$

(c)

$$|\psi'\rangle = L_z S_z |\psi\rangle$$

$$= \sum_{\varepsilon} \int d^3r \; \langle \mathbf{r}, \varepsilon | L_z S_z | \psi \rangle \, |\mathbf{r}, \varepsilon\rangle$$

$$\langle \mathbf{r}, \varepsilon | L_z S_z | \psi\rangle = -i\hbar \frac{\partial}{\partial\varphi} \langle \mathbf{r}, \varepsilon | S_z | \psi\rangle$$

$$= -i\hbar \frac{\partial}{\partial\varphi} \left[\varepsilon \frac{\hbar}{2} \langle \mathbf{r}, \varepsilon | \psi\rangle \right]$$

$$= \left(\frac{\hbar}{2}\varepsilon\right) -i\hbar \frac{\partial}{\partial\varphi} \left[\langle \mathbf{r}, \varepsilon | \psi\rangle \right]$$

$$\Rightarrow \quad \psi'_+(\mathbf{r}) = \left(\frac{\hbar}{2}\right) -i\hbar\frac{\partial}{\partial\varphi} \langle \mathbf{r}, + | \psi\rangle = \frac{\hbar}{2} \cdot \left(-i\hbar \frac{\partial \psi^+}{\partial\varphi}\right)$$

$$\psi'_-(\mathbf{r}) = \left(-\frac{\hbar}{2}\right) -i\hbar\frac{\partial}{\partial\varphi} \langle \mathbf{r} - | \psi\rangle = -\frac{\hbar}{2} \left(-i\hbar \frac{\partial \psi^-}{\partial\varphi}\right)$$

$$\Rightarrow \quad [\psi'](\mathbf{r}) = \frac{\hbar}{2} \begin{pmatrix} -i\hbar\frac{\partial}{\partial\varphi} & 0 \\ 0 & i\hbar\frac{\partial}{\partial\varphi} \end{pmatrix} [\psi](\mathbf{r})$$

Dado $\quad |\psi\rangle = \int \left[\psi_+(\mathbf{r}) \, |\mathbf{r}+\rangle + \psi_-(\mathbf{r}) \, |\mathbf{r}-\rangle \right] d^3r$

$$\mathcal{P}(+) = \int |\langle \mathbf{r}+|\psi\rangle|^2 \, d^3r = \int |\psi_+(\mathbf{r})|^2 \, d^3r$$

$$\mathcal{P}(-) = \int |\langle \mathbf{r}-|\psi\rangle|^2 \, d^3r = \int |\psi_-(\mathbf{r})|^2 \, d^3r$$

$$\mathcal{P}(\mathbf{r} \to \mathbf{r}+d\mathbf{r}) = \sum_{\varepsilon} |\langle \mathbf{r}\varepsilon|\psi\rangle|^2 \, d^3r = \left[|\psi_+|^2 + |\psi_-|^2 \right] d^3r$$

$\psi_{\pm}(\mathbf{r})$ = amplit. prob. de encontrar a partícula entre $\mathbf{r}$ e $\mathbf{r}+d^3r$ com spin $\pm$

Exemplo : Stern - Gerlach.

$$H = \frac{p^2}{2\mu} - \vec{B} \cdot \vec{M} \quad ; \quad \vec{B} = (B_0 z)\hat{z}$$

$$\vec{M} = \frac{2\mu_0}{\hbar}\vec{S} \; ; \; \mu_0 = \frac{e\hbar}{2m_e}$$

$$= \frac{p^2}{2\mu} - \frac{2B_0\mu_0}{\hbar} z S_z$$

$$= \begin{pmatrix} -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} - B_0\mu_0 z & 0 \\ 0 & -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial z^2} + B_0\mu_0 z \end{pmatrix}$$

$$\langle z | \Psi(0) \rangle = \langle z | \varphi_0 \rangle \otimes \frac{1}{\sqrt{2}}\left[|+\rangle + |-\rangle \right]$$

$$= \frac{1}{\sqrt{2}}\left[\varphi_0(z)|+\rangle + \varphi_0(z)|-\rangle \right] = \frac{1}{\sqrt{2}}\begin{bmatrix} \varphi_0(z) \\ \varphi_0(z) \end{bmatrix}$$

$\langle z | \varphi_0 \rangle$ = pacote Gaussiano

$$i\hbar \frac{d|\Psi\rangle}{dt} = H|\Psi\rangle$$

Força $= B_0\mu\hat{z}$

$$i\hbar\frac{d\Psi^+(z)}{dt} = -\frac{\hbar^2}{2\mu}\frac{\partial^2\Psi^+(t)}{\partial z^2} - B_0\mu_0 z\Psi^+(t)$$

$$i\hbar\frac{d\Psi^-(t)}{dt} = -\frac{\hbar^2}{2\mu}\frac{\partial^2\Psi^-}{\partial z^2} + B\mu_0 z\Psi^-(t)$$

Força $= -B_0\mu\hat{z}$