

Mecànica Quàntica: Formulari

H Pauli: $\hbar = \frac{h}{2\pi} = 1.0546 \cdot 10^{-34} \text{ J}\cdot\text{s}$ $\mu_B = \frac{e\hbar}{m_e} = 9,274 \cdot 10^{-24} \text{ J/T}$ $\vec{\mu} = -g \frac{\mu_B}{\hbar} \vec{S}$ $g \approx 2$ $\vec{S} = \frac{\hbar}{2} \vec{\sigma}$

$$H = -\vec{\mu} \cdot \vec{B} = g \frac{\mu_B}{2} \vec{\sigma} \cdot \vec{B}$$

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

$$[\sigma_i, \sigma_j] = 2i \epsilon_{ijk} \sigma_k$$

$$\sigma_i \sigma_j + \sigma_j \sigma_i = 2 \delta_{ij} I$$

$$|S_x+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |S_x-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad |S_y+\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} \quad |S_y-\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \quad |S_z+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad |S_z-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

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

Operators:

$$[A, B] = AB - BA \quad [A, BC] = [A, B]C + B[A, C] \quad \text{si } [[A, B], B] = 0 \Rightarrow [A, f(B)] = [A, B] \cdot f'(B)$$

$$\langle \alpha v_1 | \beta v_2 \rangle = \alpha^* \beta \langle v_1 | v_2 \rangle \quad \langle e_i | A | e_j \rangle = \alpha_{ij} \Rightarrow \langle e_i | A^\dagger | e_j \rangle = \alpha_{ji}^*$$

VAP: $A \Rightarrow \det(A - \lambda I) = 0 \Rightarrow \{\lambda_i\} \Rightarrow \text{VEP: } A |v_i\rangle = \lambda_i |v_i\rangle$; si $A = A^\dagger \Rightarrow \lambda_i \in \mathbb{R}$

Π projector $\Leftrightarrow \Pi = \Pi^\dagger$ i $\Pi^2 = \Pi$, $\lambda_i = \{0, 1\}$ U unitari $\Leftrightarrow UU^\dagger = I \Rightarrow \lambda_i = e^{i\phi_i}$ $U = e^{iA}$ (si $A = A^\dagger$)

$$A = \sum_{i=1}^{n=\#\{\lambda_i\}} \lambda_i |\lambda_i\rangle \langle \lambda_i| = \sum_{k=1}^{m=\#\{\lambda_k \text{ diferents}\}} \lambda_k \Pi_k \quad [A, B] = 0 \Rightarrow e^{A+B} = e^A e^B \quad [A, [A, B]] = 0 \Rightarrow e^{A+B} = e^A e^B e^{-\frac{1}{2}[A, B]}$$

$$e^A = \sum e^{\lambda_i} |\lambda_i\rangle \langle \lambda_i| \quad O' = e^{iA} O e^{-iA} = e^{[A, \cdot]} O \quad e^{-i\frac{\alpha}{2} \vec{n} \cdot \vec{\sigma}} = \cos \frac{\alpha}{2} I - i (\vec{n} \cdot \vec{\sigma}) \sin \frac{\alpha}{2} \quad \vec{n} \cdot \vec{\sigma} = \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}$$

$$P_{|\psi\rangle}(A: \lambda_i) = \|\Pi_i |\psi\rangle\|^2 \quad \langle A \rangle = \sum_{\forall \lambda_i} \lambda_i P_{|\psi\rangle}(A: \lambda_i) = \bar{\lambda}$$

$$\sigma_A^2 = \sum_{\forall \lambda_i} (\lambda_i - \bar{\lambda})^2 P_{|\psi\rangle}(A: \lambda_i) = \langle \psi | A^2 | \psi \rangle - \langle \psi | A | \psi \rangle^2 = \|(A - \bar{\lambda} I) | \psi \rangle\|^2 \quad A \text{ ct moviment} \Leftrightarrow [A, H] + i\hbar \frac{\partial A}{\partial t} = 0$$

