Orbitais atômicos reais e complexos

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Definindo algumas constantes

$$\Gamma = \left(\frac{Z}{a_0}\right)^{\frac{3}{2}}$$

$$a_0 = \frac{\varepsilon_0 h^2}{m e^2 \pi} = 0{,}529\ \text{Å} = 0{,}529 \times 10^{-10}\ \text{m}$$

Os orbitais atômicos são o produto de três funções:

função radial × função angular em θ × função angular em ϕ

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)\Theta_{l,m_l}\Phi_{m_l}$$

$$\psi_{n,l,m_l}(r,\theta,\phi) = R_{n,l}(r)Y^{l}_{m_l}(\theta,\phi)$$

$Y^{l}_{m_l}(\theta,\phi)$ são os Harmônicos Esféricos

Orbitais atômicos reais

Número quântico magnético, $m_l = 0$

Orbitais s, $l = 0$

$$Y^{l}_{m_l}(\theta, \phi) = Y^{0}_{0} = \frac{1}{\sqrt{2\pi}}$$

Então, $$\psi_{n,0,0}\,(r, \theta, \phi) = R_{n,0}(r) Y^{0}_{0}$$

Orbitais atômicos reais – orbitais s ($l = 0; m_l = 0$)

$$\psi_{1,0,0} = \psi_{1s} = \frac{1}{\sqrt{\pi}} \Gamma \frac{1}{e^{\frac{Zr}{a_0}}}$$

$$\psi_{2,0,0} = \psi_{2s} = \frac{1}{4\sqrt{2\pi}} \Gamma \left(2 - \frac{Zr}{a_0}\right) \frac{1}{e^{\frac{Zr}{2a_0}}}$$

$$\psi_{3,0,0} = \psi_{3s} = \frac{1}{81\sqrt{3\pi}} \Gamma \left(27 - 18\frac{Zr}{a_0} + 2\left(\frac{Zr}{a_0}\right)^2\right) \frac{1}{e^{\frac{Zr}{3a_0}}}$$

Considerando o H

$Z = 1$

Então, Z será omitido nas fórmulas para os orbitais s e nas fórmulas para os outros orbitais.

Orbitais atômicos reais – orbitais s ($l = 0; m_l = 0$)

$$\psi_{1,0,0} = \psi_{1s} = \frac{1}{\sqrt{\pi}}\Gamma\frac{1}{e^{\frac{r}{a_0}}}$$

$$\psi_{2,0,0} = \psi_{2s} = \frac{1}{4\sqrt{2\pi}}\Gamma\left(2-\frac{r}{a_0}\right)\frac{1}{e^{\frac{r}{2a_0}}}$$

$$\psi_{3,0,0} = \psi_{3s} = \frac{1}{81\sqrt{3\pi}}\Gamma\left(27-18\frac{r}{a_0}+2\left(\frac{r}{a_0}\right)^2\right)\frac{1}{e^{\frac{r}{3a_0}}}$$

Orbitais atômicos reais

Número quântico magnético, $m_l = 0$

Orbitais p, $l = 1$

$$Y^l_{m_l}(\theta, \phi) = Y^1_0 = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos\theta$$

