Formulário de Mecânica Quântica I

LEFT, 3º ano
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CONSTANTES FÍSICAS:

– Velocidade da luz no vácuo: $c = 2.9979 \times 10^8$ m/s
– Carga do eletrão: $e = 1.602 \times 10^{-19}$ C
– Constante de Planck reduzida:
$\hbar = h/(2\pi) = 1.055 \times 10^{-34}$J s
$= 6.582 \times 10^{-22}$ MeV s
– Massa do eletrão: $m_e = 9.109 \times 10^{-31}$Kg
$= 0.511\,\mathrm{MeV}/c^2$
– Massa do neutrão: $m_n = 1.675 \times 10^{-27}$Kg
$= 939.566\,\mathrm{MeV}/c^2$
– Constante de Planck: $h = 6.626 \times 10^{-34}$Js
– Aceleração da gravidade: $g = 9.8067$ m/s^2
– $\hbar c = 197.327$ Mev fm
– Constante de estrutura fina: $\alpha = 1/137.036$
– Constante de Rydberg: $\mathcal{R} = 13.606$ eV
– Massa do protão: $m_p = 1.673 \times 10^{-27}$Kg
$= 938.272\,\mathrm{MeV}/c^2$
– Constante da Gravitação:
$G = 6.674 \times 10^{-11}$ m^{3}Kg^{-1}s^{-2}

- **Eq. Schrödinger:** $i\hbar\dfrac{\partial\psi(\vec{r},t)}{\partial t} = -\dfrac{\hbar^2}{2m}\nabla^2\psi(\vec{r},t) + V\psi(\vec{r},t)$

- **Poço de potencial infinito:** $V(x) = 0\,(0 < x < a)$ e $V(x) = \infty\,(x < 0, x > a)$, com $n = 1, 2, 3, ...$

  – Funções e energias próprias: $u_n(x) = \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{n\pi}{a}x\right)$, $E_n = \dfrac{\pi^2\hbar^2 n^2}{2ma^2}$

- **Poço de potencial infinito simétrico:** $V(x) = 0\ (|x| < a/2)$ e $V(x) = \infty\ (|x| > a/2)$, com $n = 1, 2, 3, ...$

  – Funções e energias próprias ímpares: $u_n^-(x) = \sqrt{\dfrac{2}{a}}\sin\left(\dfrac{2n\pi}{a}x\right)$, $E_n^- = \dfrac{\pi^2\hbar^2(2n)^2}{2ma^2}$, $n = 1, 2, 3, ...$

  – Funções e energias próprias pares: $u_n^+(x) = \sqrt{\dfrac{2}{a}}\cos\left[\dfrac{(2n-1)\pi}{a}x\right]$, $E_n^+ = \dfrac{\pi^2\hbar^2(2n-1)^2}{2ma^2}$

- **Oscilador harmónico:** $H = \dfrac{p^2}{2m} + \dfrac{1}{2}m\omega^2 x^2$

  – Funções próprias: $u_n(x) = \left(\dfrac{m\omega}{\pi\hbar}\right)^{1/4}\dfrac{1}{\sqrt{2^n n!}}H_n(y)\,e^{-y^2/2}$, $y = \sqrt{\dfrac{m\omega}{\hbar}}x$, $n = 0, 1, 2, ...$

  onde $H_n(y)$ são os polinómios de Hermite:

  $$H_0(y) = 1\,,\ H_1(y) = 2y\,,\ H_2(y) = 4y^2 - 2\,,\ H_3(y) = 8y^3 - 12y\,,$$

  $$H_4(y) = 16y^4 - 48y^2 + 12\,,\ H_5(y) = 32y^5 - 160y^3 + 120y\,, ...$$

  . – Energias próprias: $E_n = (n + 1/2)\hbar\omega\,, n = 0, 1, 2, 3, ...$

  – Operadores $\hat{a}$ e $\hat{a}^+$: $\hat{H} = \hbar\omega(\hat{a}^+\hat{a} + 1/2)$ com $\hat{a} = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} + i\dfrac{\hat{p}}{\sqrt{2m\omega\hbar}}$, $\hat{a}^+ = \sqrt{\dfrac{m\omega}{2\hbar}}\hat{x} - i\dfrac{\hat{p}}{\sqrt{2m\omega\hbar}}$

  Invertendo: $\hat{x} = \sqrt{\dfrac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^+)$, $\hat{p} = -i\sqrt{\dfrac{\hbar m\omega}{2}}(\hat{a} - \hat{a}^+)$

  – Estados próprios: $|n\rangle = \dfrac{1}{\sqrt{n!}}(\hat{a}^+)^n|0\rangle$ com $\hat{a}|0\rangle = 0$ e $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, $\hat{a}^+|n\rangle = \sqrt{n+1}|n+1\rangle$

- **Momento angular**

  – Relações de comutação: $[L_i, L_j] = i\hbar\varepsilon_{ijk}L_k$, $[L_+, L_-] = 2\hbar L_z$, $[L_z, L_\pm] = \pm\hbar L_\pm$ com $L_\pm = L_x \pm iL_y$.