Ev. temporal:

$$i\hbar \frac{\partial}{\partial t} |\psi[t]\rangle = H(t) |\psi[t]\rangle \Rightarrow |\psi[t]\rangle = e^{-\frac{i}{\hbar} H t} |\psi[0]\rangle \quad |\psi[t]\rangle = T e^{-\frac{i}{\hbar} \int_0^t dt' H(t')} |\psi[0]\rangle \quad U(t) = e^{-\frac{i}{\hbar} H t}$$

$$X = \int dx x |x\rangle \langle x| \quad |\psi\rangle = \int dx \langle x | \psi \rangle |x\rangle \quad I = \int dx |x\rangle \langle x| \quad \langle p | X | \psi \rangle = i\hbar \frac{\partial \tilde{\Psi}(p)}{\partial p} \quad \langle x | P | \psi \rangle = -i\hbar \frac{\partial \psi(x)}{\partial x}$$

$$\tilde{\Psi}(p) = \int dx \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p x} \psi(x, t) \quad \psi(x) = \int dp \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} p x} \tilde{\Psi}(p, t) \quad \sigma_A \sigma_B \geq \frac{1}{2} \|\langle \psi | [A, B] | \psi \rangle\|$$

$$[X_i, X_j] = [P_i, P_j] = 0 \quad [X, P] = i\hbar I \quad [X^n, P] = i\hbar n X^{n-1} \quad [P^n, X] = -i\hbar n P^{n-1}$$

$$\frac{d}{dt} \langle x \rangle(t) = \frac{1}{m} \langle p \rangle(t) \quad \frac{d}{dt} \langle p \rangle(t) = -\langle \vec{\nabla} V \rangle(x) \quad \psi_n(x, t) = \psi_n(x) e^{-\frac{i}{\hbar} E_n t}$$

Osc. Harmònic: $H = \frac{P^2}{2m} + \frac{1}{2} m \omega^2 X^2 \quad E_n = \hbar \omega \left(n + \frac{1}{2} \right) \quad b = \sqrt{\frac{\hbar}{m\omega}} \quad \tilde{X} = \frac{X}{b} \quad \tilde{P} = \frac{b}{\hbar} P$

$$a = \frac{1}{\sqrt{2}} (\tilde{X} + i\tilde{P}) \quad a^\dagger = \frac{1}{\sqrt{2}} (\tilde{X} - i\tilde{P}) \quad X = \frac{b}{\sqrt{2}} (a + a^\dagger) \quad P = \frac{-i\hbar}{\sqrt{2}b} (a - a^\dagger) \quad \psi_1(x) = \frac{\sqrt{2}}{b} x \psi_0(x)$$

$$\begin{matrix} a |n\rangle = \sqrt{n} |n-1\rangle \\ a^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \end{matrix} \quad \begin{matrix} N = a^\dagger a \\ N |n\rangle = n |n\rangle \end{matrix} \quad [a, a^\dagger] = I \quad \psi_0(x) = \frac{1}{(\pi b^2)^{1/4}} e^{-\frac{1}{2} \left(\frac{x}{b}\right)^2} \quad \psi_n(x) = \frac{1}{\sqrt{2^n n!}} H_n \left(\frac{x}{b}\right) \psi_0(x)$$

Imatges: $O(t)$ Operator unitari

$$H_{est}'(t) = i\hbar \frac{\partial O(t)}{\partial t} O^\dagger(t) + O(t) H(t) O^\dagger(t) \rightarrow i\hbar \frac{\partial}{\partial t} |\psi'(t)\rangle = H_{est} |\psi'(t)\rangle$$

$$H_{op}(t) = -i\hbar \frac{dO(t)}{dt} O^\dagger(t) \rightarrow i\hbar \frac{d}{dt} A'(t) = [A'(t), H_{op}(t)]$$

Heisenberg: $H_{est} = 0 \quad H_{op} = U^\dagger(t) H(t) U(t)$ Dirac: $H = H_0 + H_1 \quad \begin{matrix} H_{est} = U_0^\dagger(t) H_1 U_0(t) \\ H_{op} = U_0^\dagger(t) H_0 U_0(t) \end{matrix}$

Schrödinger: $O(t) = I$

Simetries: $|\psi(t)\rangle$ solució Eq.Sch. $O_s(t)$ simetria $\Leftrightarrow |\psi'(t)\rangle = O_s(t)|\psi(t)\rangle$ solució Eq.Sch.

