

Formulário de Mecânica Quântica

- **Poço de potencial infinito**

$V = 0$ para $0 < x < a$ e $V = \infty$ para $x < 0$ e $x > a$. As funções próprias do operador Hamiltoniano H (i.e. da energia) são:

$$u_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad , \quad E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2 .$$

- **Poço de potencial infinito simétrico**

$V = 0$ para $-a/2 < x < a/2$ e $V = \infty$ para $x < -a/2$ e $x > a/2$. As funções próprias do operador Hamiltoniano H (i.e. da energia) são ($n = 1, 2, 3, \dots$):

$$\begin{aligned} u_n^-(x) &= \sqrt{\frac{2}{a}} \sin\left(\frac{2n\pi}{a}x\right) & E_n^- &= E_0 (2n)^2 \\ u_n^+(x) &= \sqrt{\frac{2}{a}} \cos\left[(2n-1)\frac{\pi}{a}x\right] & E_n^+ &= E_0 (2n-1)^2 \end{aligned} \quad E_0 = \frac{\pi^2 \hbar^2}{2ma^2} .$$

- **Primitivas para os problemas do poço infinito**

$$\int dy \sin^2(y) = \frac{1}{2}y - \frac{1}{4}\sin(2y)$$

$$\int dy \sin(ny) \sin(my) = \frac{1}{2(m-n)} \sin[y(m-n)] - \frac{1}{2(m+n)} \sin[y(m+n)] \quad ; \quad m \neq n$$

$$\int dy y \sin^2(ny) = \frac{y^2}{4} - \frac{\sin(2ny)y}{4n} - \frac{\cos(2ny)}{8n^2}$$

$$\int dy y \sin(ny) \sin(my) = \frac{1}{2} \left(\frac{\cos((m-n)y)}{(m-n)^2} - \frac{\cos((m+n)y)}{(m+n)^2} + \frac{y \sin((m-n)y)}{m-n} - \frac{y \sin((m+n)y)}{m+n} \right) \quad ; \quad m \neq n$$

- **Oscilador harmónico: Polinómios de Hermite**

As funções próprias são

$$u_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(y) e^{-y^2/2}$$

onde $y = \sqrt{\frac{m\omega}{\hbar}}x$ e os primeiros polinómios de Hermite, $H_n(y)$, são:

$$\begin{aligned} H_0 &= 1 & H_1 &= 2y \\ H_2 &= 4y^2 - 2 & H_3 &= 8y^3 - 12y \\ H_4 &= 16y^4 - 48y^2 + 12 & H_5 &= 32y^5 - 160y^3 + 120y \end{aligned}$$

As energias são dadas por

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega \quad n = 0, 1, 2, 3, \dots$$

- **Oscilador harmónico: Operadores A e A^+**

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 = \hbar\omega \left(A^+ A + \frac{1}{2} \right)$$

onde

$$A = \sqrt{\frac{m\omega}{2\hbar}}x + i\frac{p}{\sqrt{2m\omega\hbar}}, \quad A^+ = \sqrt{\frac{m\omega}{2\hbar}}x - i\frac{p}{\sqrt{2m\omega\hbar}}$$

com

$$[A, A^+] = 1$$

As relações inversas são

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

Os estados correctamente normalizados são

$$|n\rangle = \frac{1}{\sqrt{n!}} (A^+)^n |0\rangle$$

com $A|0\rangle = 0$ e

$$A|n\rangle = \sqrt{n}|n-1\rangle, \quad A^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

• **Momento Angular e Harmônicas Esféricas**

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k, \quad L_{\pm} = L_x \pm iL_y, \quad [L_+, L_-] = 2\hbar L_z, \quad [L_z, L_{\pm}] = \pm\hbar L_{\pm}$$

$$L^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle, \quad L_z |l, m\rangle = \hbar m |l, m\rangle, \quad L_{\pm} |l, m\rangle = \hbar \sqrt{l(l+1) - m(m \pm 1)} |l, m \pm 1\rangle$$