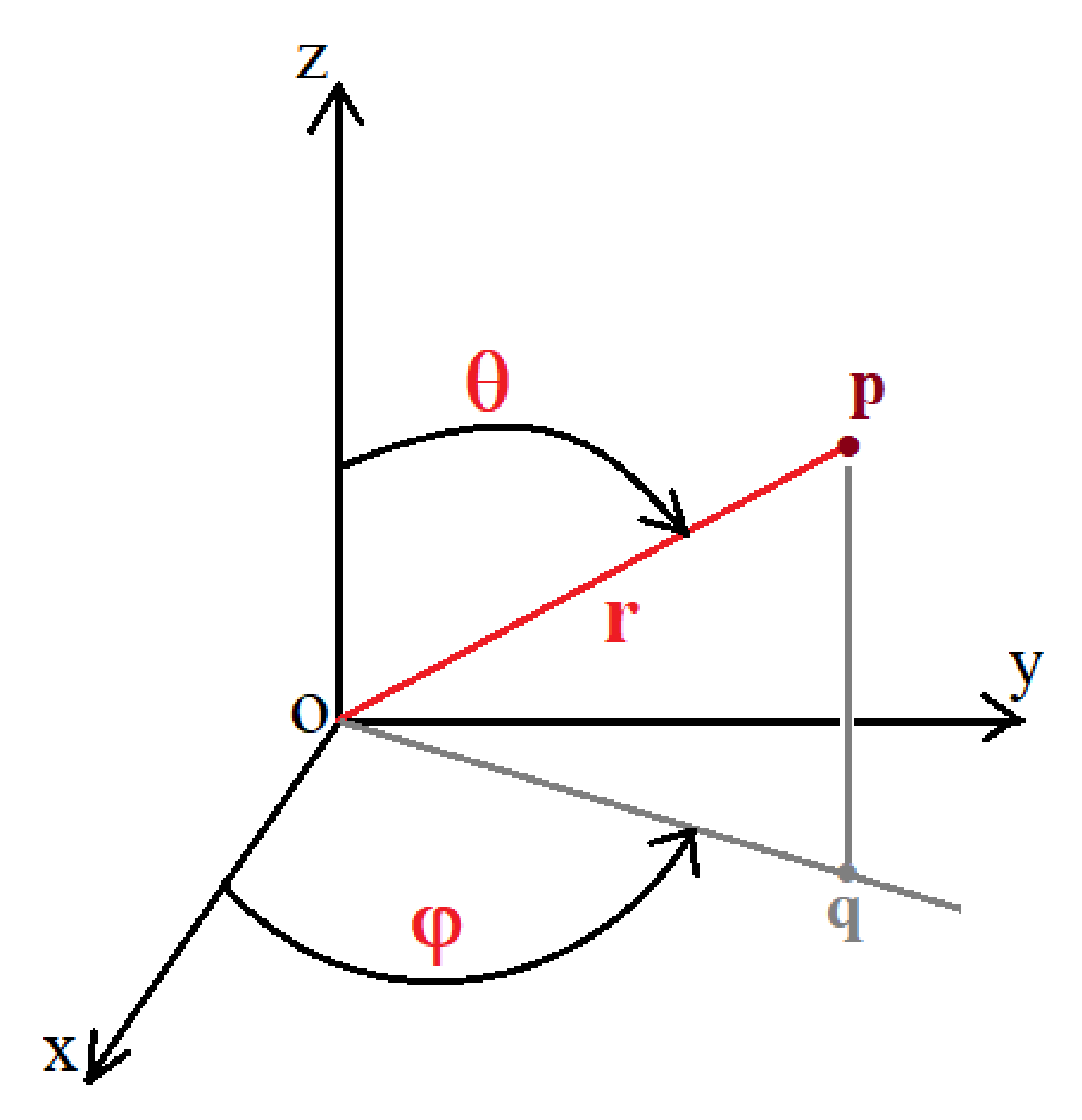
Então, $$\psi_{n,0,0}\,(r, \theta, \phi) = R_{n,0}(r)Y^1_0$$

Orbitais atômicos reais – orbitais p$_z$ $(l = 1; m_l = 0)$

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \Gamma \frac{r}{a_0} \frac{1}{e^{\frac{r}{2a_0}}} \cos\theta$$

$$\psi_{3,1,0} = \psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \Gamma \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} \frac{1}{e^{\frac{r}{3a_0}}} \cos\theta$$

Coordenadas polares



$x = r \operatorname{sen} \theta \cos \phi$

$y = r \operatorname{sen} \theta \operatorname{sen} \phi$

$z = r \cos \theta$

$0° \leq \theta \leq 180°$

$0° \leq \phi \leq 360°$

$$\cos \theta = \frac{z}{r}$$

Orbitais atômicos reais – orbitais p_z $(l = 1; m_l = 0)$

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \Gamma \frac{r}{a_0} \frac{1}{e^{\frac{r}{2a_0}}} \frac{z}{r}$$

$$\psi_{3,1,0} = \psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \Gamma \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} \frac{1}{e^{\frac{r}{3a_0}}} \frac{z}{r}$$