$O_s(t)$ invertible, conserva P.E $O_s(t) = e^{iSA(t)}$

Tr. Espacial: $O_a(t) = e^{\frac{-i}{\hbar} \vec{a} \cdot \vec{p}} \rightarrow O_a(t) |\vec{x}\rangle = |\vec{x} + \vec{a}\rangle$

Rotació: $\vec{L} = \vec{X} \times \vec{P} \quad O(t) = e^{\frac{-i}{\hbar} \gamma \hat{n} \cdot \vec{L}} \rightarrow O_\gamma(t) |\vec{x}\rangle = |R(\gamma, \hat{n}) \vec{x}\rangle$

$$\begin{cases} [L_i, L_j] = i\hbar \epsilon_{ijk} L_k \\ [L_i, X_j] = i\hbar \epsilon_{ijk} X_k \\ [L_i, P_j] = i\hbar \epsilon_{ijk} P_k \end{cases} \quad [L_i, L^2] = 0$$

$L, S \rightarrow J : [J_i, J_j] = i\hbar \epsilon_{ijk} J_k \quad [J_i, J^2] = 0 \quad J^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle \quad J_z |j, m\rangle = \hbar m |j, m\rangle \quad m = \{-j, \dots, j\}$

$J_\pm = J_1 \pm iJ_2 \quad J_+^+ = J_- \quad J_- J_+ = J^2 - J_3^2 - \hbar J_3 \quad J_+ J_- = J^2 - J_3^2 + \hbar J_3$

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

Rep. Posicions: $\vec{L} = \vec{X} \times \vec{P} = -i\hbar \vec{x} \times \vec{\nabla}$

$L_x = i\hbar \left(\sin \varphi \partial_\theta + \frac{\cos \varphi}{\tan \theta} \partial_\varphi \right) \quad L_y = i\hbar \left(-\cos \varphi \partial_\theta + \frac{\sin \varphi}{\tan \theta} \partial_\varphi \right) \quad L_z = -i\hbar \partial_\varphi$

$$\begin{cases} L_z \phi(\varphi) = \hbar m \phi(\varphi) \\ \phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \end{cases}$$

$L^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \partial_\theta (\sin \theta \partial_\theta) + \frac{1}{\sin^2 \theta} \partial_\varphi^2 \right] \quad L^2 Y_{l,m}(\theta, \varphi) = \hbar^2 l(l+1) Y_{l,m}(\theta, \varphi) \quad \text{P.164 Schaum}$

$\vec{J} = \vec{L} + \vec{S} : \langle J^2 \rangle = \langle L^2 \rangle + \langle S^2 \rangle + 2 \langle \vec{L} \cdot \vec{S} \rangle \quad \vec{L} \cdot \vec{S} = L_z S_z + \frac{1}{2} (L_+ S_- + L_- S_+)$

$|\vec{x}\rangle \otimes |j, m\rangle = |\vec{x}, m\rangle \quad \Psi_m(\vec{x}) = \langle \vec{x}, m | \Psi \rangle \quad |\Psi'\rangle = U(R) |\Psi\rangle \quad \Psi_m'(x) = D_{m,m'}(R(\gamma, \hat{n})) \Psi_m'(R^{-1} \vec{x})$

$D_{m,m'}(R(\gamma, \hat{n})) = e^{\frac{-i}{\hbar} \gamma \hat{n} \cdot S_{m,m'}} \quad S_{m,m'} = \langle j, m | \vec{S} | j, m' \rangle$

Euler: $R(\varphi, \hat{n}) = R(\alpha, \hat{k}) R(\beta, \hat{j}) R(\gamma, \hat{k}) \Rightarrow D_{m,m'}^{(j)} = \langle j, m | U(R) | j, m' \rangle = e^{-i(\alpha m + \gamma m')} d_{m,m'}^{(j)}(\beta)$

Clebsch-Gordan: $|j_1, m_1\rangle \otimes |j_2, m_2\rangle \rightarrow |j_1, j_2; j, m\rangle \quad j = \{|j_1 - j_2, \dots, j_1 + j_2\} \quad m = \{-j, \dots, j\}$
 $|j_1, j_2; j, m\rangle = \sum_{m_1, m_2} (\langle j_1, m_1 | \otimes \langle j_2, m_2 |) | j_1, j_2; j, m \rangle (| j_1, m_1 \rangle \otimes | j_2, m_2 \rangle)$