As primeiras harmônicas esféricas são:

$$Y_{00} = \frac{1}{\sqrt{4\pi}} \qquad Y_{11} = -\sqrt{\frac{3}{8\pi}} e^{i\varphi} \sin \theta$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta \qquad Y_{22} = \sqrt{\frac{15}{32\pi}} e^{i2\varphi} \sin^2 \theta$$

$$Y_{21} = -\sqrt{\frac{15}{8\pi}} e^{i\varphi} \sin \theta \cos \theta \qquad Y_{20} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1)$$

com

$$Y_{l,-m} = (-1)^m Y_{lm}^* \quad \text{e} \quad \int d\Omega |Y_{lm}(\theta, \varphi)|^2 = 1$$

• **Equação Radial**

Para um potencial esfericamente simétrico a equação radial é

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2} (V(r) - E) \right] R(r) = 0$$

Fazendo a mudança de variável $u(r) = r R(r)$ temos

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2} (V(r) - E) \right] u(r) = 0$$

• **Átomo de Hidrogénio e Funções Radiais**

A solução geral é

$$\psi_{nlm}(r, \theta, \varphi) = R_{nl}(r) Y_{lm}(\theta, \varphi), \quad \text{com energias} \quad E_n = -\frac{1}{2} mc^2 \alpha^2 \frac{1}{n^2}, \quad \alpha^{-1} = 137.036$$

As primeiras funções radiais são

$$R_{10} = 2 \left(\frac{1}{a_0} \right)^{3/2} e^{-r/a_0} \qquad R_{20} = 2 \left(\frac{1}{2a_0} \right)^{3/2} \left(1 - \frac{r}{2a_0} \right) e^{-r/2a_0}$$

$$R_{21} = \frac{1}{\sqrt{3}} \left(\frac{1}{2a_0} \right)^{3/2} \frac{r}{a_0} e^{-r/2a_0} \qquad R_{30} = 2 \left(\frac{1}{3a_0} \right)^{3/2} \left(1 - \frac{2r}{3a_0} + \frac{2r^2}{27a_0^2} \right) e^{-r/3a_0}$$

$$R_{31} = \frac{4\sqrt{2}}{3} \left(\frac{1}{3a_0} \right)^{3/2} \frac{r}{a_0} \left(1 - \frac{r}{6a_0} \right) e^{-r/3a_0} \qquad R_{32} = \frac{2\sqrt{2}}{27\sqrt{5}} \left(\frac{1}{3a_0} \right)^{3/2} \left(\frac{r}{a_0} \right)^2 e^{-r/3a_0}$$

Os valores médios de algumas potências de r

$$\langle r^k \rangle \equiv \int_0^\infty dr r^{2+k} R_{nl}^2(r) \qquad \langle r \rangle = \frac{a_0}{2} [3n^2 - l(l+1)]$$

$$\langle r^2 \rangle = \frac{a_0^2 n^2}{2} [5n^2 + 1 - 3l(l+1)] \qquad \left\langle \frac{1}{r} \right\rangle = \frac{1}{a_0 n^2} \qquad a_0 = \frac{\hbar}{m c \alpha}$$

$$\left\langle \frac{1}{r^2} \right\rangle = \frac{2}{a_0^2 n^3 (2l+1)} \qquad \left\langle \frac{1}{r^3} \right\rangle = \frac{2}{a_0^3 n^3 l(2l+1)(l+1)}$$

• **Átomos Hidrogenóides**

Para os átomos com Z prótons e um electrão, basta fazer

$$\alpha \rightarrow Z\alpha, \quad \text{e portanto} \quad a_0 \rightarrow \frac{1}{Z} a_0, \quad E_n = -\frac{1}{2} mc^2 (Z\alpha)^2 \frac{1}{n^2}$$

• **Integrais Oscilador Harmónico e Átomo Hidrogénio**

$$\int_0^\infty x^{\alpha-1} e^{-x} dx = \Gamma(\alpha), \quad \int_0^\infty x^{2\alpha-1} e^{-x^2} dx = \frac{1}{2} \Gamma(\alpha), \quad \Gamma(\alpha+1) = \alpha \Gamma(\alpha), \quad \Gamma(1) = 1, \quad \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

- **Spin 1/2**

1. Os vectores próprios do operador $S_n = \vec{S} \cdot \vec{n}$, onde, $\vec{n} = \sin \theta \cos \varphi \vec{e}_x + \sin \theta \sin \varphi \vec{e}_y + \cos \theta \vec{e}_z$, são

$$\psi(S_n = +\hbar/2) = \begin{pmatrix} \cos \frac{\theta}{2} \\ e^{i\varphi} \sin \frac{\theta}{2} \end{pmatrix} \quad \psi(S_n = -\hbar/2) = \begin{pmatrix} \sin \frac{\theta}{2} \\ -e^{i\varphi} \cos \frac{\theta}{2} \end{pmatrix}$$