Orbitais atômicos reais – orbitais p_z $(l = 1; m_l = 0)$

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}}\Gamma\frac{1}{a_0}\frac{1}{e^{\frac{r}{2a_0}}}z$$

$$\psi_{3,1,0} = \psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}}\Gamma\left(6-\frac{r}{a_0}\right)\frac{1}{a_0}\frac{1}{e^{\frac{r}{3a_0}}}z$$

E por isso chamados de orbitais p_z

Orbitais atômicos imaginários ($m_l \neq 0$)

Orbitais p, $l = 1$

$$\Upsilon_{m_l}^{l}(\theta, \phi) = \Upsilon_{1}^{1} = -\sqrt{\frac{3}{8\pi}}\,\mathrm{sen}\,\theta\; e^{i\phi}$$

$$\Upsilon_{m_l}^{l}(\theta, \phi) = \Upsilon_{-1}^{1} = \sqrt{\frac{3}{8\pi}}\,\mathrm{sen}\,\theta\; e^{-i\phi}$$

Fórmulas de Euler

$$e^{i\phi} = \cos\phi + i\,\mathrm{sen}\,\phi$$

$$e^{-i\phi} = \cos\phi - i\,\mathrm{sen}\,\phi$$

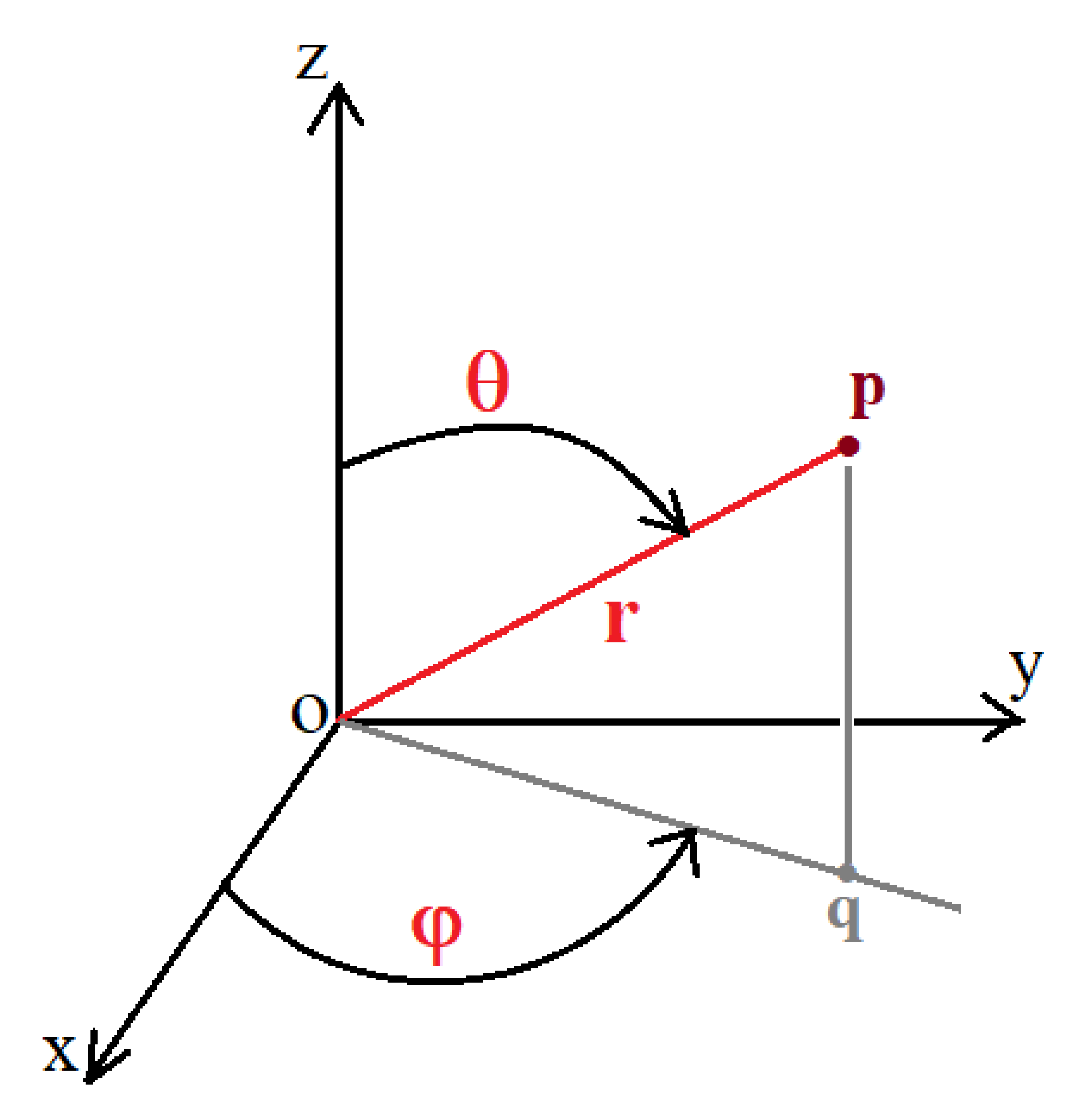
Orbitais atômicos imaginários ($m_l \neq 0$)