  – Estados próprios:

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

  – Harmónicas esféricas: $Y_{l,-m} = (-1)^m Y_{l,m}^*$, $\int Y_{l,m}^*(\theta,\varphi)Y_{l',m'}(\theta,\varphi)d\Omega = \delta_{ll'}\delta_{mm'}$

$$Y_{0,0}=\frac{1}{\sqrt{4\pi}}\,,\qquad Y_{1,0}=\sqrt{\frac{3}{4\pi}}\cos\theta\,,\qquad Y_{1,1}=-\sqrt{\frac{3}{8\pi}}e^{i\varphi}\sin\theta\,,$$
$$Y_{2,0}=\sqrt{\frac{5}{16\pi}}(3\cos^2\theta-1)\,,\quad Y_{2,1}=-\sqrt{\frac{15}{8\pi}}e^{i\varphi}\sin\theta\cos\theta\,,\quad Y_{2,2}=\sqrt{\frac{15}{32\pi}}e^{2i\varphi}\sin^2\theta$$

- **Equação radial para potencial central** $V(r)$**:** $\left[-\frac{\hbar^2}{2\mu}\frac{d}{dr}\left(r^2\frac{d}{dr}\right)+\frac{l(l+1)\hbar^2}{2\mu}+V(r)\right]R(r)=ER(r)$

  Definindo $u(r)=rR(r)$ tem-se $-\frac{\hbar^2}{2\mu}\frac{d^2u(r)}{dr^2}+\left[\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]u(r)=Eu(r)\quad,\quad V_{\text{eff}}=\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)$

- **Átomos Hidrogenóides:** $V(r)=-\frac{Ze^2}{4\pi\epsilon_0 r^2}$

  – Funcões próprias: $\psi_{nlm}(r,\theta,\varphi)=R_{n,l}(r)Y_{l,m}(\theta,\varphi)$

  – Energias próprias: $E_n=-\frac{m_e}{2\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\frac{1}{n^2}=Z^2\frac{E_1}{n^2}\ ,\ E_1=-13.6$ eV

  – Algumas funções radiais:

$R_{10}=2a^{-3/2}\exp(-r/a)$	$R_{30}=\frac{2}{3\sqrt{3}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$
$R_{20}=\frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$	$R_{31}=\frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$
$R_{21}=\frac{1}{2\sqrt{6}}a^{-3/2}\left(\frac{r}{a}\right)\exp(-r/2a)$	$R_{32}=\frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$

  onde $a=\frac{4\pi\epsilon_0\hbar^2}{Zm_e e^2}=a_0/Z\ ,\ a_0=0.529\times10^{-10}$ m (raio de Bohr)

  – Alguns valores esperados de potências de r:

$$\langle r^n\rangle=\int_0^\infty r^{2+n}R_{nl}^2\,dr\ \longrightarrow\ \langle r\rangle=\frac{a}{2}[3n^2-l(l+1)]\ ,\ \langle r^2\rangle=\frac{a^2n^2}{2}[5n^2+1-3l(l+1)]\,,$$

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

- **Primitivas/Integrais úteis:**

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

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

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

$$[\,a>0\text{ daqui em diante e }k\in\mathbb{R}]:\ \int x^n e^{-ax}\,dx=\frac{n!}{a^{n+1}}\quad,\quad\int_0^\infty x^{2n}e^{-ax^2}\,dx=\frac{1.3.5...(2n-1)}{2^{n+1}a^n}\sqrt{\frac{\pi}{a}}\,,$$

$$\int_0^\infty x^{2n+1}e^{-ax^2}\,dx=\frac{n!}{2a^{n+1}}\quad,\quad\int_0^\infty x^n e^{-(a+ki)\,x}dx=\frac{n!}{(a+k\,i)^{n+1}}\,,\quad\int_{-\infty}^{+\infty}e^{-ax^2}e^{-ikx}dx=\sqrt{\frac{\pi}{a}}\,e^{-k^2/(4a)}\,,$$

$$\int_{-\infty}^{+\infty}\frac{dx}{k^2+x^2}=\frac{\pi}{k}$$