2. As matrizes de Pauli são

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

- **Adição de Momento Angular**

$$\vec{J} = \vec{J}_1 + \vec{J}_2, \quad J_i^2 |j_1, m_1\rangle = \hbar^2 j_i(j_i + 1) |j_1, m_1\rangle, \quad J^2 |j, m_j\rangle = \hbar^2 j(j + 1) |j, m_j\rangle, \quad J_z |j, m_j\rangle = \hbar m_j |j, m_j\rangle$$

1. Os valores possíveis para j são

$$j_1 + j_2, j_1 + j_2 - 1, \dots, |j_1 - j_2|$$

2. Qualquer estado $|j, m_j\rangle$ se pode exprimir como uma combinação linear dos produtos dos estados $|j_1, m_1\rangle$ e $|j_2, m_2\rangle$ na seguinte forma

$$|j, m_j\rangle = \sum_{m_1+m_2=m_j} C(j, m_j; j_1, m_1, j_2, m_2) |j_1, m_1\rangle |j_2, m_2\rangle$$

onde $C(j, m_j; j_1, m_1, j_2, m_2)$ são os coeficientes de Clebsch-Gordon e estão dados na Fig. 1 para os valores mais baixos de j_1 e j_2 .

3. A relação inversa é (os coeficientes de Clebsch-Gordon são reais)

$$|j_1, m_1\rangle |j_2, m_2\rangle = \sum_j C(j, m_j; j_1, m_1, j_2, m_2) |j, m_j\rangle$$

4. Para o átomo de Hidrogénio ($\vec{J} = \vec{L} + \vec{S}$)

$$\begin{aligned} \psi_{l+1/2, m_j} &= \sqrt{\frac{l+m_j+1/2}{2l+1}} Y_{l, m_j-1/2} \chi^+ + \sqrt{\frac{l+1/2-m_j}{2l+1}} Y_{l, m_j+1/2} \chi^- \\ \psi_{l-1/2, m_j} &= -\sqrt{\frac{l+1/2-m_j}{2l+1}} Y_{l, m_j-1/2} \chi^+ + \sqrt{\frac{l+m_j+1/2}{2l+1}} Y_{l, m_j+1/2} \chi^- \end{aligned}$$

- **Teoria de Perturbações**

No caso não degenerado, para uma perturbação com Hamiltoniano H_1 ,

$$\Delta E_n^{(1)} = \langle \phi_n | H_1 | \phi_n \rangle, \quad \Delta E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_n | H_1 | \phi_k \rangle|^2}{E_n^{(0)} - E_k^{(0)}}, \quad |\psi_n\rangle = |\phi_n\rangle + \sum_{k \neq n} \frac{\langle \phi_k | H_1 | \phi_n \rangle}{E_n^{(0)} - E_k^{(0)}} |\phi_k\rangle$$

- **Constantes Físicas**

$$\hbar = 1.05457266(63) \times 10^{-34} \text{ Js}$$

$$e = 1.60217733(49) \times 10^{-19} \text{ C}$$

$$c = 1/\sqrt{\epsilon_0 \mu_0} = 2.99792458 \times 10^8 \text{ m/s}$$

$$\mu_0 = 4\pi \times 10^{-7} \text{ H/m}$$

$$m_e = 9.1093897(54) \times 10^{-31} \text{ kg} = 0.510998918(44) \text{ MeV}$$

$$m_p = 1.6726231(10) \times 10^{-27} \text{ kg} = 938.272029(80) \text{ MeV}$$

$$m_n = 1.6749286(1) \times 10^{-27} \text{ kg} = 939.565360(81) \text{ MeV}$$

$$hc = 1240 \text{ nm.eV}, \quad \hbar c = 197.35 \text{ nm.eV}$$

$$a_0 = 0.5291772108(18) \times 10^{-10} \text{ m}$$

$$\alpha^{-1} = 137.03599911(46)$$

$$\mu_B = \frac{e\hbar}{2m_e} = 5.788 \times 10^{-5} \text{ eV/T}$$

35. CLEBSCH-GORDAN COEFFICIENTS, SPHERICAL HARMONICS, AND d FUNCTIONS

Note: A square-root sign is to be understood over every coefficient, e.g., for $-8/15$ read $-\sqrt{8/15}$.