Orbitais p, $l = 1$

$$Y^{l}_{m_l}(\theta, \phi) = \ Y^{1}_{1} = -\sqrt{\frac{3}{8\pi}}(\operatorname{sen}\theta\cos\phi + i\operatorname{sen}\theta\operatorname{sen}\phi)$$

$$Y^{l}_{m_l}(\theta, \phi) = \ Y^{1}_{-1} = \sqrt{\frac{3}{8\pi}}(\operatorname{sen}\theta\cos\phi - i\operatorname{sen}\theta\operatorname{sen}\phi)$$

Coordenadas polares



$x = r \operatorname{sen} \theta \cos \phi$

$y = r \operatorname{sen} \theta \operatorname{sen} \phi$

$z = r \cos \theta$

$$\cos \phi = \frac{z}{r}$$

$$\operatorname{sen} \theta \cos \phi = \frac{x}{r}$$

$$\operatorname{sen} \theta \sin \phi = \frac{y}{r}$$

Orbitais atômicos imaginários ($m_l \neq 0$)

Orbitais p, $l = 1$

$$\Upsilon_{m_l}^{l}(\theta, \phi) = \Upsilon_{1}^{1} = -\sqrt{\frac{3}{8\pi}}\left(\frac{x + iy}{r}\right)$$

$$\Upsilon_{m_l}^{l}(\theta, \phi) = \Upsilon_{-1}^{1} = \sqrt{\frac{3}{8\pi}}\left(\frac{x - iy}{r}\right)$$

Os orbitais reais são obtidos pela soma ou subtração dos harmônicos esféricos, de forma a eliminar a parte imaginária.

Orbitais atômicos imaginários $(m_l \neq 0)$

Orbitais p, $l = 1$

$$\frac{1}{\sqrt{2}}(Y_{-1}^{1} - Y_{1}^{1}) = \frac{1}{4}\sqrt{\frac{3}{\pi}}\left(\frac{x - iy}{r} - \left(-\frac{x + iy}{r}\right)\right) =$$

$$= \frac{1}{4}\sqrt{\frac{3}{\pi}}\frac{2x}{r} = \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{x}{r}$$

E por isso chamado de orbital p_x

Orbitais atômicos imaginários ($m_l \neq 0$)

Orbitais p, $l = 1$

$$\frac{i}{\sqrt{2}}\left(Y_{-1}^{1} + Y_{1}^{1}\right) = \frac{i}{4}\sqrt{\frac{3}{\pi}}\left(\frac{x - iy}{r} + \left(-\frac{x + iy}{r}\right)\right) =$$

$$= \frac{i}{4}\sqrt{\frac{3}{\pi}}\left(\frac{-2iy}{r}\right) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\frac{y}{r}$$

E por isso chamado de orbital p_y

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