Pertorbacions: $H = H_0 + \lambda H_1 \quad \langle \Phi_n(\lambda) | \Phi_n^{(i)} \rangle = 0 \quad \forall i > 0$

$H_0 | \Phi_n^{(0)} \rangle = E_n^{(0)} | \Phi_n^{(0)} \rangle \quad | \Phi_n \rangle = | \Phi_n^{(0)} \rangle + \lambda | \Phi_n^{(1)} \rangle + \dots$

No degenerat: $E_n^{(1)} = \langle \Phi_n^{(0)} | H_1 | \Phi_n^{(0)} \rangle \quad E_n^{(2)} = \langle \Phi_n^{(0)} | H_1 | \Phi_n^{(1)} \rangle = \sum_{m \neq n} \frac{\langle \Phi_n^{(0)} | H_1 | \Phi_m^{(0)} \rangle \cdot \langle \Phi_m^{(0)} | H_1 | \Phi_n^{(0)} \rangle}{E_n^{(0)} - E_m^{(0)}}$

Degenerat: $E_n^{(0)}, | \Psi_{n,r}^{(0)} \rangle \quad | \Psi_n(\lambda) \rangle = \alpha_r | \Psi_{n,r}^{(0)}(\lambda) \rangle + \lambda | \Psi_n^{(1)}(\lambda) \rangle + \dots$

$H_{r,r'} = \langle \Psi_{n,r}^{(0)} | H_1 | \Psi_{n,r'}^{(0)} \rangle \Rightarrow (H_{r,r'} - E_n^{(1)} \delta_{r,r'}) \alpha_r = 0 \Rightarrow E_n^{(1)} \text{ VAP. Si } \# E_n^{(1)} = r \text{ Trenquem degeneració}$

Mètode variacional: $H | \Phi_n \rangle = E_n | \Phi_n \rangle \quad \langle H \rangle$ estacionari vora $| \Phi(a) \rangle$ de prova

$$\langle H \rangle = \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} \quad \frac{\partial \langle H \rangle}{\partial a} = 0 \rightarrow \begin{cases} \langle H \rangle \\ \Phi(a) \end{cases}$$

Cas: $H = H_0 + \lambda V(t) \quad | \Psi(0) \rangle = | \Psi_i(0) \rangle \quad | \Psi(t) \rangle = \sum_n \gamma_n(t) | \Psi(t) \rangle \Rightarrow \gamma_k^{(0)} = \delta_{ki}$

$i\hbar \dot{\vec{\gamma}}(t) = \lambda \tilde{V}(t) \vec{\gamma}(t)$

$\tilde{V}(t) = \tilde{V}_{m,n}(t) = \langle \Psi_m(t) | V(t) | \Psi_n(t) \rangle \quad \vec{\gamma}(t) = T e^{\frac{-i}{\hbar} \lambda \int_0^t \tilde{V}(t') dt'} \vec{\gamma}(0)$

$\gamma_k^{(1)}(t) = \frac{1}{i\hbar} \int_0^t dt' \tilde{V}_{ki}(t')$ $\tilde{V}_{ki}(t) = \langle \Psi_k(t) | V(t) | \Psi_i(t) \rangle = e^{\frac{i\hbar}{\hbar} (E_k - E_i) t} \langle \Psi_k(0) | V(t) | \Psi_i(0) \rangle = e^{\frac{i\hbar}{\hbar} (E_k - E_i) t} \tilde{V}_{ki}(t)$

$P_{|\Psi\rangle}(H : E_f) = \| \langle \Psi_f(t) | \Psi(t) \rangle \|^2 = \lambda^2 \left\| \frac{1}{i\hbar} \int_0^t \tilde{V}_{fi}(t') e^{\frac{-i\hbar}{\hbar} (E_i - E_f) t'} \right\|^2$

Integrals útils: $\Gamma(1/2) = \sqrt{\pi}; \quad \Gamma(3/2) = \frac{\sqrt{\pi}}{2} \quad \int_0^\infty x^m e^{-ax^2} dx = \frac{\Gamma((m+1)/2)}{2a^{m/2}} \quad \int_0^\infty x^n e^{-ax} dx = \frac{\Gamma(n+1)}{a^{n+1}}$