Notation:

J	J	\dots
M	M	\dots

$Y_0^0 = \sqrt{\frac{3}{4\pi}} \cos \theta$

$Y_1^1 = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}$

$Y_2^0 = \sqrt{\frac{5}{4\pi}} \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$

$Y_2^1 = -\sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{i\phi}$

$Y_2^2 = \frac{1}{4} \sqrt{\frac{15}{2\pi}} \sin^2 \theta e^{2i\phi}$

$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$

$d_{m,0}^\ell = \sqrt{\frac{4\pi}{2\ell+1}} Y_\ell^m e^{-im\phi}$

$\langle j_1 j_2 m_1 m_2 | j_1 j_2 JM \rangle$
 $= (-1)^{J-j_1-j_2} \langle j_2 j_1 m_2 m_1 | j_2 j_1 JM \rangle$

$d_{m',m}^j = (-1)^{m-m'} d_{m,m'}^j = d_{-m,-m'}^j$

$d_{0,0}^1 = \cos \theta$

$d_{1/2,1/2}^{1/2} = \cos \frac{\theta}{2}$

$d_{1/2,-1/2}^{1/2} = -\sin \frac{\theta}{2}$

$d_{1,1}^1 = \frac{1 + \cos \theta}{2}$

$d_{1,0}^1 = -\frac{\sin \theta}{\sqrt{2}}$

$d_{1,-1}^1 = \frac{1 - \cos \theta}{2}$

$d_{3/2,3/2}^{3/2} = \frac{1 + \cos \theta}{2} \cos \frac{\theta}{2}$

$d_{3/2,1/2}^{3/2} = -\sqrt{3} \frac{1 + \cos \theta}{2} \sin \frac{\theta}{2}$

$d_{3/2,-1/2}^{3/2} = \sqrt{3} \frac{1 - \cos \theta}{2} \cos \frac{\theta}{2}$

$d_{3/2,-3/2}^{3/2} = -\frac{1 - \cos \theta}{2} \sin \frac{\theta}{2}$

$d_{1/2,1/2}^{3/2} = \frac{3 \cos \theta - 1}{2} \cos \frac{\theta}{2}$

$d_{1/2,-1/2}^{3/2} = -\frac{3 \cos \theta + 1}{2} \sin \frac{\theta}{2}$

$d_{2,2}^2 = \left(\frac{1 + \cos \theta}{2} \right)^2$

$d_{2,1}^2 = -\frac{1 + \cos \theta}{2} \sin \theta$

$d_{2,0}^2 = \frac{\sqrt{6}}{4} \sin^2 \theta$

$d_{2,-1}^2 = -\frac{1 - \cos \theta}{2} \sin \theta$

$d_{2,-2}^2 = \left(\frac{1 - \cos \theta}{2} \right)^2$

$d_{1,1}^2 = \frac{1 + \cos \theta}{2} (2 \cos \theta - 1)$

$d_{1,0}^2 = -\sqrt{\frac{3}{2}} \sin \theta \cos \theta$

$d_{1,-1}^2 = \frac{1 - \cos \theta}{2} (2 \cos \theta + 1)$

$d_{0,0}^2 = \left(\frac{3}{2} \cos^2 \theta - \frac{1}{2} \right)$

Figure 35.1: The sign convention is that of Wigner (*Group Theory*, Academic Press, New York, 1959), also used by Condon and Shortley (*The Theory of Atomic Spectra*, Cambridge Univ. Press, New York, 1953), Rose (*Elementary Theory of Angular Momentum*, Wiley, New York, 1957), and Cohen (*Tables of the Clebsch-Gordan Coefficients*, North American Rockwell Science Center, Thousand Oaks, Calif., 1974). The coefficients here have been calculated using computer programs written independently by Cohen and at LBNL.

Figure 1: Coeficientes de Clebsch-Gordan para $j_i = 1/2, 1, 3/2, 2$. Fonte: Particle Data Group web page, <http://pdg.lbl.gov/2007/reviews/clebrpp.pdf>